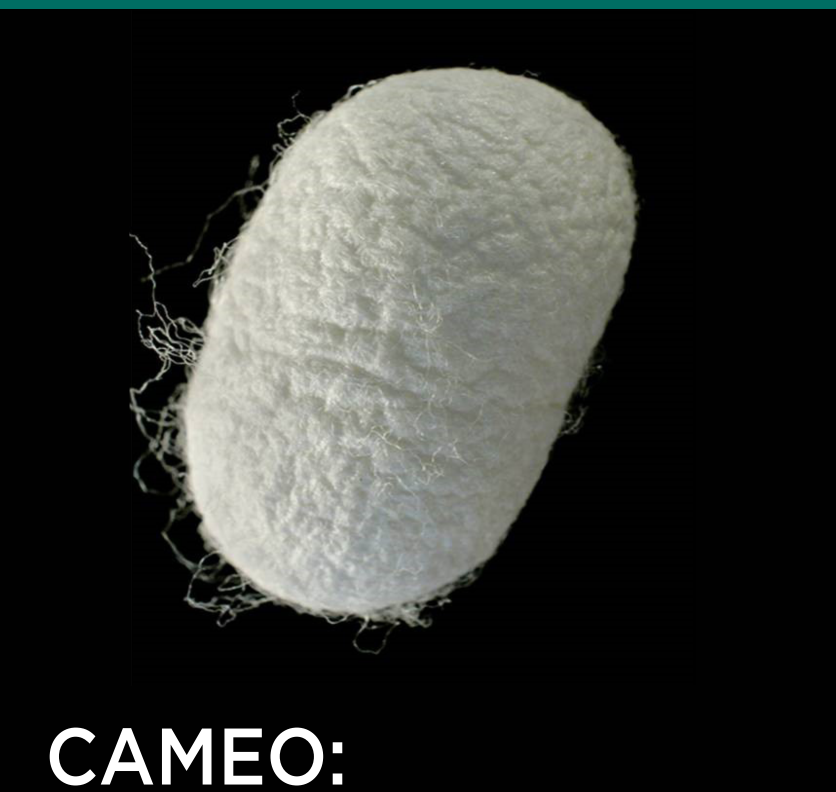
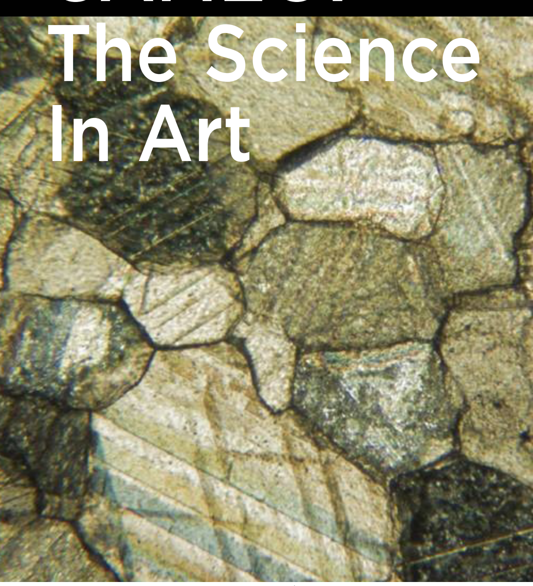
CHEMISTRY International

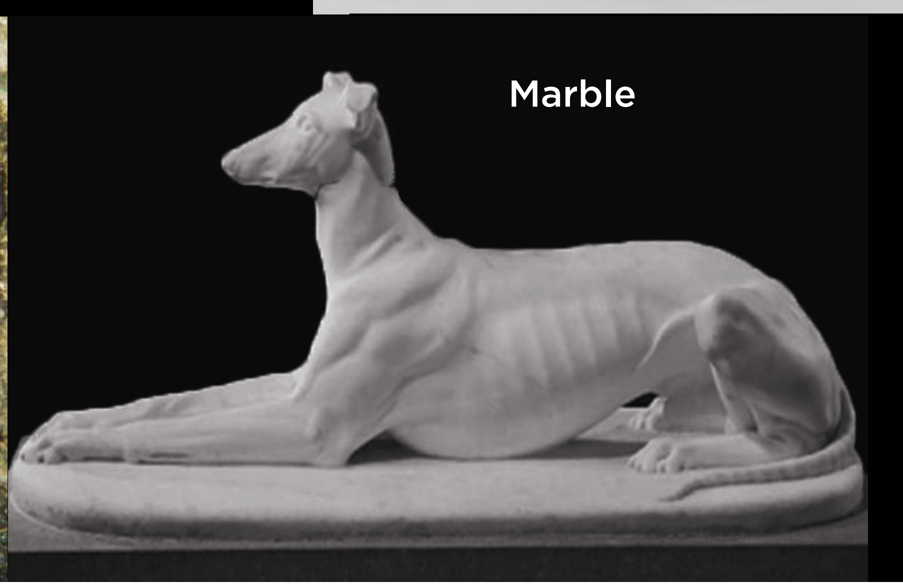
The News Magazine of IUPAC

September-October 2016
Volume 38 No. 5



CAMEO: The Science In Art





The Art of Building Small ►

The Discovery of Phytochrome ►

INTERNATIONAL UNION OF
PURE AND APPLIED CHEMISTRY

Chemistry International

CHEMISTRY International

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

All information regarding notes for contributors, subscriptions, Open Access, back volumes and orders is available online at www.degruyter.com/ci

Managing Editor:
Fabienne Meyers
IUPAC, c/o Department of Chemistry
Boston University
Metcalf Center for Science and Engineering
590 Commonwealth Ave.
Boston, MA 02215, USA
E-mail: edit.ci@iupac.org
Phone: +1 617 358 0410

Production: Joshua Gannon
Printed by: Sheridan Communications

Subscriptions
Six issues of Chemistry International (ISSN 0193-6484) will be published bimonthly in 2016 (one volume per annum) in January, March, May, July, September, and November. The 2016 subscription rate is USD 110.00 for organizations and USD 65.00 for individuals. IUPAC Affiliate Members receive CI as part of their Membership subscription, and Members of IUPAC bodies receive CI free of charge.

ISSN 0193-6484, eISSN 1365-2192
Periodicals postage paid at Durham, NC 27709-9990 and additional mailing offices. POSTMASTER: Send address changes to *Chemistry International*, IUPAC Secretariat, PO Box 13757, Research Triangle Park, NC 27709-3757, USA.

Cover: The Conservation and Art Materials Encyclopedia Online (CAMEO) is a database that compiles, defines, and disseminates technical information on the distinct collection of terms, materials, and techniques used in the fields of art conservation and historic preservation. From silk to marble, CAMEO offers valuable resources to everyone interested in art and sciences, and the science in art. See feature page 8.

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The Art of Building Small

by Ben L. Feringa

Beginning a fantastic voyage beyond the frontiers of contemporary chemical sciences, the creative power of synthetic chemistry imbues chemists with the confidence needed to enter many unknown molecular worlds. The beauty of Nature's functional molecular structures offers, of course, a fantastic source of inspiration, yet chemists are not limited by the molecular building blocks selected by evolution to sustain the intricate systems of a living organism. Nature has developed on the principle of the minimal chemistry set—imagine what we can achieve with the whole of chemistry available to us.

Chemistry has already demonstrated its potential, creating, for example, the diverse materials that allow a modern airplane to transport hundreds of people at high speed over thousands of miles. One should note, however, that the materials, as well as the principles of flight, are distinct from those of a bird. In all modesty, we have so far failed to build even a single cell of a pigeon. Biological function is usually the result of complex molecular systems built on a very simple set of principles and components. Although highly effective, these systems are far from efficient. As the frontiers in chemistry shift from structure to function and from molecules to molecular systems, chemists must explore novel strategies to create functional molecular systems. Major challenges include discovering novel functions emerging from the collective behavior of molecules, exploring the dynamic properties of molecular systems, integrating synthetic and biological systems, and studying far-from-equilibrium behavior. This exploration will open unimagined opportunities to address future challenges in materials, sustainable processes, energy carriers, and biomedical applications.

From Molecules to Dynamic Molecular Systems

Confronted with the question of how to realize complex molecular systems with specific dynamic functions, we should reflect on the multifaceted nature of the problem. Besides the obvious structure, reactivity, and functionality of individual molecular components, their correct assembly and organization are crucial to the proper functioning of such dynamic systems. Interfacial phenomena are important, as is elegantly illustrated by membrane-embedded motors and filament-guided transporters in biology, as well as by electronic and sensing devices based on organic-inorganic systems. In integrating structure and function and interfacing the nanoscopic-world with the macroscopic-world, control at different hierarchical levels and length scales, *i.e.*, supramolecular, mesoscopic, and macromolecular, offer additional challenges. An especially intriguing aspect is how we can amplify effects induced at the molecular level via the cooperative action of the individual molecular components. This ability will provide fascinating opportunities, for instance in the design of responsive materials such as artificial muscles, smart surfaces and coatings, and soft robotics.

Responsive behavior also asks for triggering, addressing, and sensing functions, not only to allow one to remotely influence the molecular system, but also to provide the ability to detect as well as act on demand in response to a change in the environment, a specific external signal, or a particular property that is desired. Chemical systems with adaptive or emergent behavior may already be within reach. We should note that biological systems operate far-from-equilibrium and the move from thermodynamic to kinetic, far-from-equilibrium control is the next major step for (supra-) molecular chemistry. In the broader context, synthetic chemistry has only scratched the surface of "chemistry as an information science", which will become particularly evident as we enter the era of systems chemistry. Signal transduction, feedback loops, repair mechanisms, and autonomous processes are just a few of the additional aspects we have to deal with on our future journey into the world of dynamic molecular systems.

Two examples from our program, although still primitive compared to the sophisticated molecular machinery found in a living cell, illustrate the approaches we take to building responsive molecular systems at the nanoscale. In order to construct a light-responsive nano-valve to enable controlled drug delivery, a switchable MSCL channel protein complex was designed. Here, the MSCL channel of *E. Coli.* was re-engineered to accommodate synthetic photo-responsive units at specific positions in the protein complex. The whole system was assembled in an artificial membrane, *i.e.*, a giant vesicle, that can be loaded with a molecular cargo, *i.e.*, a drug. When the system is illuminated, the MSCL channel opens a 3 nm pore and the drug is released. In the second example, the focus was on autonomous translational movement. A carbon nanotube was decorated with carboxylic acid groups that allowed covalent anchoring of two enzymes, glucose oxidase and catalase. While the first enzyme converts glucose, generating hydrogen peroxide, the catalase rapidly converts this into molecular oxygen and water. The cooperative action of the two enzymes and the use of glucose as the chemical fuel induces an autonomous propulsion of the carbon nanotube. In this way, taking advantage of biology and synthesis, we built complex nano-systems that operate in an aqueous environment in which the individual components act together and respond to an external optical signal, or a chemical fuel, to perform a novel function. In the first example it is opening-closing of a nano-valve, while in the second example autonomous movement is accomplished by "burning" glucose. In these dynamic systems, we merge biological and synthetic components and integrate them to create advanced functions. With progress in synthetic biology, organic synthesis, and supramolecular chemistry, together with the opportunities offered by photo-and electro-chemistry and catalysis to power motility, the future of hybrid dynamic systems is particularly bright.

Molecular Switches and Responsive Materials

In materials science and nanotechnology, the use of molecular switches is particularly attractive, as they enable the introduction of responsive behavior and can function as information storage units and basic elements in optoelectronic devices. Again, Nature serves as a source of inspiration—human vision is based on arguably one of the most elegant natural responsive molecular systems, taking advantage of the retinal photo-isomerization as the elementary switching process. Key parameters in designing molecular switches for information technology are robustness in switching behavior, non-destructive read-out, and long-term stability. Although molecular switching can be triggered by a variety of input signals, *e.g.*, redox, light, pH, temperature, or metal ion binding, light offers the distinct advantage as being a non-invasive trigger for a switching process. We built chiroptical molecular switches based on helical-shaped overcrowded alkenes, in which excellent photoreversibility is combined with high fatigue and non-destructive read-out. Here the interconversion of molecules with distinct chirality and shape define a zero-one digital information storage system at the molecular level. Future prospects are high-density nano-scale information storage systems.

In alternative approaches, advantage can be taken of reversible changes in the electronic properties of molecules. Numerous synthetic systems have been reported in the quest for the bottom-up approach toward molecular electronics, but major challenges remain in both the design of novel robust switching elements and the integration of molecular switches in microarray electronic devices. Organic photochromic compounds are attractive as photoswitches, as they have the potential to integrate optics (speed) and electronics, provided switching is not compromised by integrating the organic molecules in semiconductor devices. For example, our program achieved the construction of single molecule optoelectronic switching elements and the integration of photoswitches in large array devices. These, and related photo- and redox- active molecules, offer ample opportunity to explore molecular switches for information technology, but also for imaging and sensing applications.

Supramolecular chemistry is a field that can benefit from responsive functions and molecular switches. A next major step is the introduction of intrinsic switching functions in the components that are designed to undergo self-assembly to form larger supramolecular systems enabling responsive behavior. It will allow the system to react to an external signal, and, for example, adapt and reconfigure into a new assembly with a different function. For instance, we introduced photo-switches in small molecular gelators and could modulate the material between different gel states using a non-invasive light signal. Particularly fascinating is that, with these light-responsive gels, metastable states and out-of-equilibrium assemblies of soft materials can be reached. The introduction of photo-switches in the core part of special designed amphiphiles resulted in multicomponent self-assembled nano-objects, including vesicle capped nanotubes and nanotube enclosed vesicles, that show highly selective responsive properties. Illustrative of more complex responsive behavior at the nanoscale are systems designed to switch between a vesicle and a nanotube structure. The introduction of optical switches in soft matter, polymers, and supramolecular systems is expected to bring a wealth of novel responsive materials. In addition, these and related approaches will likely play a major role in the development of smart surfaces, *e.g.*, for coatings, cell growth, tissue engineering, and sensing applications.

Light on Medicine

Exciting opportunities for the use of light responsive molecules in the biomedical field have emerged in recent years. While photodynamic therapy and a range of sophisticated fluorescence imaging techniques have found widespread application in the clinic, recent developments such as optogenetics, that allow, for instance, the control of neural functions, take advantage of photoactive proteins and have opened up entirely new avenues. From a synthetic perspective the design of small light-responsive bioactive compounds is largely uncharted territory. The introduction of photocleavable groups to existing or new drugs offers opportunities in precision therapy. In more complex molecular systems, sensing, delivery, and therapeutic function are combined, which make theranostics applications possible. The need for more effective medical

Chemistry for the Future Solvay Prize

On November 19, 2015, the second "Chemistry for the Future Solvay Prize" of 300000 Euros was awarded to Professor Ben Feringa (University of Groningen, the Netherlands) for his work on unidirectional molecular motors. Professor Feringa has opened a new field of research which could pave the way for the development of new therapeutic and technological applications. Within the next twenty or thirty years, his research will likely lead to the introduction of nanorobots—microscopic robots which can accurately target specific molecules during therapeutic treatment. It may also enable a new generation of scientists to design artificial muscles or further optimize the storage of information on a molecular scale.

The Prize-giving Ceremony took place in Brussels, at the Palace of Academy. The award was presented by Queen Mathilde of Belgium and Jean-Pierre Clamadieu, CEO of Solvay, at the end of a stimulating afternoon in the presence of a large audience.

Following a presentation by Laure Twyffels, a young, talented biochemist who told us with enthusiasm why she is so committed to research, Ben Feringa, recognizing the contribution of his research team, spoke of his conviction that synthetic chemistry will

Professor Feringa receives the Solvay Prize. (From L to R) Nicolas Boel, Solvay Chairman of the Board; Maryem van den Heuvel, the ambassador of Holland in Belgium; Professor Ben Feringa; Queen Mathilde; Jean-Pierre Clamadieu, Solvay CEO; and Professor Hakan Wennerstrom, chairman of the jury.

therapies and responses to major challenges such as antibiotic resistance, stimulates the use of unconventional approaches. For example, photopharmacology can play a major role, combining the power of synthetic chemistry with the precision of light-responsive function. Photopharmacology is based on small molecule bioactive compounds, *i.e.*, a “smart drug” with a photoswitchable function that allows the activation-deactivation of the drug. The photoswitch unit can be appended to an existing drug or built into the design of the pharmaceutical to become an integral part of its structure. The major advantage of photoresponsive molecules is that light allows non-invasive activation of the drug with high spatio-temporal precision. We have focused on light-activated antibiotics to fight antibiotic resistance. Activation with high precision at the point of infection and auto-deactivation away from it prevents the active form of the drug from entering the environment and may both enhance efficacy and provide a novel approach to fight the buildup of bacterial resistance. An additional benefit of the photopharmacological approach is the reduction of side effects, such as being harmful to benificial bacteria in the organism. The incorporation of an azobenzene photoswitch in a broad spectrum quinolone antibiotic not only enabled activation by light, but the

bring solutions unimaginable today to society in the future.

The scope and applicability of Professor Feringa’s research underlines why the Chemistry for the Future Solvay Prize is so important. It’s all about creativity and innovation, two things that have been embedded in the culture of Solvay for more than 150 years, and that enable us to deliver new solutions, improving life for people around the world.

It takes about nine months to designate the Solvay Prize laureate. First, a number of candidates are nominated by members of the Solvay International Institutes’ Chemistry Councils, as well as scientific academies, organizations, and selected individuals from all over the world. After a step-by-step process to whittle this long list of nominations down to a shortlist of candidates, Ben Feringa was selected as the 2015 Solvay laureate by a jury including Nobel laureates Jean-Marie Lehn and Gerhard Ertl, eminent scientists Chris Dobson (Cambridge) and Paul Chaikin (New York University), and the 2013 prize laureate, Peter Schultz. The jury was chaired by Hakan Wennerstrom (Lund University, Sweden) assisted by two Solvay secretaries, Paul Baekelmans and Patrick Maestro.

The word that comes up continually during the jury’s deliberations is excellence. The second criteria is the candidate’s contribution to the transformation of science into potential applications. Both are equally important criteria, as the growing reputation of the Chemistry for the Future Solvay Prize will largely depend on the quality of the laureates.

One of the most creative chemists of our time, Professor Feringa is an eminent laureate who fulfills the ambitions of the Chemistry for the Future Solvay Prize. As such, Professor Feringa has already been recognized by several scientific academies, and has won many other awards for his innovative research.

Professor Ben Feringa, Queen Mathilde and Jean-Pierre Clamadieu, Solvay CEO

During the process of selecting the 2015 Chemistry for the Future Solvay laureate, we were accompanied by two students in chemistry from Paris who covered the selection process and Prize presentation on social media. Together with young Belgian researchers they had the opportunity to talk and exchange their views with Queen Mathilde of Belgium after the ceremony. We felt that it was very important to involve young scientists in this process and it has been amazing to see their enthusiasm for chemistry. We hope that their enthusiasm will help to inspire another generation of scientific innovators.

Dr. Paul Baekelmans
Science Adviser/Secrétariat Général Solvay Group

stability of the antibiotic's on-state could also be tuned by molecular design to allow the drug to switch to the off state automatically after a set time. The opportunities offered for high precision therapy go far beyond antibacterial agents, as is illustrated with photoresponsive antitumor agents such as a switchable SAHA anticancer drug. Here the main challenge is to avoid the severe side effects of the more commonly used chemotheurapeutic agents. Once proven effective, a potential future scenario is to translate the information from molecular imaging to guide laser activation of a switchable chemotheurapeutic compound for high precision treatment in a clinical setting. Recently, we have demonstrated patterning of bacterial growth using light activated drugs and interference with bacterial communication and biofilm formation using switchable quorum sensing molecules, while other groups have focused on restoring vision, interfering with neural processes, and controlling cell division, among others. Although the prospects of photopharmacology are bright, major challenges remain, for instance, how to achieve switching with visible and near-IR light to reduce potential toxicity and achieve high tissue penetration. Also, the design of orthogonal photoswitching units in molecular systems to control several biological functions in parallel and achieve up and down regulation of selected pathways in complex biological networks will provide exciting new opportunities at the interface of synthetic chemistry and biology.

Molecular Motors

In our body, many of the essential functions are controlled by biomolecular motors, ranging from ATP synthesis to muscle function and cell division. In modern society, the motors that power our machines, cars, and planes are ubiquitous. However, synthetic chemists have only recently begun to design molecular systems that show motor function at the nanoscale. At the heart of the nano-machines and robots of the future will be molecular motors providing the power for these systems to do work. In taking up the challenge to exploit motion at the nanoscale to perform useful tasks, one should realize that these systems operate at low Reynolds numbers in an environment of continuous Brownian motion. Furthermore, a comparison between machines and robots in the macroworld and those in the cell should be taken into account in design strategies aimed towards molecular motors and machines. Whereas in macromachines size, friction, and inertia play a dominant role, these parameters are insignificant in molecular machines, where inter-and intra- molecular interactions and interfacial phenomena are key. By translating lessons taken from nature into the design of synthetic molecular motors, we were able to demonstrate for the first time unidirectional rotary motion in a molecular system powered by light. Here the complexity is not so much in the molecular structure, but in the multitude of parameters that enable controlled rotary motion. These include chirality to control directionality of motion, multiple isomerization processes to achieve continuous rotation, and photo-responsive behaviors to power the motor by light. With the principle of a rotary molecular motor established, the foundation was laid for several generations of molecular motors with expanded properties and functions. For instance, the power of synthetic chemistry is shown once again with the construction of motors whose rotary speed could be controlled over several orders of magnitude. Meanwhile rotary motors have been used to control polymer folding and the organization of molecules in liquid crystal films in a dynamic way, driving these systems out of equilibrium. It is a fascinating experience to see how the availability of molecular rotary motors opens unforeseen possibilities, such as the transmission and amplification of motion, as was also demonstrated with light-driven rotating micro-objects and adaptive self-assembled nanostructures. Taking advantage of the cooperative action of rotary motors, a nanocar was constructed, enabling the conversion of rotary motion into directional translational motion on a surface at the nanoscale. Motors can be used as multistage responsive systems to control function, as was shown in multitasking chiral catalysts for enantioselective synthesis. In a typical Dutch design, "a nanoscale windmill park", comprising self-assembled monolayers of rotary motors, was constructed with the prospect of responsive and adaptive surfaces and nanoscale energy converters.

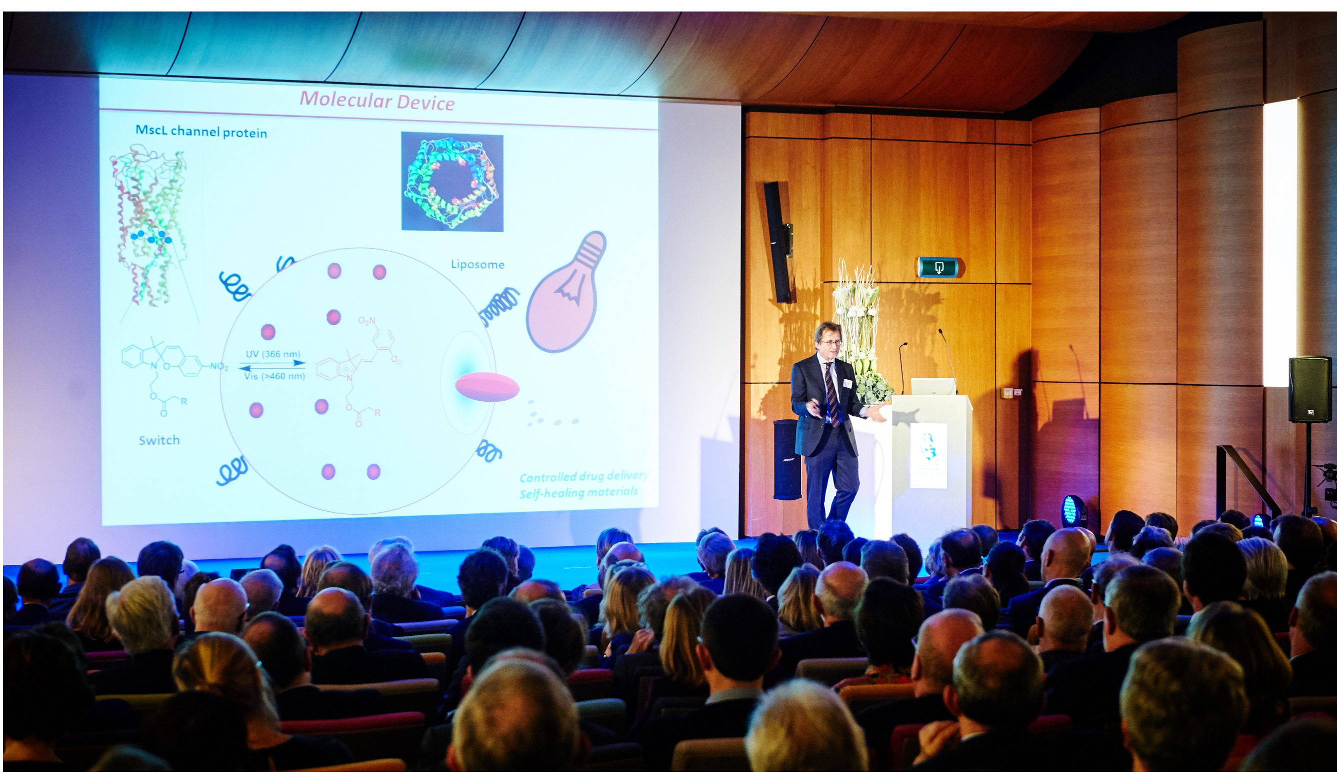
In dynamic molecular systems based on rotary molecular motors, many of the key elements discussed earlier merge. These elements range from the essential parameters that govern rotary motion in the motor structure itself to the control elements that allow, for instance, the assembly and proper functioning of a collection of motors on a surface or in a liquid crystal thin film. With the discovery of the first molecular motor and the development by other groups of molecular systems that show controlled translational and rotary motion, the question arises as to what opportunities these systems offer. Molecular motors are arguably a fascinating starting point for the bottom-up construction of molecular machines and nano-robots. Although some might consider this the domain of science fiction, the fact that chemists are now able to design, control, and use motor-type function at the molecular level sets the stage for entirely new possibilities in science and industry. Programming molecules to enable responsive and adaptive functions cumulating in controlled motion is a major step from molecules to dynamic molecular systems. Incorporating dynamic functions in novel materials offers exciting opportunities for responsive surfaces and coatings, self-healing polymers, biomedical materials for tissue engineering, and the control of cell growth, among others. The integration of information technology and responsive materials will open an exciting new domain for the "synthesis of function", especially when these systems are biocompatible. Roving sensors, smart delivery systems, responsive implants, and precision therapy are areas where dynamic molecular function can likely offer entirely new perspectives.

Conclusion

The beauty and strength of synthetic chemistry is that we can build our own molecular world, as evident in the wealth of chemical products that sustain modern society. Facing the challenges of sustainable processes and products and of our future materials, medical, and energy needs, the practitioner of the art of building small will need to reach new levels of sophistication. Dynamic molecular systems, responsive functions, and control of motion offer fascinating opportunities, as illustrated above and in elegant examples that can be found in recent literature. In this endeavor, Nature's motors and machines can guide the molecular explorer. However, at the start of our next journey we should remind ourselves of the words of Leonardo da Vinci *"Where Nature finishes producing its own species man begins, with the help of Nature, to create an infinity of species".*

Ben L. Feringa (b.l.feringa@rug.nl) is Jacobus van 't Hoff Distinguished Professor of Molecular Sciences at the Stratingh Institute for Chemistry, University of Groningen, The Netherlands. www.benferinga.com

Essay based on the presentation of the "Chemistry of the Future Solvay Prize 2015" awarded to Professor Ben L. Feringa, Brussels, Belgium, November 2015.



CAMEO: The Science in Art

by Michele Derrick

What is Coade Stone? When was Bakelite invented? What is the chemical structure of indigo? Is it safe to use mineral spirits? The answer to all of these questions and much more can be found in CAMEO, the Conservation and Art Materials Encyclopedia Online, available at www.cameo.mfa.org, [1] a set of Internet databases that serve art-related professionals as well as the general public.

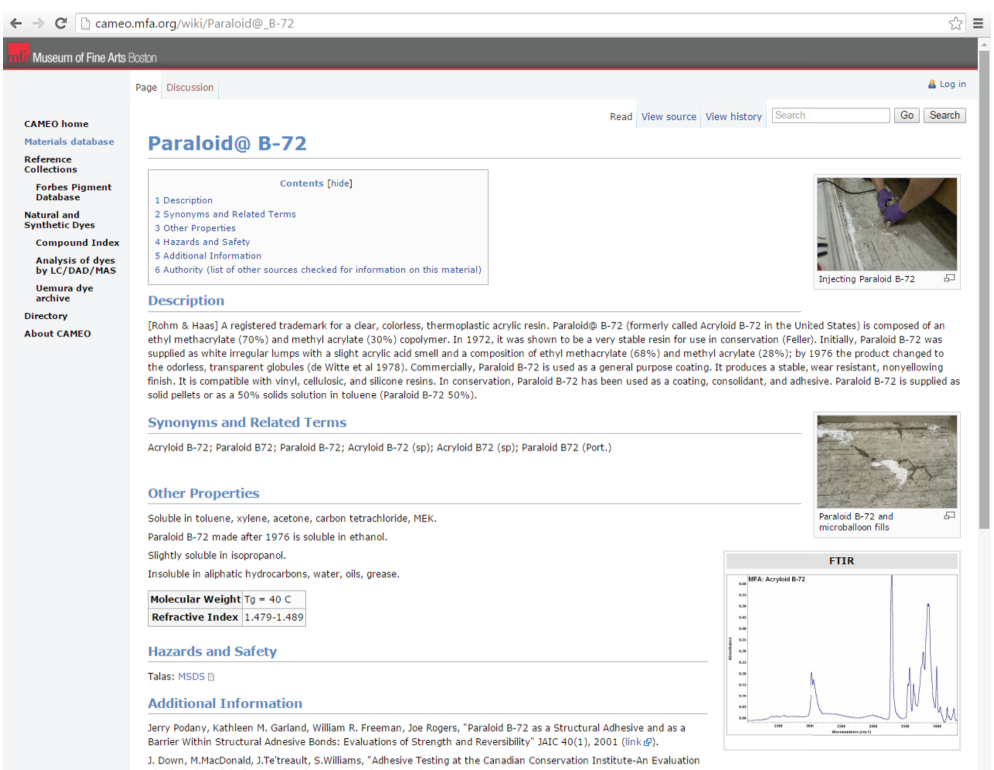
Started in 1999 by the Museum of Fine Arts, Boston, the primary CAMEO database combines technical, historical, chemical, and visual information on historic and contemporary materials used in the preservation and production of artistic, architectural, and archaeological artifacts. With more than 10000 records, the knowledge base is broad—artifacts, sites, and treatment methods can include any combination of materials that have been used in the history of mankind. Additionally, the information required for conservation is becoming ever more complex and technical due to factors such as an increased availability of analytical techniques, the better understanding of deterioration processes, a wider selection of treatment materials, the new emphasis placed on preventive conservation, and ever-growing concerns about health and safety.

CAMEO entries include materials such as pigments, minerals, binders, coatings, adhesives, fibers, dyes, solvents, corrosion inhibitors, woods, pollutants, insects, pesticides, and storage materials. Each term was selected based on its mention in conservation literature, regardless of whether its use on objects or in museums is now considered 'good', such as Paraloid B-72, [2] or 'bad', such as DDT [3] or Soluble nylon. [4]

Examples of more materials and related terms in the encyclopedia include:

- Materials used in the production, conservation, or analysis of historic and processed materials (stainless steel, eosin, Portland cement, plywood, Art-Sorb, acoustic tile, *etc.*)
- Compositional groups (oil, alcohol, acrylic, aniline dye, polymer, *etc.*)
- Chemical and physical classes (abrasive, detergent, sealant, absorbent, insecticide, *etc.*)
- Analytical tools (hygrometer, X-ray fluorescence analysis, infrared spectroscopy, *etc.*)
- Material characterization terms (hardness, gloss, porosity, refractive index, *etc.*)

Figure 1. An example page for the commercial product Paraloid B-72



- Selected devices (Solander box, smoke detector, laser pointer, fluorescent lamp, *etc.*)

The primary description pages for each record contain a brief but comprehensive text about the general class of material along with its major use or biological source (see Fig. 1). For a natural product, its native geographical region is listed. Information is supplied about the material's production, manufacturer, historical availability, appearance, and uses. For searching purposes, alternative, foreign, and archaic names are included in a synonym field, along with common misspellings.

Because of the condensed format of these descriptions, references, such as review articles, book chapters, and books, are included to direct the reader to more extensive information. Some of the references, such as the manufacturer's Web pages, cited articles for the Journal of the American Institute for Conservation (JAIC), and Safety Data Sheets (SDSs), have direct hyperlinks to other Web sites on the Internet.

Several thousand images have also been added to CAMEO (see Fig. 2). Online thumbnail images can be enlarged with a click. These images provide an essential record of a material's characteristics and include photographs and drawings of a material's outward appearance, as well as analytical image records of a material's microscopic and spectroscopic characteristics.

Examples of images in CAMEO are:

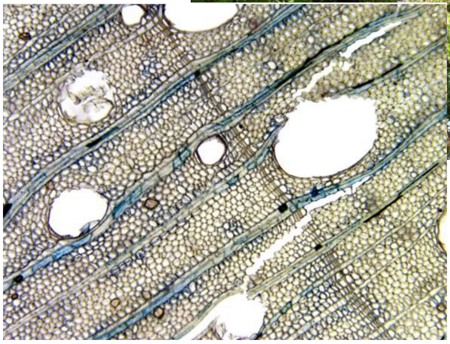
- Images of artwork from the MFA's collection that contain the material or have been treated or affected by the subject of the record (*e.g.*, indigo, black walnut [see Fig. 2]).
- Photographic images or drawings of minerals, gemstones, corrosion products, insect, animals, trees, and plants as well as processed products from these raw materials (*e.g.*, quartz, ant).
- Micrographs of minerals, metals, pigments, wood sections, and fibers, as well as positive and negative microanalytical results for spot tests and fluorescent staining (*e.g.*, oak, cotton)
- UV/Vis, infrared and Raman spectra of oils, resins, gums, waxes, proteins, pigments, dyes, and polymers (*e.g.*, polyethylene, beeswax, realgar).
- XRD patterns for minerals, pigments, and corrosion products (*e.g.*, calcite, brochantite)

Figure 2. Examples of images that are found in the record for black walnut

Black walnut chest: Boston, about 1715-1726, MFA 1986.240

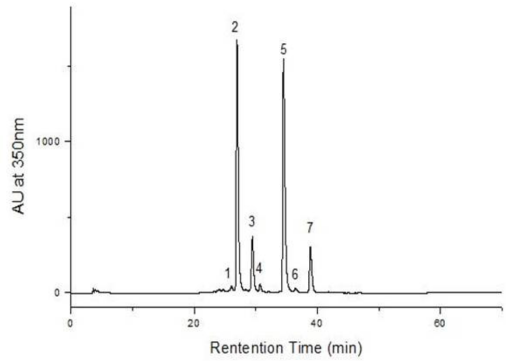
Black walnut tree, Juglans nigra, Arnold Arboretum

Black walnut reference sample



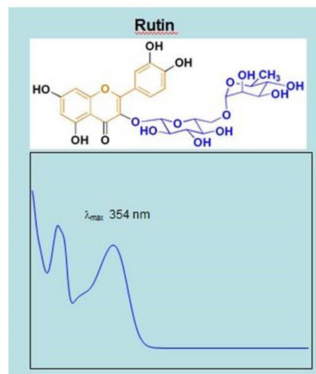
Transmitted light micrograph of transverse thin section from black walnut (Juglans nigra)

Figure 3. Excerpt from the pagoda tree bud record in the Natural and Synthetic Dyes database of CAMEO showing a pagoda tree, the chromatogram for the dye extract, along with the UV/Vis spectra for one of the identified compounds.



Identified compounds

Compound	RT (min.)	MW	UV/vis	Other
rutin	27.0	610	278,352	Comments here
quercetin	34.6	302	280,395,370	
kaempferol	39.0	286	280,395,368	
isorhamnetin	39.0	316	280,395,368	



References

- Zhang, X., and , R. A., Development of Mild Extraction Methods for the Analysis of Natural Dyes in Textiles of Historical Interest Using LC-Diode Array Detector-MS. Analytical Chemistry 77, 2022-2025 (2005).
- Zhang, X., Corrigan, K., MacLaren, B., , M., and , R. A., Characterization of Yellow Dyes in Nineteenth Century Chinese Textiles. Studies in Conservation 52, 211-220 (2007).

Comparative charts showing aging studies, stress curves, and product comparisons are also available. See for example, the records for blue pigments, gemstones, solvents and Paraloid.

Database Development

In 2013, the CAMEO database was transferred from proprietary software and placed on a MediaWiki platform that resides on a cloud server. This transformation provided two significant changes for the active maintenance and growth of the database. First, it opens the database to data entry by many volunteer editors, whose updates provide the flexibility to keep editorial restrictions while also allowing easier, widespread contributions for revising and expanding the scope and content of our multi-functional information source. CAMEO currently has over 60 editors and that number is continually growing. Scientists interested in adding to the database are welcome to contact this author.

Secondly, the cloud server provides for virtually unlimited growth, which has placed CAMEO in the unique position to offer homes to small collaborative databases that benefit the conservation and museum communities. Two of the new major information resources are related to the use and analysis of natural and synthetic dyes in works of art. The first resource is the documentation of the Uemura collection of dyed fabrics that was acquired by the MFA in 2008. A database containing the original Japanese text with its English translation was created by Masumi Kataoka, Sherman Fairchild Fellow in Textile Conservation. Images of all of the dyed samples were collected by Keith Lawrence, scientific photographer. The second new resource is seminal to the scientific art analysis world because it provides critical analytical parameters for the analysis of synthetic and natural dyes using state-of-the-art liquid chromatographic and mass spectrometric equipment. This database initially will contain analyses carried out over the past ten years by Richard Laursen and collaborators at Boston University, comprising extensive work on many natural dye raw materials. Results from analyses of the Uemura archive carried out by Richard Newman at the MFA will also be included. It is anticipated that analyses from other researchers around the world will also be included in the future, making this CAMEO database an invaluable resource for high-quality information on the compositions of raw dye materials used throughout history, as well as samples from works of art that contain those dyes (see Fig. 3).

International Scope

In 2006, the MFA formed a collaborative agreement with EU-Artech (Access, Research and Technology for the conservation of European Cultural Heritage) [5] to increase the international scope of CAMEO. In 2010, this partnership was redeveloped and extended with the CHARISMA (Cultural Heritage Advanced Research Infrastructures) [6] European research project consortium that focuses on providing transnational access, doing cooperative research, and networking applications in the field of cultural heritage conservation.

With this partnership, CHARISMA members have provided systematic review, correction, and update of the material records, including the introduction of records concerning examination and analysis techniques. The working group contributed European language synonyms, resulting in the addition of about 10000 non-English synonyms to the database as an aid for searching records. Now users can enter either English or non-English terms into the MATERIAL search box. Both the primary name and the synonym list are searched simultaneously, allowing for records to be retrieved by their Dutch, French, German, Greek, Italian, Portuguese, or Spanish names.

This collaboration helped expand the reach of the website into a broadly-used international resource. During the five year timeline of the CHARISMA working group project, CAMEO logged more than 1.5 million page hits in 219 countries. Further breakdown on the user distribution by Google Analytical statistics (Table 1) illustrates the impact that the CHARISMA work had on increasing the transnational use of CAMEO. The values for two one-month periods, January 2010 and January 2015, show the number and distribution of users of CAMEO at the beginning and end of the CHARISMA partnership. By percentages, the total number of users increased by 80%, and the relative percentage of the user pool outside the U.S. increased by 13%.

Table 1. Google Analytic Statistics for two separate one-month periods of online access to the CAMEO database. These months represent equivalent times at the beginning and end of the CHARISMA partnership with CAMEO.

Time Period	Sessions	Users	Countries	% Users Outside the U.S.
January 2010	5454	4111	97	48%
January 2015	8910	7428	128	61%

Preventive Conservation

Why is the technical information in CAMEO important for museums, and how is it used? Identification of materials in art is a significant consideration, but factors dealt with in the specialized field of preventive conservation can provide some insight into a few specific problems. An important goal of museums is to preserve their collections for future generations. In preventive conservation, the basic guidelines are to provide optimal environments for objects, thereby minimizing the causes of deterioration. These practices are widely considered critical for the cost effective preservation of large collections and are applied to the objects in storage as well as those on display.

To this effect, when sensitive objects go on display, they are placed in air-tight vitrines or display cases to provide physical safety while also creating controlled microenvironments that diminish pollutants, temperature and humidity fluctuations, and UV light exposure. Both high-tech and low-tech methods are used to create the environments. For example, some valuable organic materials, such as the Declaration of Independence, are stored in hermetically sealed cases that use oxygen scavengers to maintain an anoxic atmosphere. Also, it is common for display cases to be buffered at optimal levels using silica gel that has been conditioned to very specific moisture levels using saturated salt solutions. Controlled humidities are extremely important in many cases, such as where an archaeological ceramic with absorbed salts or a corroded sculpture with bronze disease must be kept at low humidities to minimize the formation of salt accretions or further corrosion. Additionally, vitrines containing objects made of silver or combinations of metals may contain scavengers, such as Corrosion Intercept, to hinder surface reactions.

Extreme care is used to examine all materials used in display case construction, since levels of any volatile components introduced in a contained atmosphere will be higher than levels found outside of it. Since the interior of a display case essentially creates a microclimate for the object, it can be disastrous if the materials used in the construction of the case release pollutants. For example, a common construction material is wood, but hardwoods, such as oak, release acetic acid, and some laminated woods, such as plywood, release formaldehyde and other reactive compounds. Vitrines can still be made with wood, as long as it is sealed with a barrier film, *i.e.*, impermeable laminating material, such as MarvelSeal 360. A video on the Marvelseal 360 record illustrates the correct method for the application of this heat-seal laminate. [7]

It is standard practice to test all materials that go into a display case, whether it is the base, gasket, adhesive, fabric, or display label. For decades, a low tech method, called the Oddy test, [8] has been used to evaluate display case materials by placing them in a sealed test tube with small coupons of silver, lead, and bronze, then waiting for 6 weeks to see if any corrosion or tarnish occurs. Attempts to evaluate off-gassing of deleterious materials by other methods, including residual gas analyzers and sorbent tubes, have not been successful. Current hopes are leaning in the direction of a colorimetric sensor array developed by the Suslick group at the University of Illinois at Urbana-Champaign that uses an array of chemically reactive dyes that are specifically reactive to potential pollutants, resulting in a visual indicator of aerosol problems (see text box and references therein).

Summary

CAMEO is a readily accessible resource that defines, characterizes, and increases our understanding of the materials found in historic and artistic works. It provides a time saving resource for the conservation field, where knowledge regarding material properties, reactivity, and history can be crucial to success and safety. It also enables all interested persons to access vast amounts of technical and visual material data. This is especially beneficial to labs or museums with

Colorimetric Sensor

by Kenneth S. Suslick

The Suslick Research Group at the University of Illinois Urbana-Champaign created an extremely sensitive and portable "optoelectronic nose" used in the detection of toxic gases and other substances [1-4]. It is also developing cumulative colorimetric sensor arrays which are inexpensive, and cross-reactive, using a wide range of chemical interactions with analytes (*i.e.*, not just physical adsorption): an optical analog of mammalian olfaction. A composite response to volatiles in the environment can be measured quantitatively by digitally monitoring the change in color of each spot on an easily printed array (Fig. 1). These new colorimetric sensor arrays are 100s of times more sensitive than conventional passive monitoring diffusion tubes. The use of a disposable array permits the use of stronger chemical interactions, which dramatically improves both sensitivity and specificity compared to any prior e-nose technology. Importantly the sensor array has been specifically engineering to be insensitive to humidity changes. The sensor array has been successfully used for detection of toxic gases at ppb levels, for identification of cultured pathogenic bacteria (and their antibiotic resistance), and for discovery of explosives including peroxide based compounds such as TATP (triacetone triperoxide, the explosive used in the recent terrorist bombings in Paris and Brussels).

A compact reader (the size of a double-deck of cards) for these arrays is available for active sensing and uses a color contact image sensor (a line imaging unit used for portable business card and paper scanners). In addition, cell phone camera imaging was used to monitor artwork after passive exposure in situ during a Disney Animation Research Library exhibition, "Drawn from Life: the Art of Disney Animation Studios", in Beijing. Sensor arrays monitoring pollutant exposure were placed in the exterior and interior environments of passe partout frames during the course of the

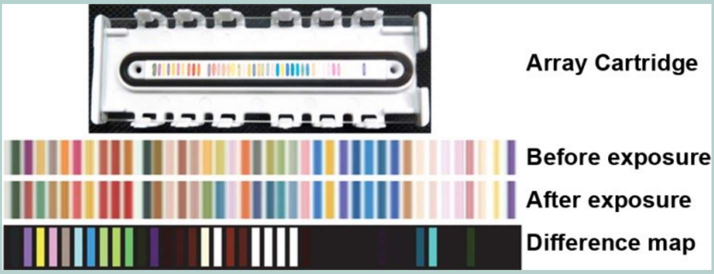


Fig. 1. Color difference maps of the colorimetric sensor array are "molecular fingerprints" and quantitatively identify pollutants, even at part per billion concentrations.

limited personnel or resources, as all sections of the database are free to users on the World Wide Web.

The database is now based on a MediaWiki platform and resides on a cloud server, placing CAMEO in the unique position to offer homes to small collaborative databases that benefit the conservation and museum communities. Continually growing, CAMEO has established a collaborative agreement with an EU working group of museum scientists to enhance the content, breadth, and transnational accessibility of the database. CAMEO currently has over 60 editors and that number is continually growing. Scientists interested in adding to the database are welcome to contact this author. The MFA is committed to providing CAMEO as an outreach program, with numerous benefits for professional conservators, the museum community, and the general public.

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In November 2015, CAMEO was the subject of a online presentation hosted by Robert Belfort and part of the CCCE Fall Newsletter: http://confchem.ccce.divched.org/2015FallCCCENL. This feature for Chem. Int. was inspired by that presentation.

Michele Derrick <MDerrick@mfa.org> is Schorr Family Associate Research Scientist at Museum of Fine Arts, Boston.

exhibition and inside shipping crates during transport (Fig. 2). This work, a collaboration between the Getty Conservation Institute (GCI) and the University of Illinois, was previously supported by a National Science Foundation grant.

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Fig. 2. Placement of colorimetric sensor arrays on the back side of passe partout frames for the 2015 "Drawn from Life", the first traveling exhibit from the Walt Disney Corp. to China; artwork © Disney.

The Discovery of Phytochrome

Unlocking the Secrets of Plants and Their Connection to Light

by James A. Poulos, Robert J. Griesbach, Cathleen J. Hapeman, Stephen O. Duke, and Kevin L. Armbrust

The US Department of Agriculture (USDA) Beltsville Agricultural Research Center (BARC) in Beltsville, Maryland, USA was recently designated an American Chemical Society National Historic Chemical Landmark for the seminal work of USDA scientists in the discovery of phytochrome, the ubiquitous plant pigment that controls plant growth and development in response to light. The discovery team was inspired by the work of Harry A. Borthwick and Marion W. Parker in the 1930s, which quantified photoperiodic phenomena and recruited Sterling B. Hendricks into the search for a chemical basis for non-photosynthetic responses of plants to light. Hendricks was a world famous soil chemist and member of the National Academy of Sciences before he became engaged in plant science. He hypothesized the existence of a photoreversible pigment that controls photoperiodism in flowering, seed germination, and many photomorphogenic processes in plants. Karl Norris and Warren Butler created the specialized spectrophotometer that was needed to detect the pigment in vivo. Harold W. (Bill) Siegleman provided the biochemical expertise to isolate the pigment. The scientific stars aligned in one place, as they rarely do, to make the discovery complete.

The discovery of phytochrome (a tetrapyrrole pigment coupled to a protein), and the proof that it controls almost every aspect of a plant's response to light was a critical discovery for plant science. The ripple effects of their historic research have been tremendous, resulting in many laboratories and scientists worldwide focusing on phytochrome-related research.

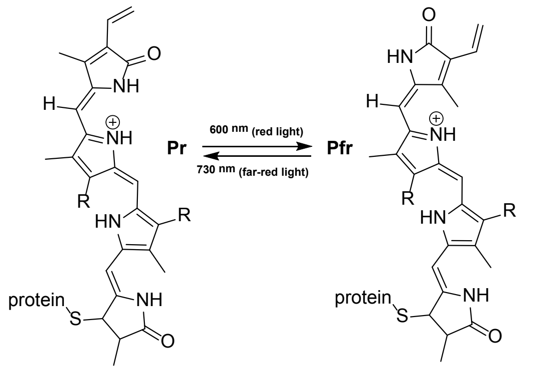
Historical Significance

The discovery of phytochrome in 1959 by scientists at BARC was a crucial advance towards understanding how plants control their growth and development. The presence of phytochrome, a photoreceptive pigment found throughout plant species and in all higher plants, controls their germination, stem growth, leaf growth, and flowering. Understanding the role of phytochrome in plant development allows horticulturists to grow a variety of commercial crops in seasons and latitudes not previously possible and has impacted plant breeding by widening the availability of plants with desirable traits.

The identification of phytochrome was a major turning point in the understanding of plant photoperiodism and, more broadly, plant growth and development. The discovery was the culmination of 40 years of research into plant response to light by USDA scientists. From 1919 until the mid-1940s, research into photoperiodism was mostly based in botany. When chemist Sterling B. Hendricks joined the Agricultural Research Service (ARS) team in 1944, the search for the pigment responsible for photoperiodism using chemical and physical theories and methods began. By increments, the team learned of the pigment's properties: it was engaged by red and far-red light, meaning that it would be green or blue in color; it was rarer and more brightly colored than chlorophyll, the pigment that gives green leaves their color and allows plants to absorb sunlight during photosynthesis; it would be photoreversible, meaning that in one form it would absorb light in the red spectrum and in another in the far-red spectrum; and that the pigment was an enzyme and therefore a protein.

USDA Scientists Harry Borthwick and Sterling B. Hendricks around 1950 (USDA-ARS Information Staff).

"On April 9, 1952, the loose-knit team of scientists came up with another magnificently simple find. Seed hit with red light germinated unless it was then hit with far-red; but if red again ensued, it would germinate. Incredibly, all that mattered was which color came last, even if the seed was struck by 100 alternating cycles of red and far-red." [1] Hendricks proposed that the pigment exists in two inter-convertible forms, one absorbing in the red (Pr) spectrum and one absorbing in the far red (Pfr) spectrum, and concluded that the red and far-red light causes transformation between the two forms—a photoreversible pigment or a photoreversible reaction:



This photoreversibility provided Hendricks and colleagues the tool for establishing the presence of the pigment. [2] Hendricks also "proposed from the absorption spectrum that the chromophore of Pr was an open-chain tetrapyrrole, similar to that allophycocyanin." He further proposed, "based on low intracellular concentrations, that the pigment was an enzyme, and therefore a protein." [3] Hendricks also concluded that Pfr was the active form of the enzyme, because germination of seed, with accompanying respiration, takes place only after Pr has been converted to Pfr. [4]

At a symposium in 1957 on plant and animal photoperiodism in Gatlinburg, Tennessee, the majority in attendance believed that phytochrome "was two separate chemicals." [2] because photoreversible compounds were not known to exist in living things. Some resorted to calling it "this pigment of the imagination." In addition, the compound was evading detection because its concentration in plants and seeds was present "at very low concentrations," 10^{-6} to 10^{-7} M^2. Light and darkness turned it from one form to the other, chlorophyll in green leaves masked its presence, and the instrumentation was not available. "Commercial spectrophotometers, designed to assay solutions, were inadequate for [use with] light scattering materials, such as seedlings." [2]

It fell upon two additional scientists working at Beltsville, Karl H. Norris and Warren L. Butler, to introduce the photoperiod-team to spectrophotometers that they had designed and modified, respectively, allowing for placing a photometer in the spectrophotometer right on top of small samples, close enough to collect most of the scattered light. This close-up

USDA agricultural engineer Karl Norris developed near-infrared spectroscopy in 1963. Here, in May 1981, Norris prepares to analyze fiber content of a grain sample with the near-infrared equipment behind him. Photo by Fred Witt.

allowed for the detection of weak signals generated, for instance, by a pigment or enzyme present in small quantities.

Almost forty years after photoperiodism was identified, Hendricks and Butler, armed with this recording, single-beam spectrophotometer, demonstrated the presence of a photoreversible pigment in intact tissue (dark-grown turnip seedlings and maize seedlings). Siegleman was able to separate the pigment from maize plant tissue. "The pigment was immediately shown to be a protein." [5] The photoreversibility of phytochrome was lost on denaturation, indicating its dependence on interaction of the chromophore with native protein (inactivated by heat).

"Cleavage of the chromophore, or prosthetic group, from isolated phytochrome verified that the compound is an open chain tetrapyrrole related to the bile pigments," [6] such as the biliprotein allophycocyanin. This was confirmed by comparing absorption spectra of the phytochrome and the allophycocyanin chromophores; the two chromophores also had similar RF values in several solvent systems on thin layer chromatography. Their zinc complexes would not fluoresce. The presence of two carboxylic side groups were revealed by chromatography after partial esterification with methanol. [6]

For many years after 1959, when phytochrome was isolated and purified, it was the only characterized and purified photoreceptor. We now know that in the plant kingdom phytochrome is "ubiquitously present in all species and in cyanobacteria." Today it is also known in non-photosynthetic organisms such as eubacteria.

BARC botanist Harry A. Borthwick, a part of the team that discovered phytochrome, studied the effect of different light wavelengths on Biloxi soybeans using a huge carbon arc light salvaged from a Baltimore burlesque theater. Photo by National Agricultural Library, USDA.

Contributions to Agriculture and Society

From 1929 to 1939 soybean production in the US increased by ten-fold, going from 9 million bushels to 91 million bushels. (Editorial note: A bushel is a non SI measure used for dry goods and the equivalent; in the US, 1 million bushels is about 35×10^3 m^3) The existence of phytochrome explained why a single variety of soybean plants flower at the same time no matter how many days a farmer staggered plantings, thereby preventing a staggered harvest. But instead of covering plants to block sunlight to manipulate flowering, which is impractical across multiple acres, crops could now be chosen for the suitability to different latitudes, which of course is the foundation of the world soybean industry. The soybean is now divided into thirteen maturity groups, based upon their photoperiodic response, and a photoperiod insensitive group. This allows soybeans to be grown from Brazil to Canada, as well as throughout the world. Soybeans contain the highest amount of protein of any seed crop and have become one the world's major food crops. In addition, they contain substantial amounts of fat, carbohydrates, dietary fiber, vitamins, minerals, and phytochemicals.

The ability to synchronize flowering of species differing in day-length response has increased the ability to make interspecific crosses, which results in an increased spectrum of horticultural traits, including bloom time, bloom color, size and appearance, and a wider range of cultivars available to both growers and gardeners, with obvious economic benefits. Before this research, nearly all commercial chrysanthemums were short-day plants that flowered during the winter and were not winter-hardy. Because of both the effects of breeding on natural flowering time, and the ability to manipulate flowering time by shading plants or by extending day length with supplemental light, consumers can now purchase plants in flower for immediate impact in the landscape over a far longer season (chrysanthemum being perhaps the best example), and for cut-flower production year-round rather than just in-season.

It may be too early to identify all of the benefits of the discovery of photochrome to society; however, while the impact of temperature itself is probably of far more immediate concern, as climate change progresses there will be increasing need for both agronomic crop varieties and ornamentals that can flower and produce effectively and efficiently at different latitudes than they have been able to grow in previously. As crop zones expand towards the poles, there will be an increased need for plants that can produce under longer days and shorter growing seasons, as day length will not be affected by climate change. While that is not a direct effect on the plant hardiness zone system, this will affect productivity – it's not much use being able to grow a crop plant further north if it is not able to produce economic yield because it does not flower early enough for grain or other types of seed to mature before temperatures fall.

In addition, the analyses of transgenic plants over-expressing phytochrome may have highlighted a few of the potential implications. For example, transgenic tobacco plants, which over-express oat phytochrome A show an improved harvest index by alleviating the shade-avoidance response in a densely planted plot. In potatos, over expression of *Arabidopsis* phytochrome B improved photosynthetic performance and increased life span leading to higher yields of tubers.

Dedication Ceremony

A dedication ceremony to mark this honor was held at BARC on 21 October 2015 and was followed by a symposium on past, present, and future research related to phytochrome. The keynote speaker was Peter H. Quail, professor, Department of Plant and Microbial Biology, University of California, Berkeley and research director of the Plant Gene Expression Center, Albany, California. His talk was titled "A Pigment of the Imagination". Karl Norris, a member of the original ARS phytochrome discovery team and developer of near-infrared reflectance spectroscopy, described his experiences. Also presenting were USDA scientists David Horvath, Sunflower and Plant Biology Research Laboratory, Fargo, North Dakota and Johnnie Jenkins, Genetics and Sustainable Agriculture Research Unit, Mississippi State, Mississippi; Joanne Chory, Howard H. and Maryam R. Newman Chair in Plant Biology, professor and director of the Plant Biology Laboratory at the Salk Institute for Biological Studies; and Dr. Richard Vierstra, Emeritus Professor at University of Wisconsin-Madison.

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James A. Poulos, III, Technology Transfer Coordinator, USDA-ARS, Beltsville, MD, USA; Robert J. Griesbach, Deputy Assistant Administrator, Office of Technology Transfer, USDA-ARS, Beltsville, MD USA; Cathleen J. Hapeman, Research Chemist, USDA-ARS, Beltsville, MD, USA; Stephen O. Duke, Research Leader, USDA-ARS, University, MS, USA; Kevin L. Armbrust, Professor, Louisiana State University, Baton Rouge, LA, USA

Stamps International

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

Raman's Gift to the Art World

Chandrasekhara Venkata Raman (1888-1970), a resourceful physicist, prolific writer, and generous mentor, is best known for the discovery of the light-scattering effect that bears his name. He was the sole recipient of the 1930 Nobel Prize in Physics, an honor bestowed upon him less than two years after the phenomenon was first observed. Interest in Raman spectroscopy grew exponentially within years and, by 1937, close to 1800 papers had been published on the subject.

Since its inception, Raman spectroscopy has been used to probe the vibrational states of the chemical bonds present in an incredible variety of molecular compounds and solid-state materials and is therefore a versatile method for chemical analysis and characterization. Not surprisingly, applications of this spectroscopic technique range from the identification of gemstones and minerals and the remote sensing of explosives to the study of complex biomolecules and drug polymorphs in the pharmaceutical industry.

The Indian stamp illustrated here, issued only a year after Raman's death, features a portrait of the renowned scientist, his signature, a diamond (a crystalline substance he studied extensively), and the Raman spectrum of carbon tetrachloride (*i.e.*, tetrachloromethane in IUPAC parlance).

As a very sensitive and non-destructive method that requires minimal sample preparation, Raman spectroscopy is a widespread technique used to investigate the composition of works of art and objects of cultural heritage, including paintings, ceramics, glasses, manuscripts, textiles, metals, and even biomaterials such as hair, skin, teeth, and bones. For example, the unequivocal identification of the original pigments used in a painting provides useful information regarding the artist's working method and facilitates its present-day preservation and authentication.

Interestingly, a recent article in a Royal Society of Chemistry journal (E. Imperio, G. Giancane and L. Valli, *Analyst* 2015, **140**:1702-1710) describes the use of Raman spectroscopy to analyze the printing inks of Italian stamps produced since 1862. This could potentially help in the detection of forgeries of rare or valuable stamps, which I personally think is a beautiful example of analytical chemistry in the service of philately!

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

Kicking off the Preparations for the IUPAC Centenary

In 2019, IUPAC will celebrate 100 years. A Centenary is a notable milestone and a unique opportunity to recognize what we have accomplished and to acknowledge our role and responsibility in the future of chemistry.

As we start planning for the celebrations, volunteers and members of the IUPAC Bureau have outlined a vision for the Centenary, providing the following background and offering initial ideas. Members at large, including individuals and National Adhering Organizations, are invited to take note and share ideas. Over the coming months, specific initiatives will be announced, inviting everyone to participate.

Background

As the curtain rose on the 20th century, chemistry was already a mature science and a thriving industry. But communication within the industry was difficult. There were few generally-accepted norms for the naming of chemical compounds and chemists routinely did so according to their own personal preferences, resulting in multiple names for a single, unique compound. This lack of a universally accepted language in chemistry created a major barrier to the sharing of information, ultimately hindering efficient research and the rapid advancement of scientific discovery. Aware of this major barrier to the growth of scientific knowledge, a group of eminent chemists and visionaries from France, Belgium, Italy, UK, and USA gathered in 1919 to create IUPAC.

The IUPAC founders were also aware that chemical instrumentation and methodologies were continuously evolving towards greater precision and that more tools were being developed to assess the chemical and physical properties of substances. Therefore, IUPAC was given the charter not only to create a nomenclature that would facilitate communication within the chemistry community, but also to develop standards and norms for the calibration and normalization of chemical substances.

What may have seemed a distant and perhaps unachievable goal in 1919, is today a reality. Thanks to the efforts of a legion of chemists over many decades, advances in scientific research have escalated due to the creation of universally accepted standards, terms, and nomenclature.

IUPAC as a Creator of the Common Language of Chemistry

Conceived as an international organization, IUPAC was born in the aftermath of the First World War—an event that negatively impacted the public's perspective of science in general, and of chemistry in particular, leading them to question the peacetime role of chemistry and the societal benefits that it provides. Through the organization of regularly-scheduled scientific meetings worldwide, IUPAC has nurtured an international community that has dealt with all aspects of chemistry, pure as well as applied.

Today, one hundred years later, IUPAC and the field of chemistry jointly face many interwoven challenges, such as globalization, the energy crisis, climate change, and other environmental challenges. The IUPAC Centenary offers an opportunity not only to commemorate this century-old organization, but also to rethink how IUPAC can better promote and advance the evolving field of chemistry. It is an opportune time to take a critical and ambitious look at IUPAC in order to prepare the global chemistry community for the future.

Chemistry is a major contributor to the well-being of humankind, from the ongoing evolution of better and more effective medicines to the production of safe, clean water. Some of its major breakthroughs, such as the fixation of nitrogen to make fertilizer or the synthesis of nylon as a new material, have greatly contributed to health and security, but there are still major challenges to be met. From societal challenges such as climate change to alternatives to fossil fuels, chemistry has a significant role to play in the invention of new solutions for a better and more sustainable future for all. Today's United Nations Sustainable Development Goals [https://sustainabledevelopment.un.org/sdgs] are both a call to and a source of inspiration for chemists. IUPAC, as the international organization of chemistry, should play a major role in creating the platform, providing the resources and the network for delivering the needed solutions more effectively and in a collaborative and open manner.

IUPAC's legacy is very rich and one that should be celebrated. After a century of activity and growth, IUPAC has helped to shape a very dynamic field of knowledge. Chemistry has reinvented itself several times since 1919, reorganizing its structure through the creation of new sub-disciplines, fostering new topics at the crossroads of well-rooted specialties, and forging multidisciplinary communities for the resolution of contemporary problems, such as the creation of new materials and environmental studies. Along with its constant effort to shape and constantly improve the language of chemistry to reflect new developments, IUPAC has also been instrumental in the support of education and in the global growth of chemistry. IUPAC remains an indispensable resource for chemistry.

Events and Activities

In July 2019, IUPAC will meet in Paris for the World Congress and General Assembly. This is not a coincidence! When offering the venue, our French colleagues made the point of wanting to celebrate the IUPAC centenary in the City of Light.

Several ideas for activities and events have been put forth as follows:

The Celebration of IUPAC's role in creating the common language of chemistry. This is recommended as the main theme of the Centenary activities. The 150th anniversary of Mendeleev's periodic table will also take place in 2019 and this would be highlighted in the celebration. The organizers of the 2019 World Chemistry Congress (WCC) plan several events celebrating the IUPAC Centenary. These events include sessions focused on IUPAC's role in the evolution of chemistry, the revolution of instrumentation in chemistry, the education and training in chemistry, and some of the scientists who have worked for IUPAC.

Establishment of an International IUPAC Day. IUPAC will approach International partners and invite the recognition an International IUPAC Day in celebration of IUPAC Centenary. Using social media, IUPAC members and chemists worldwide will create a virtual handshake.

Logo competition. Prior to the Centenary, students worldwide will be invited to design a logo as part of the celebration.

Youth Activities. Examples include the creation of trading cards featuring chemical elements and molecules, highlighting key facts, *etc.*; competitions focused on the language of chemistry or the periodic table.

The IUPAC100 Celebrations will provide a unique opportunity for IUPAC and all its Members to highlight the importance of chemistry in an international enterprise. How will you celebrate?

www.iupac.org/iupac100

IUPAC Elections for the 2018–2019 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/who-we-are/organizational-guidelines).

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-year term that will start in 2018. 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 **15 February 2017**. An online submission form will be available starting 1 January 2017. Elections for each committee will take place during the second trimester of 2017 and the 2018–2019 memberships for all committees will be finalized during the next IUPAC General Assembly in July 2017. Individuals interested in becoming officers on the IUPAC Bureau should contact their NAOs. Nominations for officers (*i.e.* Vice President or President Elect for 2018-2019) 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 in Brazil.

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

IUPAC Announces the Winners of the 2016 IUPAC-Solvay International Award for Young Chemists

The International Union of Pure and Applied Chemistry and Solvay announce the winners of the 2016 IUPAC-Solvay International Award for Young Chemists, presented for the best Ph.D. theses in the chemical sciences, as described in 1000-word essays.

The five winners are:

Matthew Ross Golder, Ph.D., University of Oregon, USA: "Synthesis and Characterization of Small Molecule Carbon Nanotube Fragments";
Andreas Thomas Haedler, Ph.D., University of Bayreuth, Germany: "Synthesis, Self-Assembly and Photophysical Properties of Multichromophoric Systems";
Luyao Lu, Ph.D., University of Chicago, USA: "Understanding the Mechanism and Exploring the Optimization Strategies for Organic Solar Cells";
Sebastian Angel Suarez, Ph.D, University of Buenos Aires, Argentina: "HNO Chemistry: Generation, Detection and Quantification in Bioinorganic Systems"; and
Ekaterina V. Vinogradova, Ph.D., Massachusetts Institute of Technology, USA: "Development of New Catalytic Transformations and Reagents for the Construction of C-N and C-S Bonds"

The winners, who are from five different countries, will each receive a cash prize of USD 1000 and travel expenses to the 46th IUPAC World Chemistry Congress, 9-14 July 2017, in Sao Paulo, Brazil. Each winner will also be 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 of the 2016 and 2017 competitions during the Opening Ceremony of the Congress.

There were fourteen applications from individuals receiving their Ph.D. degrees from institutions in eight countries. The award selection committee, chaired by Dr. Mark C. Cesa, IUPAC Past President, comprised members of the IUPAC Bureau and a senior science advisor from Solvay, all of whom have a wide range of experience in chemistry.

In view of the many high-quality applications, the Committee also decided to award an Honorable Mention to **Dawei Feng**, Ph.D., Texas A&M University, USA; B.S., Peking University, China.

Dr. Feng will receive a copy of Principles of Chemical Nomenclature – A Guide to IUPAC Recommendations. The book is published by the Royal Society of Chemistry (UK) and is offered with the compliments of RSC Publishing.

The call for applications for the 2017 IUPAC-Solvay International Award for Young Chemists is now opened. Eligible candidates must have received a Ph.D. or equivalent degree in any of the countries that have National Adhering Organizations or Associate National Adhering Organizations in IUPAC during the year 2016.

www.iupac.org/2017-iupac-solvay-international-award-for-young-chemists/

Volker Hessel Is Awarded the 2016 IUPAC ThalesNano Prize for Flow Chemistry

Professor Volker Hessel has been awarded of the 2016 IUPAC ThalesNano prize for flow chemistry, prize coordinated by the IUPAC Committee on Chemistry and Industry (COCI). The prize will be presented at International Conferences on MicroREaction Technology (IMRET14) in Beijing on 14 September 2016. The prize consists of an award of $10,000 US Dollars. At the awards ceremony Professor Hessel will make a short technical presentation.

Professor Hessel has been active in flow chemistry from 1994 and thus has a 22 years engagement in flow chemistry which is longer than for any other researcher in the field. Professor Hessels group (at the early stage at IMM Institut fuer Mikrotechnik Mainz, Germany and later at the Technical University Eindhoven, The Netherlands) created outstanding methodologies for organic syntheses, especially at micro-flow conditions, including catalysis, photochemistry, application of plasma catalysis, and multiphase flow, to name only a few.

Professor Hessel is one of the most important scientist in the field of Microreaction Technology. He brought the idea from the "high p,T" processing into the lab-scale life and later successfully into the industrial scale. Professor Hessel has published several textbooks which are in world-wide use as basics for micro-flow research and also for advanced teaching. His multidisciplinary work is published numerous papers. His number of citations approaches 9000 and his highest cited review paper (*Angew. Chem.*) will soon have 1000 citations. His work spans the fields of chemistry and engineering.

Professor Hessel holds a PhD in Chemistry from Johannes-Gutenberg University of Mainz. He is full professor "Micro Flow Chemistry & Process

Technology" at Eindhoven University of Technology, Group Micro Flow Chemistry & Process Technology, Department Chemical Engineering and Chemistry. He has relationships with many organizations and industrial contacts.

Dan Kunkel to Receive the IUPAC International Award for Advances in Crop Protection Chemistry

On 21 March 2016, the IUPAC Division on Chemistry and the Environment announced that the 2016 "IUPAC International Award for Advances in Harmonized Approaches to Crop Protection Chemistry" will be presented to Dr. Daniel L. Kunkel of the IR-4 Project based at Rutgers University, New Jersey, USA.

The award recognizes individuals in government, intergovernmental organizations, industry, and academia who have exercised personal leadership for outstanding contributions to international harmonization for the regulation of crop protection chemistry. Awardees receive a USD 3000 honorarium, plus travel and per diem reimbursement to attend the award presentation ceremony. Corporate sponsorship for the award is provided by Dow AgroSciences. The 2016 award will be presented to Dr. Kunkel during a symposium to be organized by the Agrochemicals Division as part of the American Chemical Society's national meeting in Philadelphia, USA, during 21-25 August.

Dr. Kunkel has been active for the past 25 years in advancing innovative research and harmonized approaches for regulation of crop protection chemicals and establishment of food residue standards supporting minor uses and specialty crops. He currently serves as Associate Director of IR-4's Food and International Programs, where he has been on staff since 1991. The IR-4 Project is a publicly funded (USDA) research program that provides safe and effective pest management tools to growers of specialty crops through the generation of high quality data for regulatory approvals. For many years, Dr. Kunkel and the IR-4 Project have led efforts to develop field residue trial data to achieve registration approvals and support harmonized maximum residue limits (MRLs) for specialty crops as established by U.S. EPA and other national regulatory authorities to support trade. In the process, he has promoted adoption of cross-regional data sharing, streamlined assessment approaches, and worked tirelessly to resolve scientific issues. One of the hallmarks of Kunkel's efforts has been the highly collaborative nature of his work. As noted by one of his nominators: "Dan has played a pivotal role in coordinating efforts of the grower community, government regulators, crop protection industry, academic researchers and institutions, and policymakers worldwide in garnering, maintaining and improving support for crop protection uses for specialty products."

Dr. Kunkel's early international efforts were focused on harmonization projects involving Canada, Mexico, and the U.S. as a lead scientist with the NAFTA Technical Working Group. He also has been active in promoting the development of harmonized approaches for minor use registrations through IR-4's cooperative agreements with Canada and other countries including Brazil, Colombia, Costa Rica, and New Zealand, and in addition has supported development of a minor use program in the EU. Kunkel's global influence has been applied for the past decade through his active engagement with intergovernmental organizations including OECD and Codex. Through the OECD's Expert Group on Minor Uses he has contributed to development of a number of critical guidance documents and surveys, and through several working groups operating under the Codex Committee on Pesticide Residues he has advanced the establishment of improved assessment processes that include more minor use Codex MRL standards of global significance.

Leadership of global cooperation efforts through the Global Minor Use Summit (GMUS) has been one of Kunkel's most significant international contributions. Three of these unique gatherings, involving hundreds of participants from more than 50 countries, have yielded new global consensus and collaborative action plans for advancing harmonization efforts related to minor use registrations and MRLs. As recognized by other award nominators "Dr. Kunkel has been a champion of international harmonization of regulatory standards..." and "Dan personally has been relentless in developing the infrastructure and personal relationships around the globe to facilitate mutual understanding and respect in addressing MRL issues." For all these reasons IUPAC is pleased to recognize Dr. Daniel L. Kunkel as the 2016 recipient of the IUPAC International Award for Advances in Harmonized Approaches to Crop Protection Chemistry.

Ali Maleki Is Awarded the 2016 IUPAC-CHEMRAWN VII Prize for Green Chemistry

Ali Maleki (Iran) has been awarded the 2016 IUPAC-CHEMRAWN VII Prize for Green Chemistry. Dr. Ali Maleki received this award in recognition of his outstanding contributions to the field of green chemistry.

The CHEMRAWN VII Prize was first announced in August 2008 and since, has been awarded every two years at the IUPAC International Conference on Green Chemistry. The Prize of USD 5000 is granted to a young investigator (less than 45 years of age) from an emerging region who is actively contributing to research in Green Chemistry. The 2016 CHEMRAWNVII Prize will be presented to Dr Maleki at the 6th IUPAC Conference on Green Chemistry that will be held in Venice, Italy on 4-8 September 2016.

Ali Maleki received his Ph.D. in organic chemistry from Shahid Behesti University, Tehran, Iran and he is currently an Associate Professor in the Department of Chemistry at Iran University of Science and Technology. Dr Maleki's research focuses on the use of green reaction media such as solvent-free, water, ethanol and ionic liquids; green and clean catalysts and catalytic reactions (magnetically recyclable and reusable heterogeneous nanocatalysts); one-pot multicomponent reactions (least reaction steps and side-reactions or by-products, high yields, saving energy, high atom economy and bond forming efficiency in the synthesis of organic compounds); and bionanomaterials (natural and synthetic biopolymers).

The IUPAC CHEMRAWN VII Prize has previously been awarded to Noureddine Yassaa (Algeria) in 2010, Rashimi Sanghi (India) in 2012, and Vania G. Zuin (Brazil) in 2014.

2016 Andrei Sakharov Prize Awarded to Zafra Lerman

Zafra Lerman has been named a recipient of the 2016 Andrei Sakharov Prize for her outstanding leadership and achievements upholding human rights. The Andrei Sakharov Prize is awarded every second year by the American Physical Society (APS) since 2006. The recipients are chosen for "outstanding leadership and/or achievements of scientists in upholding human rights". The prize is named after Andrei Sakharov (1921-1989), Soviet nuclear physicist, dissident and human rights activist.

Lerman received the Prize "For life-long devotion to the scientific freedom and human rights of scientists throughout the world and for compelling leadership in using science as a bridge to peace in the Middle East." The $10,000 prize was presented on 17 April 2016, at the APS meeting in Salt Lake City. Lerman's presentation titled "Human Rights and Peace - A Personal Odyssey" captured her life-long as endeavor as a science educator and humanitarian.

Zafra Lerman received her award from APS President Homer A. Neal.

Lerman is a founder and president of the Malta Conferences Foundation which organizes the Biennial Malta Conferences promoting international scientific cooperation and diplomacy as a bridge to peace in the Middle East. The conferences bring scientists from Middle Eastern nations together with several Nobel laureates to explore regional problems, establish cross-border collaborations and build relationships of trust. See report on the recent Malta 2015 conference, page 35.

In Memoriam—Paul De Bièvre

Paul De Bièvre was born in Blankenberge (Belgium) on 7 July 1933. He obtained his PhD from Gent University in 1959 where he continued to work as a lecturer until 1961. In 1961 he joined the Central Bureau for Nuclear Measurements of the European Commission (renamed Institute for Reference Materials and Measurements in 1994) where

he was Head of the Isotope Measurement Unit until 1998 and Advisor to the Director until 2002.

In IUPAC, in addition of being for many years, an active member of the Belgian delegation present at the IUPAC Council, Paul was active in several Divisions and Committees, including the Inorganic Chemistry Division, the Analytical Chemistry Division, and the Committee on Chemistry and Industry. Paul attended his first Commission on Isotopic Abundances and Atomic Weights (CIAAW) meeting in Washington D.C. in 1971 and was elected Associate Member. He remained active member of the Commission throughout the next five decades. At the 1973 Munich meeting, Paul (and Norman E. Holden) proposed to form a Working Party to review the data on isotopic abundance measurements and their impact on atomic weights. This started an eight-year project for IUPAC on the assessment of our knowledge of the isotopic composition of the elements and led to what is now known as the Subcommittee on Isotopic Abundance Measurements with Paul as its inaugural Chair. Until earlier this year, Paul was also an active member of the Analytical Chemistry Division which meeting he attended this past March in Bratislava.

Paul's early work in the Central Bureau for Nuclear Measurements focused on the isotope dilution method and he pioneered the uncertainty analysis in this area. The textbook equation describing the optimal sample-to-spike ratio in isotope dilution analysis (the geometric mean) derives, in fact, from his seminal analysis of isotope dilution equations in 1965 (with Debus). From the 1980s, he directed IRMM work on the improved measurements of the Avogadro constant through the single crystal route. This work, now led by PTB (Germany), forms an integral part of the proposed new International System of units (SI) which is set to be changed in 2018.

Paul was very active in the international activities of chemistry and he was a charter member of many international chemistry organizations, including the BIPM Consultative Committee on the Amount of Substance (CCQM). He was co-founder (1989) and President (1993-1995) of EURACHEM, co-founder (1992) of CITAC ("Co-operation on International Traceability in Analytical Chemistry") (1992). In 1988 he was elected President of the National Committee on Chemistry of the Royal Academies of Belgium (1988-2006). He represented IUPAC to the Joint Committee for Guides in Metrology and has been active contributor to the 1998-2008 revision of the International Vocabulary of Metrology.

Paul had a penchant for philosophy of science and he believed that great measurements start with great thinking. His writings on metrology in chemistry appeared frequently in Accreditation and Quality Assurance (ACQUAL, Springer) of which he was the Founding Editor-in-Chief (1995). He was a straightforward, cheerful person and his colleagues fondly remember his passion for science. Talking science over hours in the rain at a bus stop was not unusual for those who were fortunate enough to have met him. He was an inspiration to generations of analytical chemists and his passion for the highest quality measurements and accuracy in communication will be lasting memories. Paul loved a good debate and this quality placed him at the centre of the decade-long discussions and debates on the redefinition of the SI unit for the amount of substance, the mole. Fittingly, he lived only 10 km away from the city called Mol.

Paul passed away on 14 April 2016 in Leuven at the age of 82.

"One of my Editorials in ACQUAL was triggered by the visit to Aveiro and Lisboa during which we made a walk along the Atlantic sea coast near Aveiro. That gave rise to an Editorial in ACQUAL with the title "Definitions of metrological concepts are lighthouses"*. I still see before my eyes the lighthouse at the entrance of the small port of that coastal village, serving as a beacon to create the metrological clarity with smallest possible target measurement uncertainty, needed for a safe "realization" of the set goal. You are co-guilty of that walk resulting in an enduring description of the function of a light tower in metrology and its understanding by the public."

--Extract of Paul De Bièvre's letter of 29 Feb 2016 to Filomena Camoes,
former President of the IUPAC Analytical Chemistry Division.
**Accreditation and Quality Assurance*, Dec 2010
http://dx.doi.org/10.1007/s00769-010-0726-1

Guide (and Brief Guide) to Polymer Semiconductors

A new project, in association with the IUPAC Polymer Division, will develop both a full guide and a brief guide to clarify new terminology and nomenclature specific to macromolecular optoelectronics, device fabrication, and standard methods of characterization. This project will help to bring awareness of the chemical/technological advances to the widest audience, inspire the next generation of scientists, and to clarify terms used between disparate but inter-related science around polymer optoelectronics. Specifically, the full *Guide to Polymer Semiconductors* will introduce researchers, students, and a general scientific audience to common polymer semiconductor materials, their nomenclature, and terms used for the applications and standard methods used to characterize newly synthesized materials. This project will also result in the preparation of a concise 2- to 3-page *Brief Guide to Polymer Semiconductors* document that will act as a basic guide to studying the terminology for polymer semiconductors and will be readily accessible for new researchers. Journals and society magazines publishing in polymer science and related sciences will be encouraged to participate in the project.

The task group, chaired by Assistant Professor Michael G. Walter (University of North Carolina at Charlotte), will work with several researchers heavily involved in the field of polymer semiconductors, many of whom have already made significant contributions to the IUPAC Sub-Committee on Polymer Terminology and the Polymer Division.

For further information, contact the Task Group Chair Michael G. Walter <michael.walter@uncc.edu>
www.iupac.org/project/2015-014-1-400

Critical Evaluation of Equilibrium Constants of 4f Metal Mixed Complexes with Acidic (Chelating) Ligands in Combination with Various Organophosphorus O-donor Molecules

A critical evaluation survey of equilibrium constants concerning the complexation of 4f-ions by acidic (chelating) ligands in combination with organophosphorus O-donor molecules in various molecular or ionic diluents with particular regard to synergism will be done during the execution of a project under IUPAC auspices. Stability constants of metal complexes are extremely important for academic and industrial research and are widely used in analytical chemistry. The subject is of utmost importance, and this contribution has the potential for wide application (geology, material science, metallurgy, metal recycling, industrial wastewater treatment, handling of radioactive waste, *etc.*). Solvent extraction is a distinguished process for metal refining that stands at the frontier between organic synthesis, analytical, physical, coordination, and green chemistry and is the only industrial technology for lanthanoids separation. Therefore, developing a database review containing useful information of already applied synergistic systems will offer opportunities to the scientists of diversified fields in chemistry and chemical technology to make comparisons, draw conclusions, and choose better ideas when planning their next research investigations. In terms of the increase of safety, prevention of pollution, and improvement of extraction efficiency, the research, development, and implementation of innovative green chemical technologies is indispensable. The very limited set of data available today concerning metal behavior in ionic liquids raise the hope for greater extraction efficiencies accompanied with increased selectivity.

This project is part of a series titled "Critical evaluation of stability constants of metal complexes in solution".

For further information, contact the Task Group Chair Maria A. Petrova <ma@uctm.edu>
www.iupac.org/project/2016-003-1-500

Network for Heterocyclic Chemistry among Countries of the Mediterranean Sea Area, Including Europe and North Africa

The Strategic Planning for a new Network for Heterocyclic Chemistry among Countries of the Mediterranean Sea Area, including Europe and North Africa is an umbrella project that seeks to establish a network in the Mediterranean Area. The program is designed to create world-class research hubs in selected fields within the countries of the region while fostering the next generation of leading researchers by establishing sustainable collaborative relations among research/education institutions in countries such as Spain, Portugal, France, Italy, Slovenia, Croatia, Albania, Greece, Bulgaria, Romania, Georgia, Russia, Cyprus, Turkey, Egypt, Jordan, Tunisia, Algeria, and Morocco. Under this program, core institutions will collaborate in cutting-edge fields of research and on research topics deemed to be of high international importance. The core institutions in the various countries will conduct exchanges based on a principle of equal partnership in the form of joint research, scientific meetings, and researcher exchanges. It is anticipated that the hubs formed by the core institutions will continue to carry out research activities after the funded project has ended. The scope of the project on heterocyclic chemistry includes, but is not limited to, the core areas of heterocyclic chemistry, organic synthesis methodology, and total synthesis of natural products. Research in green chemistry, bioorganic chemistry, medicinal chemistry, pharmacochemistry, structural and materials sciences, and environmental chemistry, as well as the applications of these fields to ultimately benefit the society and economy of the Mediterranean Sea Area, are also encouraged.

Within that framework, the most recent **Trans Mediterranean Colloquium on Heterocyclic Chemistry**, Tramech VIII, was held in Antalya, Turkey, 11-15 November 2015, and turned out to be particularly successful from a scientific point of view, as well as asocial and friendly gathering. The local organization proved to be very efficient, creating a friendly atmosphere. There were more than 220 participants coming from several countries, including Turkey, Algeria, Morocco, Tunisia, Greece, Slovenia, Italy, Germany, Belgium, France, Portugal, Spain, Poland, Australia, Czech Republic, Finland, Hungary, Iran, India, Republic of Korea, Romania, Russian Federation, Saudi Arabia, and the United Kingdom. With support from IUPAC, it was possible to facilitate the participation of 10 young people from different countries, giving them the opportunity to present the results of their research and the chance to strengthen already existing collaborations and start new ones. The program included 14 invited speakers, 26 oral communications, and 161 posters. The level of all the scientific presentations was very high, and discussions that followed were interesting and stimulating. The subjects of the lectures ranged from Innovative synthetic methodologies, metal-free synthesis of heterocycles, synthesis of complex heterocycles, heterocycles as organocatalysts in asymmetric synthesis, organosulfur synthons for the synthesis of heterocycles, synthesis and reactions of chromones and quinolones, and structural and conformational studies in the chemistry of strained heterocycles and synthesis of beta-aminoacids to carbon nanotubes as platforms for material chemistry and drug delivery (see the program at the webpage of the meeting: www.tramech8.org)

At the closing of TRAMECH VIII, the chair of the scientific committee announced that TRAMECH IX will be organized at Fez (Morocco) in November 2017 by the Laboratory of Organic Chemistry of the Faculty of Sciences Dhar El Mahraz using the infrastructure of the University and the City of Fez. The involvement of very distinguished speakers will be pursued and the participation of young, motivated people will be facilitated. IUPAC will provide financial support within the project 2015-027-1-300. As in the Rabat and Antalya meetings, the interactions among participants are expected to promote scientific collaborations and give young people the chance for research experience in well-established laboratories, either as PhD students or as visiting researchers.

For further information, contact the Task Group Chair Saverio Florio <florio@farmchim.uniba.it>
www.iupac.org/project/2015-027-1-300

Nomenclature for Properties and Units or NPU Terminology

Laboratory medicine has an important role in clinical decision making in healthcare everywhere. Results of sample-based patient investigations are involved in almost every decision on diagnosis or treatment and frequently make up the largest amount of data in healthcare records. Most of the results represent chemical and biochemical measurements, with increasing involvement of molecular biology.

With the advent of digital data storage and widespread communication of investigation results, new possibilities have opened for both research and patient care. The challenge is to ensure that all users have a common understanding of what is being measured, how the results are expressed, and with which unit. This demands a stable and metrological sound international standard for identifying measurement results. To support this, IUPAC and the International Federation of Clinical Chemistry and Laboratory Medicine (IFCC) have partnered to publish several recommendations and supported work on the Nomenclature for Properties and Units (or NPU) terminology and its basic principles for decades.

The NPU definitions have a uniform structure and use a referenced vocabulary for every term. The outcome of a patient examination yields information about certain properties of the patient, and the NPU terminology identifies the laboratory result by specifying these properties. It follows international standards of metrology, including IUPAC Recommendations.

Today, NPU terminology is a coding system and terminology for the identification and communication of examination results, covering most fields of clinical laboratory science.

The structured definitions describe:

- the part of the universe that is studied (the system)
- the component that is examined in that system
- the estimated kind-of-property of the component in that system
- measurement unit and specifications where relevant
- an individual code value identifying the definition

Example:

NPU03568 B—Thrombocytes; num.c. = ? × 10^9/L.

- B - is Blood and is the part of the universe that is studied (the system)
- Thrombocytes is the component that is examined in the system, Blood
- num.c. is number concentration, the estimated kind-of-property of the component in the system
- 109/L is the measurement unit and specification where relevant

NPU03568 B—Thrombocytes; num.c. = 60 × 10^9/L - means *The number of thrombocytes per litre blood is 60 × 10^9*

By using the NPU codes, the examination results will be:

- fully defined in the clinical context
- transferable between systems
- comparable to other results of the same kind
- reusable for decision support, calculations, research, statistics, *etc.*

The NPU terminology has proved useful in health informatics and health care for 15 years, and is today a National standard in Denmark, Sweden, and Norway. It is implemented in all laboratory departments at hospitals and private labs, suppliers of laboratory systems and EHRs, and National registers and databases, and is used for online requesting from the GP to the researching laboratory.

The Norwegian Directorate of eHealth has implemented the NPU terminology as a national standard for laboratories in communicating requisitions and examination results in the sector of specialized health services.

The NPU terminology has been in use in Sweden for more than 10 years and is the basis for the National Patient Summary to collect information from different healthcare systems in hospitals, GP's, and private healthcare providers and to make the information available for all users of EHR in the country.

For further information, contact Helle Moller Johannessen <hmj@sst.dk>, chair of the Subcommittee on Nomenclature for Properties and Units (SC-NPU) and member of the IUPAC Chemistry and Human Health (Div VII)

Visit the NPU website at www.npu-terminology.org

Human Errors in a Routine Analytical Laboratory—Classification, Modeling and Quantification: Overview of the IUPAC/CITAC Guide*

Ilya Kuselman and Francesca Pennecchi

******Pure and Applied Chemistry,* **2016, Volume 88, Issue 5, pp. 477–515; online 22 June 2016**
http://dx.doi.org/10.1515/pac-2015-1101

Human error in chemical analysis is any action or lack thereof that leads to exceeding the tolerances of the conditions required for the normative work of the measuring/testing (chemical analytical) system with which the human interacts. When the measuring system is dealing with sampling, the human may be the sampling inspector. On other steps of chemical analysis the human is the analyst/operator of the measuring system. The tolerances of the conditions are, for example, intervals of temperature and pressure values for sample decomposition, purity of reagents, pH values for an analyte extraction and separation, *etc.* They are formulated in a standard operation procedure (SOP) of the analysis describing the normative work, based on results of the analytical method validation study.

Human errors in a routine analytical laboratory may lead to atypical test results of questionable reliability. An important group of atypical results is out-of-specification test results—those that fall outside the established specifications in the pharmaceutical industry, or do not comply with regulatory legislation, or specification limits in other industries and fields, *e.g.*, environmental and food analysis.

Risk of human error is the combination of the likelihood of occurrence of the error and the severity of that error for quality of analytical results. Prevention, avoidance, or blocking of human error by a laboratory quality system is not easy, since *errare humanum est* (to err is human). Both correct performance and error follow from the same cognitive processes allowing us to be fast, to respond flexibly to new situations, and to juggle several tasks at once. Both are "two sides of the same theoretical coin". An example is the "syndrome" of certified reference material (CRM), when an analyst reports an analyte concentration value close to that in a CRM certificate (applied as a control sample), which is subsequently found to be incorrect. There are a number of other human errors which may occur for various reasons. A part of them seem trivial for professionals in the analysis. However, people make trivial errors in their day-to-day life. Nobody is able to change the nature of human being. Thus, protection of the analytical result quality by managing risk of human error for reduction of the error likelihood and mitigation of its severity (the risk reduction) is an important task for the quality system of any analytical laboratory. Residual risk of human error, not prevented or blocked by the laboratory quality system, decreases quality of analytical results and can be interpreted as a source of measurement uncertainty.

There is no currently available data bank (database) containing empirical values of likelihood/frequencies of occurrence of human errors in analytical chemistry, derived from relevant operating experience, experimental research or simulation studies. On the other hand, any expert in a specific chemical analysis has necessary information accumulated during his/her work. That is why this Guide discussed classification, modeling and quantification of human errors in chemical analysis using expert judgments.

Classification

The classification includes the following nine kinds of human errors, $k = 1, 2, ..., K$ ($K = 9$): seven kinds of commission errors of a sampling inspector and/or an analyst/operator (knowledge-, rule- and skill-based mistakes and routine, reasoned, reckless and malicious violations) and two kinds of omission errors (lapses and slips).

The errors may happen at any step of chemical analytical measurement/testing process, $m = 1, 2, ..., M$ (location of the error). The main steps, for example, are: 1) choice of the chemical analytical method and corresponding SOP, 2) sampling, 3) analysis of a test portion, and 4) calculation of test results and reporting. However, after sampling, a sample preparation is required in many chemical analytical methods, including the sample freezing, milling and/or decomposition. The chemical analysis may start from an analyte extraction from a test portion and separation of the analyte from other components of the extract. The analyte identification and confirmation are important in some cases. Then only calibration of the measuring system and quantification of the analyte concentration are relevant. On the other hand, choosing of an analytical method and SOP may not be necessary in a laboratory where only one method and corresponding SOP are applied for a specific task. Many chemical analytical laboratories are not responsible for sampling, *etc.*

The kind of human error and the step of the analysis, in which the error may happen, form the event scenario, $i = 1, 2, ..., I$. There are maximum $I = K \times M$

scenarios of human errors. Since $K = 9$ here, $I = 9M$. These scenarios put together generate a map of human errors in chemical analysis. Mapping human errors is necessary for quality risk management of analytical results. Examples of mapping human errors in pH measurement of groundwater, multi-residue pesticide analysis of fruits and vegetables, and ICP-MS analysis of geological samples are provided in Annex A of the Guide.

Modeling

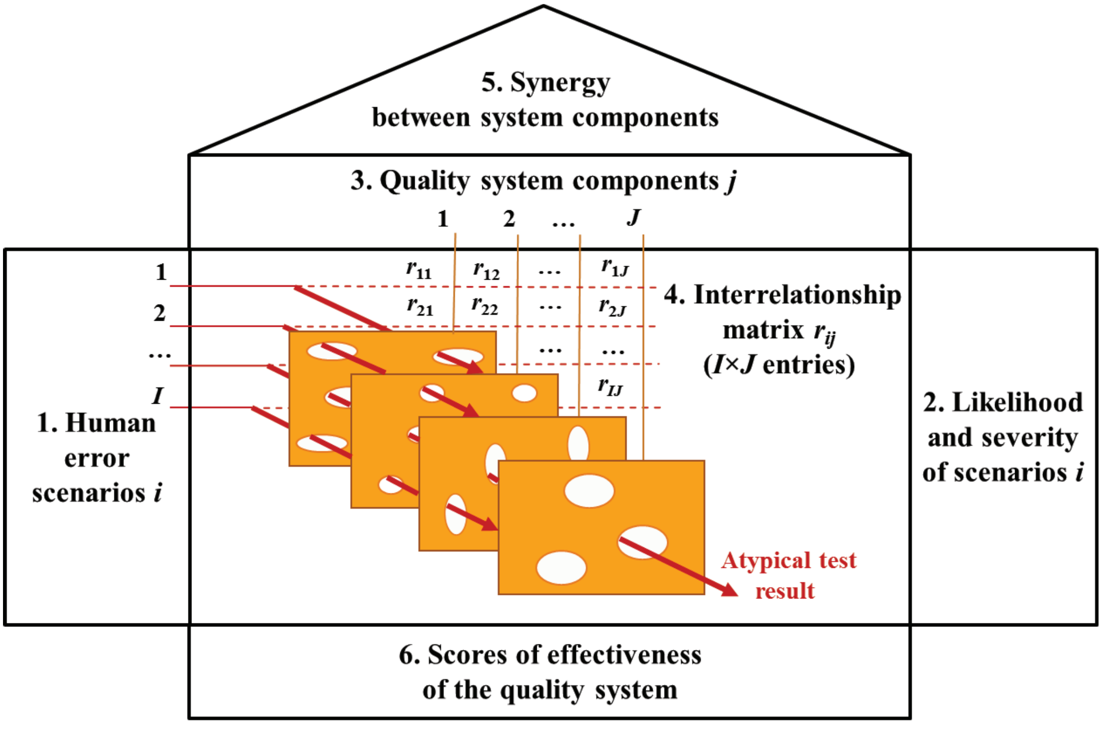
A Swiss cheese model shown in Fig. 1 is used for characterizing the errors interaction with a laboratory quality system. This model considers the quality system components $j = 1, 2, ..., J$ as protective layers against human errors. For example, the main system components are: 1) validation of the measurement/analytical method and formulation of standard operation procedures (SOP); 2) training of analysts and proficiency testing; 3) quality control using statistical charts and/or other means; and 4) supervision. Each of such components has weak points, whereby errors are not prevented, similar to holes in slices of the cheese. The presence of holes in a layer will not lead to system failure, as a rule, since other layers are able to prevent a bad outcome. That is shown in Fig. 1 as the pointers blocked by the layers. In order for an incident to occur and an atypical test result to appear, the holes in the layers must line up at the same time to permit a trajectory of incident opportunity to pass the system (through its defect), as depicted in Fig. 1 by the longest pointer. Examples of modeling human errors are available in Annex A of the Guide.

Quantification

A technique for quantifying human errors in chemical analysis using expert judgments was formulated based on the Swiss cheese model and the house-of-security approach. According to this approach, an expert may estimate likelihood p_i of scenario *i,* by the following scale: likelihood of an unfeasible scenario as $p_i = 0$, weak likelihood as $p_i = 1$, medium as $p_i = 3$, and strong (maximal) likelihood as $p_i = 9$. The expert estimates/judgments on the severity of an error by scenario i, interpreted as the expected loss l_i of quality of the analysis result, are performed on the same scale (0, 1, 3, 9). Estimates of the possible reduction r_{ij} of the likelihood and the severity of human error scenario *i* as a result of the error blocking by quality system layer *j* (degree of interaction) are made by the same expert(s) using again the same scale. The interrelationship matrix of r_{ij} has *I* rows and *J* columns, as shown in Fig. 1.

Blocking human error according to scenario *i* by a quality system component *j* can be more effective in

Fig. 1. A laboratory quality system against human errors in the house of security. Adapted from I. Kuselman et al.*, Accred. Qual. Assur. 18:459 (2013)*



presence of another component j' ($j' \neq j$) because of the synergy $\Delta^{(i)}_{jj'}$ between the two components. The synergy may be equal to 0 or 1 whenever the effect is absent or present, respectively. Estimates q_j of importance/effectiveness of quality system component j in human error reduction are calculated as $q_j = \Sigma^{I}_{i=1} p_i l_i r_{ij} s_{ij}$, where the synergy factor is

$$s_{ij} = 1 + \Sigma^{J}_{j'\neq 1} \Delta^{(i)}_{jj'}/(J-1).$$

Taking into account the synergy factor, the interrelationship matrix is to be transformed replacing r_{ij} by $\tilde{r} = r_{ij} s_{ij}$ in every cell ij of the matrix.

This technique allows to convert the semi-intuitive expert judgments on human errors and on the laboratory quality system into the following quantitative scores expressed in %:

a. likelihood score of human error in the analysis $P^* = (100\ \%/9)\ \Sigma^{I}_{i=1} p_i/I$;
b. severity (loss) score of human error $L^* = (100\ \%/9)\ \Sigma^{I}_{i=1} l_i/I$;
c. effectiveness score of a component of the laboratory quality system $q_j^* = (100\ \%)\ q_j/\ \Sigma^{J}_{j=1} q_j$; and
d. effectiveness score of the quality system, as a whole, against human error $E^* = (100\ \%/9)\ \Sigma^{J}_{j=1} q_j/\ \Sigma^{J}_{j=1} \Sigma^{I}_{i=1} p_i l_i s_{ij}$.

The effectiveness score of the quality system at different steps of the analysis can be evaluated also. Examples of the quantification are available in Annex A of the Guide.

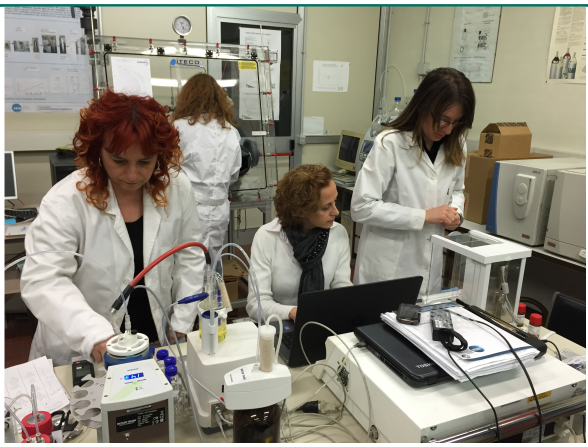
Risk Evaluation of Human Errors

Since the risk of human error is a combination of the likelihood and the severity of that error, their reduction $\tilde{r}_{ij}$ is the risk reduction. A score characterizing the risk reduction by the laboratory quality system in whole, expressed in %, is

$$r^* = (100\ \%/18IJ)\ \Sigma^{J}_{j=1} \Sigma^{I}_{i=1} \tilde{r}_{ij}$$

Then, a score of residual risk of human errors (%) which are not prevented/blocked or reduced/mitigated by the quality system, is $R^* = 100\ \% - r^*$. The fraction (%) of the quality of the analytical results which may be lost due to residual risk of human errors is $f_{HE} = (P^*/100\ \%)(L^*/100\ \%)R^*$.

In practice, a quality system is not able to prevent or block human errors completely, *i.e.*, $0\ \% < f_{HE} < 100\ \%$, and residual risk of human errors can be interpreted as a source of measurement uncertainty when human being is involved in the measurement process and human interaction with the measuring system is taken into account. Such interpretation is discussed in Annex B of the Guide. Examples of calculation of the risks, their consequences for the quality of the analytical results and corresponding contributions to the uncertainty budget are available in Annex A.



Dr. Francesca Pennecchi (at the computer) and her colleagues in their chemical lab of INRIM.

Limitations

Any expert is also a human being, and the elicitation process (by which the expert is prompted to provide error likelihood, severity and other estimates) is influenced by epistemic uncertainty, intrapersonal conflicts, *etc.* Therefore, evaluation of variability of the error quantification scores and relative risks due to the expert's inherent hesitancy, is also important. A detailed analysis of the score variability, as well as the variability of the corresponding loss of quality f_{HE}, based on Monte Carlo simulations, is presented in Annex C.

Changes in any quality system component require a re-evaluation of the quality fraction f_{HE} of the analytical results, which may be lost due to the residual risk of human errors. Either an f_{HE} increase (*e.g.*, due to the retirement of an experienced supervisor) or a decrease (*e.g.*, due to the acquisition of a new, more accurate, and more automated measuring system) is possible.

Latent errors due to a poor laboratory design, a defect in the equipment, an unsuccessful management decision not depending on the sampling inspector and/or the analyst/operator, or positive human factors are not considered in the Guide.

Implementation Remarks

Classification, modeling, and quantification of human errors in a routine laboratory show the ways for increasing the quality system effectiveness and subsequently reducing the risk of these errors in the laboratory. In particular, results of the human error study would be useful for validating the analytical method and formulation of the SOP, as well as for training and for supervision. The map of possible human error scenarios, included in the validation report, may also be useful as a checklist for the prior assessment of an analyst before assigning the task, *etc.*

References and Acknowledgments

The Guide of the International Union of Pure and Applied Chemistry (IUPAC) and the Cooperation on International Traceability (CITAC) was developed by the task group: I. Kuselman (Chair, Israel), F. Pennecchi (Italy), A. Fajgelj (Austria), S.L.R. Ellison (UK), Y. Karpov (Russia) and M. Epstein (Israel). The sponsoring bodies: IUPAC Analytical Chemistry Division, IUPAC Interdivisional Working Party on Harmonization of Quality Assurance, and CITAC.

The Guide includes 52 references to basic publications on human errors, ISO and JCGM documents, and articles of the task group on the topic.

The task group thanks E. Bashkansky, E. Kardash and P. Goldshlag (Israel) and W. Bich (Italy) for their help; Springer Science+Business Media (www.springer.com), Elsevier (www.elsevier.com), Bureau International des Poids et Mesures (BIPM) and IOP Publishing (www.ioppublishing.org) for permissions to use material from the published papers cited in the Guide.

Dr. Ilya Kuselman <ilya.kuselman@bezeqint.net> National Physical Laboratory of Israel (INPL), Jerusalem, Israel; National University of Science and Technology "MISIS", Moscow, Russia; currently Independent Consultant on Metrology. Dr. Francesca Pennecchi <f.pennecchi@inrim.it> Istituto Nazionale di Ricerca Metrologica (INRIM), Turin, Italy. Dr. Kuselman and Dr. Pennecchi are also involved in a project titled "Risks of conformity assessment of a multicomponent material or object in relation to measurement uncertainty of its test results" (IUPAC project 2016-007-1-500, initiated in June 2016, www.iupac.org/project/2016-007-1-500).

IUPAC 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 IUPAC's journal *Pure and Applied Chemistry*. Full text is available online.

Names and Symbols of the Elements With Atomic Numbers 113, 115, 117, and 118

Following earlier reports that the claims for discovery of these elements have been fulfilled [1,2], the discoverers have been invited to propose names and the following are disclosed for public review:

nihonium and symbol Nh, for the element with $Z = 113$,
moscovium and symbol Mc,for the element with $Z = 115$,
tennessine and symbol Ts, for the element with $Z = 117$,
oganesson and symbol Og, for the element with $Z = 118$.

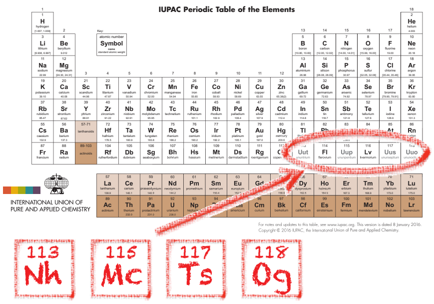
The IUPAC Inorganic Chemistry Division has reviewed and considered these proposals and recommends these for acceptance. A five-month public review is set, expiring 8 November 2016, prior to the formal approval by the IUPAC Council.

The guidelines for naming the elements were recently revised [3] and shared with the discoverers to assist in their proposals. Keeping with tradition, newly discovered elements can be named after:

(a) a mythological concept or character (including an astronomical object),
(b) a mineral or similar substance,
(c) a place, or geographical region,
(d) a property of the element, or
(e) a scientist.

The names of all new elements in general would have an ending that reflects and maintains historical and chemical consistency. This would be in general "-ium" for elements belonging to groups 1-16, "-ine" for elements of group 17, and "-on" for elements of group 18. Finally, the names for new chemical elements in English should allow proper translation into other major languages.

For the element with atomic number 113, the discoverers



at RIKEN Nishina Center for Accelerator-Based Science (Japan) proposed the name **nihonium** and the symbol Nh. Nihon is one of the two ways to say "Japan" in Japanese, and literally means "the Land of Rising Sun". The name is proposed to make a direct connection to the nation where the element was discovered. Element 113 is the first element to have been discovered in an Asian country.

For the element with atomic number 115, the name proposed is **moscovium** with the symbol Mc and for element with atomic number 117, the name proposed is **tennessine** with the symbol Ts. These are in line with tradition, honoring a place or geographical region, and are proposed jointly by the discoverers at the Joint Institute for Nuclear Research, Dubna (Russia), Oak Ridge National Laboratory (USA), Vanderbilt University (USA), and Lawrence Livermore National Laboratory (USA).

Moscovium is in recognition of the Moscow region and honors the ancient Russian land that is the home of the Joint Institute for Nuclear Research, where the discovery experiments were conducted using the Dubna Gas-Filled Recoil Separator in combination with the heavy ion accelerator capabilities of the Flerov Laboratory of Nuclear Reactions.

Tennessine is in recognition of the contribution of the Tennessee region, including Oak Ridge National Laboratory, Vanderbilt University, and the University of Tennessee at Knoxville, to superheavy element research, including the production and chemical separation of unique actinide target materials for superheavy element synthesis at ORNL's High Flux Isotope Reactor and Radiochemical Engineering Development Center.

For the element with atomic number 118, the collaborating teams of discoverers at the Joint Institute for Nuclear Research, Dubna (Russia) and Lawrence Livermore National Laboratory (USA) proposed the name **oganesson** and symbol Og. The proposal is in line with the tradition of honoring a scientist and recognizes Professor Yuri Oganessian (born 1933) for his pioneering contributions to transactinoid elements research. His many achievements include the discovery of superheavy elements and significant advances in the nuclear physics of superheavy nuclei, including experimental evidence for the "island of stability".

References:

1. P.J. Karol, R.C. Barber, B.M. Sherrill, E. Vardaci, T. Yamazaki, (2016) *Pure Appl. Chem.* **88**:139; http://dx.doi.org/10.1515/pac-2015-0502
2. P.J. Karol, R. C. Barber, B. M. Sherrill, E. Vardaci, T. Yamazaki, (2016) *Pure Appl. Chem.* **88**:155; http://dx.doi.org/10.1515/pac-2015-0501
3. W.H. Koppenol, J. Corish, J. Garcia-Martinez, J. Meija, J. Reedijk, (2016) *Pure Appl. Chem.* **88**:401; http://dx.doi.org/10.1515/pac-2015-0802

Comments by 8 November 2016

Corresponding Author: Jan Reedijk, reedijk@chem.leidenuniv.nl
www.iupac.org/recommendation/names-and-symbols-of-the-elements-with-atomic-numbers-113-115-117-and-118/

Preferred Names of Constitutional Units for Use in Structure-based Names of Polymers

A list of constitutional units (CU) used for naming polymers according to IUPAC nomenclature rules is provided. This list contains CUs of commercial and well-known polymers, as well as CUs which have been used in polymer-nomenclature-related IUPAC documents. A preferred name is provided for each constitutional unit. Other acceptable names are also listed, along with names which must not be used because they are outdated or incorrect, although they may have been correct in the past or in a different context. A second table contains the names of common polymers: structure-based, source-based, and retained traditional polymer names, as well as names that are not acceptable, again because they are outdated or incorrect. These tables supersede similar tables and names in previous documents. The rules given in those documents are still valid, but the names of constitutional units should be checked for agreement with the present document. The preferred names of constitutional units in Table 1 should be used in structure-based names of regular and irregular polymers.

Comments by 14 November 2016

Corresponding Author: Werner Mormann, mormann@chemie.uni-siegen.de
www.iupac.org/project/2008-015-1-400

Ecological Risk Assessment Workshop

by John B. Unsworth (Consultant) and Joseph O. Lalah (Technical University of Kenya, Nairobi)

The IUPAC-supported project “A Global Framework for Implementing Consistent Ecological Risk Assessment for Pesticides for Sustainable Agriculture” has elicited a great deal of interest. Following workshops in China, Colombia, and Chile, a fourth workshop was hosted by the Technical University of Kenya in Nairobi 25-26 February 2016.

Losses due to crop pests and diseases can be significant. In sub-Saharan Africa, for example, reported losses in maize can be up to 50% due to stem borers, up to 75% due to fungal attack by grey leaf spot, and up to 90% because of weed competition. [1] Pesticides are a necessary tool to reduce crop losses and increase production to feed growing populations, particularly in countries such as Kenya. However, with the use of pesticides comes the need to keep the ecological impact to a minimum. A key to the safe and sustainable use of a pesticide is to evaluate how likely it is that the environment may be impacted as a result of exposure to the pesticide. This requires carrying out an ecological risk assessment. Many countries include an ecological risk assessment in their registration requirements, but risk assessment is an evolving science, and it is important that the current best practices are understood and implemented properly, particularly in scientifically emerging regions. An ecological risk assessment can be broken down into several different steps:

- Planning
- Problem formulation
- Analysis
- Risk characterisation
- Risk management

These five major phases, together with international approaches to ecological risk assessment, were discussed in detail during the workshop, which was opened by Professor Alex Muumbo, Executive Dean, Faculty of Engineering Science and Technology, on behalf of the Vice-Chancellor of the Technical University of Kenya. Six lecturers from industry, academia, and government gave a total of 12 presentations. Closing remarks were made by Professor Shem O. Wandiga (Institute of Climate Change, University of Nairobi). The presentations were well received by the 32 participants, who came mainly from Kenya, but also from Uganda and Tanzania. After each presentation, and during breaks in the programme, participants were able to discuss all aspects of ecological risk assessment, including good modelling practices, scenario development, and local requirements. In addition, they were able to network with the experts present. Each participant received copies of the presentations and a supplementary guidance document on the development of ecological risk assessments was made available to them. They were also presented with certificates of participation. As with the previous workshops, the participants agreed that they were given much useful information that enabled them to better understand the complexities of ecological risk assessment. Thanks are due to IUPAC, ACS-AGRO, and CropLife International for supporting the Workshop.

1. Gianessi, L., 2014, Importance of Pesticides for Growing Maize in Sub-Saharan Africa, *International Pesticides Benefits Case Study No. 104,* CropLife International

For further information contact Task Group Chair J.B. Unsworth, unsworjo@aol.com. See www.iupac.org/project/2015-048-1-600

ChemCYS 2016. An Inspiring and Stimulating Conference for Young Chemists Worldwide

by Santiago Gómez-Ruiz (Universidad Rey Juan Carlos, Madrid, Spain)

In memory of Professor Sir Harold Kroto and Professor Paul De Bièvre

The **Chemistry Conference for Young Scientists** (ChemCYS) took place in Blankenberge, Belgium, 16-18 March 2016. This conference was organized by the Youth Division of the Royal Flemish Chemical Society (Jong-KVCV) and covered most current topics in Chemistry. Over three days, 341 participants from 39 countries all over the world (including 25 non-EU countries) travelled to the Belgian coastal town to take part in this conference, which offered a very productive and fresh atmosphere focused on the new generation of chemists and current scientific trends.

This excellent scientific event relied on the participation of renowned chemists, such as Prof. Dr Sir Harold Kroto (Nobel Laureate 1996), who, in a pre-recorded presentation, gave an amazing talk on diffuse interstellar bonds; Prof. Dr Karin Öberg, who introduced us to the hidden and unknown world of the Chemistry of Planet formation; and Prof. Dr Bert Meijer, who spoke about multifunctional supramolecular systems. Just as important were the six parallel sessions, with 110 inspiring talks by young chemists, and the various poster sessions, with 116 contributions. For some PhD students, this conference was the first opportunity to present their work to a specialized audience. Therefore, ChemCYS tried to create a constructive and non-intimidating atmosphere for its participants. This stimulated helpful and beneficial discussions by all participants and made the conference an excellent forum for chemists in an early stage of their careers.

The development of the participants' soft skills was taken into account by the organizers. There were sessions on job hunting, CV analysis, social media training, and reviewing, in which professionals of several companies and universities were involved. These more informal sessions helped the attendants to take decisions with respect to some important steps in their scientific careers.

Personally, I have had the honor to participate in the last two editions of this conference as an invited speaker giving different seminars on soft skills. I have observed not only the professionalism, enthusiasm, and excellent organization of Jong-KVCV, but also the motivation and willingness to learn of the attendees. I am convinced that events like ChemCYS are the best forums to assure networking and promote a generational relay in Chemistry, to maintain and improveactive levels in research.

A collection of papers based on presentations at this ChemCYS will appear in *Pure and Applied Chemistry*. Geert-Jan Graulus, President ChemCYS 2016, will act as conference editor, together with Hugh D. Burrows, *PAC* Scientific editor.

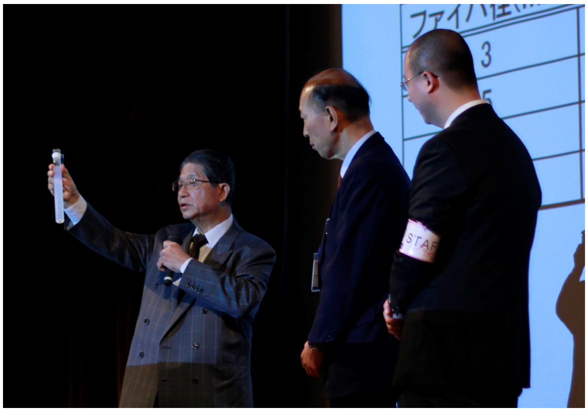
More details about the event, including a detailed program, are available at **www.chemcys.be**.

[Editorial note: Soon after the closing of the conference, we were informed of the passing of Professor Paul De Bièvre, who attended the event as an IUPAC representative. Paul was an enthusiastic supporter of involving young practitioners in the international community. In his earlier report covering the ChemCYS 2014, he concluded: "it was a very well organized conference where the average age of the participants was about 15-20 years below the average age of participants of most Conferences I have attended before. And it gave me a lot of satisfaction to be able represent IUPAC to young chemists who were not familiar with the Union."]

Photochemistry

by Axel G. Griesbeck (University of Köln, Germany)

The **XXVIth IUPAC Conference on Photochemistry** on 3-8 April 2016 in Osaka, Japan was organized by Professor Tetsuro Majima from Osaka University, together with a large group of local organizers. They chose an impressive place to gather: the Osaka City Central Public Hall, an eye-catching building in the center of Osaka featuring pale red bricks and a bronze dome. Built as a public hall for local citizens and completed in 1918, it has become a symbol of Osaka within walking distance of the impressive Osaka Central Station as well as Osaka Castle. Approximately 600 participants from all parts of the world and all areas of photochemistry, photobiology, and photophysics met in Osaka. The conference was accompanied by a pre-symposium in Hiroshima (by Prof. Manabu Abe), two post-symposia in Kyushu and Osaka (by Prof. Yoshio Hisaeda and Prof. Hiromi Yamashita), and the 12th Korean-Japan binational symposium on "Frontier Photoscience" (KJFP-2016).



Professor Akira Fujishima, Tokyo University of Science, demonstrating a photochemical experiment.

The cornerstones of this symposium were 8 plenary and 11 invited lectures, together with 291 oral presentations (including 49 young researcher and 36 student oral presentations) and 187 poster contributions. As a spectacular start to this conference, Akira Fujishima from the Tokyo University of Science, Japan, gave a talk on "Photocatalysis and CO_2 reduction". The groundbreaking work by Honda and Fujishima on the photocatalytic activities of titanium dioxide in the second half of the last century initiated the enormous research activities in the fields of semiconductor photocatalysis, photocatalytic water splitting, and oxidation technologies in surface and water purification with an impressive potential in daily life applications. Richard A. Mathies from the University of California at Berkeley, USA, presented his results on "A coherent picture of photobiology and photochemistry," demonstrating that vibrational dephasing and return to the lowest excited states as described by Kaska´s rule is no longer occurring for ultrafast reactions of excited states at the femtosecond time scale, such as the photoisomerization of the cis-retinal chromophore in the visual pigment rhodopsin that occurs in about 50 femtoseconds.

Thomas Carell from the University of Munich, Germany, lectured on "Time resolved IR and crystallographic studies of DNA photodamage and repair" and described the newest results on the complex mechanisms of repair processes of photoinduced DNA lesions, such as cyclobutane or 6-4 single bond lesions. He explained the differences in green plant photorepair enzymes and mammalian repair by nucleotide excision. Cornelia Bohne from the University of Victoria, Canada, gave her talk on "Mechanistic insights from supramolecular studies on the binding of guests with cucurbit[n]urils" and described a sophisticated study on rate constants of host-guest interactions of photoreponsive molecules with natural bile acids and cucurbiturils as host molecules.

Harry Anderson from Oxford University, England, presented "Excited state energy delocalization in synthetic porphyrin nanorings" where he described the synthesis of linear and cyclic oligometalloporphyrins by a template route that allowed the approach to hitherto unthinkable compounds with extended energy delocalizations in their excited singlet states. Dario M. Bassani from the University of Bordeaux, France, delivered a presentation of "A supramolecular approach to controlling the behavior of excited states" where he described the directionality and predictability of hydrogen-bonding as tool with which chromophores can be pre-oriented prior to photoexcitation in solution and in the solid. The products obtained from supramolecular photoreactions may exhibit affinity for a chosen template, thereby providing a route to substrate-induced receptor synthesis.

Can Li from the Dalian Institute of Chemical Physics, China, referred to "Photogenerated charge separation in artificial photosynthesis systems" and presented the research progress on solar fuel productions from artificial photosynthesis, namely photocatalysis and photoelectrocatalysis processes with the emphasis on the photogenerated charge separation. Nicola Armaroli from the National Research Council in Bologna, Italy, gave a talk on "Photoactive materials for energy conversion" and described the strategies to optimize the luminescence output, color and stability of Ir(III) and Cu(I) complexes, along with the possibility to switch from metal complexes to hybrid organic-inorganic materials and fully organic triplet luminophores.

The next IUPAC conferences on photochemistry will be organized in Dublin, Ireland in July 2018 by Prof. Miguel Garcia-Garibay, and in Amsterdam, The Netherlands, in July 2020 by Prof. Fred Brouwer. This conference series is alternating in odd years with the "International Conference on Photochemistry (ICP)," organized in 2017 in Strasbourg. These two conference series are clearly the path makers of international research in photochemistry and will be more strongly linked in the future in order to make this structure a more powerful stage for the exchange of research results and a tool to foster this important area in the natural sciences.

Research and Education in the Middle East

by Morton Z. Hoffman, Zafra Margolin Lerman, and Iona Black

More than 90 scientists and science educators, including students and early-career scientists, from universities and national institutes in 15 Middle East and North Africa (MENA) countries met at the seventh biennial **Malta Conference on Research and Education in the Middle East** (Malta VII) at the Sofitel Hotel in Rabat, Morocco, on 15-20 November 2015.

With the terrorist massacres a few days before in Beirut and Paris, the ongoing killings in Israel and the West Bank, and the further encroachment of ISIS into the area as the immediate backdrop, the continuing horrifying events within the Middle East and around the world provoked an increased determination by the participants to unite with one another to build collaborations as a bridge to peace.

The countries represented were Bahrain, Egypt, Iran, Iraq, Israel, Jordan, Kuwait, Lebanon, Morocco, Palestinian Authority, Qatar, Saudi Arabia, Syria, Turkey, and the United Arab Emirates. Amazingly, given the declared and undeclared states of war and political animosities among the MENA countries, only one person, a representative from Libya, was denied a visa to enter Morocco. Even the Syrians and Iraqis, who received their visas on the day before the Conference was to begin, managed to come and tell first-hand about the hardships they encounter on a daily basis in order to maintain their scientific research, as well as the obstacles they faced in order to travel to Morocco.

The Conference featured plenary lectures by four Nobel Laureates, keynote talks, workshops on topics of importance to the participants from the region, oral and poster presentations, and ample time for everyone to make personal and professional connections. A total of 54 oral presentations were given during the workshop sessions; 21 posters were on display throughout the entire meeting.

The plenary lectures were given by the following chemistry Nobel Laureates:

Ada Yonath (Weizmann Institute of Science, Israel; NL 2009), Borderless Science;
Dan Shechtman (Technion-Israel Institute of Technology, Israel; NL 2011), Technological Entrepreneurship, Key to World Peace and Prosperity;
Roald Hoffmann (Cornell University, U.S.; NL 1981), Two New Games for Carbon;
Martin Karplus (Harvard University, U.S.; NL 2013), Motion: Hallmark of Life From Marsupials to Molecules.

Nobel Laureates in a discussion: Roald Hoffmann (left) and Martin Karplus. (photo by Justin Kulovsek)

The following also made keynote presentations:

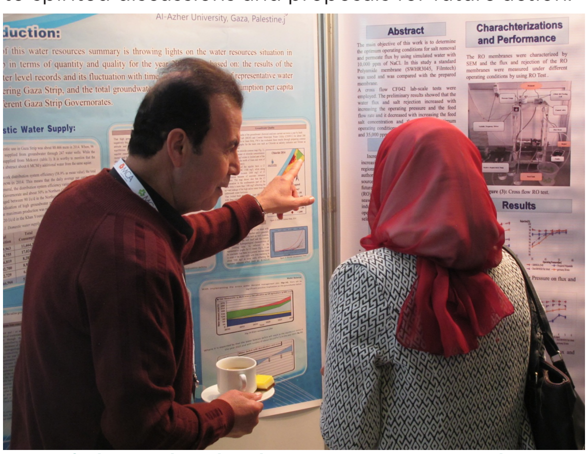
Yvonne Pope (Chemical Abstracts Services, U.K.), SciFinder—The Choice for Chemistry Research;
Nicholas Anthis (U.S. Agency for International Development), The Middle East Regional Cooperation (MERC) Program;
Fadila Boughanemi (European Commission on Research and Innovation), E.U. Builds Bridges Through Science Diplomacy;
Mohamed Ismail (Ain Shams University, Egypt), Software Demonstration of Molecular Modeling and Computer Aided Drug Design;
Donna Nelson (President-Elect, American Chemical Society), The Science Behind "Breaking Bad."

Greetings were offered at the opening ceremony by the following:

Zafra Lerman (President, Malta Conferences Foundation)
Rachid Benmokhtar Benabdellah (Minister of National Education and Vocational Training, Morocco)
Dwight Bush, Sr. (U.S. Ambassador to Morocco)
Karen Betts (U.K. Ambassador to Morocco)
Anne Vasara (Finland Ambassador to Morocco)
Are-Jostein Norheim (Norway Ambassador to Morocco)
Lahcen Haddad (Minister of Tourism, Morocco)
Fadila Boughanemi (Head, Unit for European Neighborhood, Africa and the Gulf, European Commission)
Donna Nelson (President-Elect, ACS)

Evening receptions were held during the week at the residences of Ambassadors Bush, Vasara, and Norheim. The farewell cocktail dinner was hosted by the Moroccan Ministry of National Education and Vocational Training, the Academy of the Kingdom, and the Hassan II Academy of Science and Technology.

The multi-session workshops, chaired by participants and members of the organizing committee, led to spirited discussions and proposals for future action.



Yousef Abu Mayla (Al-Azhar University, Gaza, Palestinian Authority) explaining his poster on the "Water Situation in the Gaza Strip 2015." (photo by Morton Hoffman)

Organic, Organo-metallic, and Medicinal Chemistry: A wide range of topics were covered in the presentations on bioorganic, bioinorganic, and medicinal chemistry in this workshop: the early detection of disease using electrochemical techniques, the synthesis and isolation of natural products, the early diagnosis of cancer cells through the use of electrochemiluminescence, therapeutic drug monitoring, and molecular modeling and software demonstration for drug discovery. The participants suggested the following future collaborations:

- Creation of instrument and resources directories.
- Development of student and postdoctoral exchanges in laboratories across borders.
- Sharing of technical materials.
- Establishment of career development workshops, especially for the editing of proposals and manuscripts.

Energy, Materials, and Nanotechnology for Resource Sustainability: Oral presentations were given by graduate students and faculty members from across the Middle East on topics that ranged from photovoltaic materials and devices, polyelectrolyte, sol-gel, and polymer chemistry, to heterogeneous and photo-catalysis, spintronics applications, and crystallography. The workshop also included intensive discussions and a well-attended poster session.

Environment: Air and Water Quality: The presentations focused on topics of water scarcity, quality, and disinfection, including the analysis of strategies to stabilize and restore the Dead Sea, the development of environmental technologies for reverse osmosis, electrolysis, and biogas generation from human and animal waste, as well as the impact of air-borne metallic pollutants on metabolic biochemistry. The discussion of the use of open-path FTIR to detect pesticides remotely in the air attracted a great deal of attention. Potential areas of collaboration among participants include the scaling of the Arava biogas system to larger units and the reuse of gray and black water.

Science and Technology Education: The talks covered the professional development of science teachers, curriculum development at the secondary and tertiary level, the use of technology in the classroom, and the promotion of a culture of nuclear security. Of particular interest was the presentation on providing learning support for science students with hearing impairments. The following proposals for future collaboration were introduced:

- Translation of curricular materials for secondary school teachers into other local languages.
- Creation of a web-based site for students to ask questions of chemists in English, Arabic, Hebrew, Farsi, or French.
- Development of educational modules on chemical, biological, and nuclear safety and security.
- Establishment of a chat box for teachers to examine critical and creative thinking, and informal scientific activities.

- Expansion of computer-based programs to translate sign language for science for hearing-impaired students.

Entrepreneurship and Innovation: The main themes of the entrepreneurship workshop that was conducted by Olli Vuola (Finland) were "courage," which is something both entrepreneurs and scientists need, and "fear," which must be overcome by them, especially in the process of building bridges to peace. He pointed out that fear prevents one from taking action, and the fear of becoming an outcast is strong in the Middle East. "Collaborating with the opposing side may lead to being isolated from your own community; overcoming one's fears and conquering the fear of failure is also the first step of entrepreneurship." To get a younger generation's perspective on matters, Marianne Vikkula and Ghita Wallin, both students at Aalto University (Helsinki), were part of the workshop team.

Chemical Safety and Security: This workshop addressed the factors that would influence the future of the Organisation for the Prohibition of Chemical Weapons (OPCW) and international chemical weapons conventions, the use of analytical tools in the measurement of chemicals in the environment, education and networking, ethical issues, and the development of new workshops and their funding.

In the closing session of Malta VII, the participants, many of whom had attended previous Conferences, enthusiastically endorsed the motion that Malta VIII be held in 2017. Expressed again was the embodiment of the Malta Conferences: "We have only one nationality here—and that's science."

Among the co-sponsors of Malta VII were the Carnegie Foundation of New York (U.S.), Rockefeller Brothers Fund (U.S.), Alexander von Humboldt Foundation (Germany), Korea Chemical Industry Research Group, OPCW, UNESCO, the Committee of Concerned Scientists (U.S.), the ACS and the AAAS.

The six previous Malta Conferences were held in Valletta, Malta (2003, 2005, 2013), Istanbul, Turkey (2007), Amman, Jordan (2009), and Paris, France (2011, at UNESCO headquarters as part of the celebration of the International Year of Chemistry). The Malta Conferences Foundation (MCF), a nonprofit charitable organization, organizes the Conferences and raises money for their support. More information about MCF and the Malta Conferences can be found at **maltaconferencesfoundation.org**.

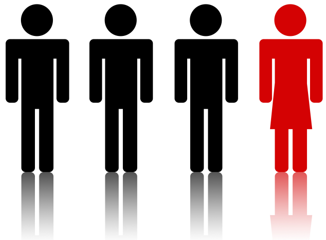
Morton Z. Hoffman, Zafra Margolin Lerman, and Iona Black are the Treasurer, President, and Secretary of the Malta Conferences Foundation, respectively.

Gender Issues in Field Research

Risks and challenges for women doing field research was the topic of a workshop organized on 27 April 2016 in Mexico City by the International Council of Science (ICSU), through its Committee of Freedom and Responsibility in Research (CFRS).

"This is a very relevant topic since gender issues prevent women's full participation in science research," said Leiv K. Sydnes, Chair of CFRS. He reminded participants that today's scientific challenges are unprecedented, including climate change and potential pandemics, and that "all the talent that we can possibly get to resolve this issues and pave the way to a sustainable future is needed; it is crucial to support women in science".

According to UNESCO statistics, women represent 53% of science graduates, however only 28% of all researchers in the world are women. Dr. Erika Pani Bano, General Secretary of the Mexican Academy of Sciences added that it is necessary to achieve transformations that guarantee gender equity in every field, including science.



The aim of the workshop was to prepare an Advisory Note about the topic to be circulated through ICSU members in order to sensitize the scientific community about gender equity. The workshop was organized with the support of the Mexican Academy of Sciences (MAS) and the ICSU Regional Office for Latin America and the Caribbean (ROLAC). The workshop was followed by a two-day meeting of ICSU CFRS during which Leiv K. Sydnes signed the UNESCO & L'Oreal Women in Science Manifesto in representation of CFRS/ICSU; Sydnes encourages everyone to sign the Manisfesto (online @ http://fondationloreal.com/categories/for-women-in-science/lang/en)

For more details about the workshop, including speakers biographies and abstracts

see www.icsu.org/news-centre/news/top-news/icsu-cfrs-workshop-on-gender-issues-in-field-research

Mark Your Calendar

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

2016

4-8 September 2016 • Green Chemistry • Venice, Italy
6th International IUPAC Conference on Green Chemistry
Prof. Pietro Tundo, Dipartimento di Scienze Molecolari e Nanosistemi, University Ca' Foscari Sede: Santa Marta, Venezia, Italy. E-mail: secretary@greeniupac2016.eu; www.greeniupac2016.eu

4-8 September 2016 • Molecule-Based Magnets • Sendai, Japan
15th International Conference on Molecule-Based Magnets (ICMM2016)
Professor Masahiro Yamashita (Chair), Professor Tomoyuki Akutagawa (Secretary), Tohoku University, Magnetism Division, IMR, Sendai, Japan, E-mail: icmm2016@t_imr.tohoku.ac.jp, www.icmm2016.imr.tohoku.ac.jp

18-23 September 2016 • Solid State Chemistry • Prague, Czech Republic
Solid State Chemistry Conference (SSC 2016)
Dr. Adriana Lančok, Institute of Inorganic Chemistry 250 68 Husinec - Řež 1001, Czech Republic,
E-mail: chair@ssc-conference.com, www.ssc-conference.com

24-27 September 2016 • Natural Products and Biodiversity • İzmir, Turkey
29th International Symposium on the Chemistry of Natural Products and the 9th International Conference on Biodiversity (ISCNP-29 & ICOB-9)
Prof. Dr. Bilge Sener (Chair), Prof. Dr. İlkay Eedogan Orhan (Secretary), The Society of Biological Diversity, P.O. Box 43, 06572 Maltepe-Ankara, Turkey,
E-mail: bioced@serenas.com.tr, www.iscnp29-icob9.org

26-30 September 2016 • General and Applied Chemistry • Ekaterinburg, Sverdlovsk region, Russia
XX Mendeleev Congress on General and Applied Chemistry
Prof. Yulia Gorbunova, A. N. Frumkin Institute of Physical Chemistry and Electrochemistry of the Russian Academy of Sciences, Moscow, Russia, Tel.: +74959554874
E-mail: mendeleev2016@gmail.com or mendeleev@prm.uran.ru; www.mendeleev2016.uran.ru

4-7 October 2016 • Advanced Polymeric Materials • Jeju, South Korea
IUPAC-PSK40 Conference on Advanced Polymeric Materials, commemorating the 40th Anniversary of the Polymer Society of Korea
Kilwon Cho, Department of Chemical Engineering, Pohang University of Science and Technology (POSTECH), Pohang, Korea, Tel.: +82-54-279-2270, E-mail: kwcho@postech.ac.kr; www.polymer.or.kr

14-19 October 2016 • Novel Materials and their Synthesis • Changsha, China
12th IUPAC International Conference on Novel Materials and their Synthesis (NMS-XII)
Prof. Yuping Wu, Conference Co-Chair, Department of Chemistry, Fudan University, No. 220 Handan Road, Shanghai 200433, China; E-mail: nms@fudan.edu.cn, www.nms-iupac.org/present

16-19 October 2016 • Bioinspired and Biobased Chemistry & Materials • Nice, France
The 3rd International Conference on Bioinspired and Biobased Chemistry & Materials, or "Nature Inspires, Chemistry Engineers" NICE 2016
Frédéric Guittard (Chair) and Elena Celia, Université de Nice Sophia Antipolis, 1-3 bd Maurice Slama, F-06200 Nice, France, E-mail: elena.celia@unice.fr, www.nice2016-conference.com

24-26 October 2016 • Biotechnology • Melbourne, Australia
17th International Biotechnology Symposium and Exhibition (IBS 2016)
National Conference and Events Manager Kirsty Grimwade,
E-mail: kgrimwade@ausbiotech.org, www.ibs2016.org

20-23 November 2016 • Australasian Polymer • Mantra Lorne, Victoria, Australia
36th Australasian Polymer Symposium
Prof Greg Qiao (Conference Chair), The University of Melbourne; Emma Harrison, Symposium Manager, c/o Leishman Associates, 113 Harrington St, HOBART TAS 7000, 170 Elgin Street, CARLTON VIC 3053
P: +61 3 6234 7844, E-mail: emma@laevents.com.au, www.36aps.org.au

11-16 December 2016 • Organic Synthesis • Mumbai, India
21st IUPAC International Conference on Organic Synthesis (ICOS 21)
Prof. Krishna P. Kaliappan, Department of Chemistry, Indian Institute of Technology Bombay, Tel.: + 91 22 2576 7177, E-mail: kpk@iitb.ac.in; www.chem.iitb.ac.in/icos21

2017

23 Jan 2017 • Validation of Test Methods • Tel Aviv, Israel
International Workshop on Validation of Test Methods, Human Errors and Measurement Uncertainty of Results, in conjunction with the Isranalytica Conference and Exhibition (24-25 Jan 2017)
Dr. Ilya Kuselman, Chairman of the International Workshop Advisory Committee, ilya.kuselman@bezeqint.net; c/o Isranalytica, Reut Lazar, Bioforum Applied Knowledge Center, E-mail: reutl@bioforum.co.il
http://bioforumconf.com/satellite-event2017 and www.isranalytica.org.il

10-13 April 2017 • Macromolecules & Materials • Stellenbosch, South Africa
14th Annual UNESCO/IUPAC Workshop and Conference on Macromolecules & Materials
Prof B Klumperman (Conference Chair), University of Stellenbosch, Department of Chemistry & Polymer Science, Private Bag X1, Matieland 7602 South Africa, E-mail: bklump@sun.ac.za;
Conference Secretariat: aef2@sun.ac.za, http://academic.sun.ac.za/unesco

19-22 April 2017 • Croatian Chemical Congress • Poreč, Croatia
25th Meeting of Croatian Chemists and Chemical Engineers (25HSKIKI)
Dr.sc. Ana Šantić, PhD, Co-chair, Department of Materials Chemistry, Ruđer Bošković Institute, Bijenička c. 54, HR-10000 Zagreb, Croatia; E-mail: asantic@irb.hr, www.25hskiki.org

21-25 May 2017 • Advanced Polymers • Ghent, Belgium
12th Advanced Polymers via Macromolecular Engineering (APME 2017)
Prof. Filip Du Prez (chair), Ghent University, Krijgslaan 281 S4-bis B-9000 Ghent, Belgium
E-mail: filip.duprez.ugent.be, www.apme2017.org

6-10 June 2017 • Supramolecular Architectures • Sochi, Russia
8th International Symposium on Macro- and Supramolecular Architectures and Materials
Prof. Eduard Karakhanov (MAM-17 chair), Lomonosov Moscow State University, Russia
E-mail: kar@petrol.chem.msu.ru, www.mam-17.org

11-16 June 2017 • Analytical Spectroscopy • Pisa, Italy
Colloquium Spectroscopicum Internationale XL (CSI-XL)
Prof. Alessandro D'Ulivo (chair) CNR, Institute of Chemistry of Organometallic Compounds, Via G. Moruzzi, 1, Pisa, Italy; E-mail: dulivo@pi.iccom.cnr.it; www.csi-conference.org

25-29 June 2017 • Organometallic Chemistry • Jeju Island, South Korea
International Symposia on Organometallic Chemistry Directed Towards Organic Synthesis (OMCOS 19)
Prof. Sukbok Chang (chair), Department of Chemistry, Korea Advanced Institute of Science and Technology (KAIST), Daejeon, Korea, E-mail: sbchang@kaist.ac.kr, website tba

2-7 July 2017 • European Polymer Congress 2017 • Lyon, France
From last trends in polymer science to cutting-edge industrial innovations
Prof. Jean-Francois GERARD, IMP CNRS UMR 5223, Université de Lyon—INSA Lyon, F-69621 Villeurbanne, France; E-mail: epf-2017-lyon@sciencesconf.org, http://epf-2017-lyon.sciencesconf.org

9-14 July 2017 • 46th IUPAC World Chemistry Congress • São Paulo, Brazil
Prof. Adriano D. Andricopulo, Brazilian Chemical Society
www.iupac2017.org

13-17 August 2017 • 200 Years of Selenium Research • Stockholm, Sweden

The 11th International Symposium on Selenium in Biology and Medicine and The 5th International Conference on Selenium in the Environment and Human Health (Se2017)

Prof. Elias Arnér, Department of Medical Biochemistry and Biophysics, Karolinska Institutet, SE-171 77 Stockholm, Sweden, E-mail: Elias.Arner@ki.se, www.se2017.se

5-9 November 2017 • HPLC 2017 • Jeju Island, Korea

46th International Symposium on High Performance Liquid Phase Separations and Related Techniques

HPLC 2017 Secretariat contact: Haengdo Lee, Department of Chemistry, Seoul National University, Seoul 151-747, Korea, E-mail: hplc2017@gmail.com; www.hplc2017-jeju.org

23-29 July 2017 • RACI Centenary Congress • Melbourne, Australia

Chemistry addressing sustainable development and other challenges of the 2020s

Dr. Roger Stapleford, CEO RACI, 21A Vale Street, North Melbourne, Australia,
E-mail: Roger.stapleford@raci.org.au; www.racicongress.com

Visas

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

How to Apply for IUPAC Endorsement

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

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