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Books of Secrets

INTERNATIONAL UNION OF
PURE AND APPLIED CHEMISTRY

Systematic Flexibility ▶
What's in a Name? ▶

CHEMISTRY International

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

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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

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Cover image: Museum visitors view paintings at the opening of the Chemical Heritage Foundation's exhibit Books of Secrets: Writing and Reading Alchemy., Photo © 2014 Conrad Erb, www.conraderb.com

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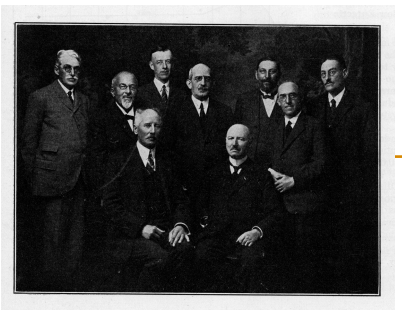

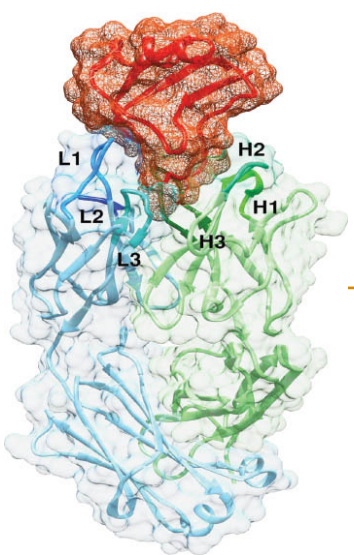

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The First IUPAC Congress in Korea

by Myung Soo Kim, Chair of the IUPAC-2015 Organizing Committee

The organizing committee is pleased to welcome scientists from around the world to the 45th IUPAC World Chemistry Congress and 48th IUPAC General Assembly (IUPAC-2015), which will be held 9-14 August 2015 in Busan, Korea. IUPAC-2015 will provide the appropriate forum to promote innovation in chemistry and related fields all over the world.

The main goals of the 45th IUPAC Congress are to:

- emphasize the central role of chemistry as a multidisciplinary science improving the quality of life and welfare through innovative scientific achievements;
- discuss current issues of mutual interest and seek insights that will be highly appropriate and beneficial in solving problems around us relating to energy, food, water, and the environment;
- provide a variety of opportunities to exchange ideas and expertise, and to network worldwide research groups;
- organize symposia attracting eminent chemists from all over the world; and
- promote collaboration in chemistry and related fields between Koreans and the world.

The theme for the IUPAC 2015 Congress is **"Smart Chemistry, Better Life"**. The Congress will include plenary and keynote lectures, oral and poster presentations, workshops, and up-to-date scientific exhibitions. Four Nobel Laureates and other distinguished chemists will participate as plenary and keynote speakers. The scientific topics of the congress are:

- Physical Chemistry
- Molecular Synthesis
- Advances in Inorganic Chemistry
- Materials for Energy and Environment
- Analytical Chemistry & Environment
- Macromolecular Science and Technology
- Chemistry of Life
- Nanoscience and Materials
- Open Innovation for Enlightening Chemistry Education
- Green Chemistry for World Needs
- Chemistry for Industry Innovation

Registration in now open and early bird discounted rates will end **30 June 2015**. The deadline for abstract submission is **30 April 2015**. Busan, the Congress venue and a bustling city of 4 million, is situated on the southeastern tip of the Korean peninsula. The natural environment of Busan is a perfect example of harmony between mountains, rivers, and sea. Its geography includes a coastline with superb beaches and scenic cliffs, mountains that provide excellent hiking and extraordinary views, and hot springs scattered throughout the city. Its natural endowments and rich history have resulted in Busan's increasing reputation as a world-class city of tourism and culture.

See you soon at Busan!

www.iupac2015.org

The IUPAC-2015 Organizing Committee at their first meeting after the 2013 Congress, on 7 October 2013; Professor Myung Soo Kim, chair of the committee, is sitting in the center of the front row. As they pledge for the success of IUPAC-2015, the committee members raise their fists as a symbol of strength and unity.

IUPAC-2015 *Busan*

48th General Assembly August 6-13, 2015
45th World Chemistry Congress August 9-14, 2015
BEXCO, Busan, Korea

Smart Chemistry, Better Life

Organized by
The Korean Chemical Society

IUPAC

KCS 대한화학회 KOREAN CHEMICAL SOCIETY

www.iupac2015.org

Registration Opens on December 1, 2014

Books of Secrets

Writing & Reading Alchemy

by Neil Gussman

On the cold, rainy night of 5 December 2014, the Chemical Heritage Foundation (CHF) opened its latest exhibit, *Books of Secrets: Writing and Reading Alchemy*. Nearly 200 visitors braved the weather to see a selection of alchemical manuscripts, chosen primarily from a large collection CHF acquired in 2013, along with rarely seen alchemical paintings from CHF's extensive fine-art collections.

James Voelkel, curator of rare books, and Amanda Shields, curator of fine art and registrar, co-curated the new exhibit. They designed *Books of Secrets* to appeal to those interested in books and manuscripts and fine art, as well as to attract those who are curious about all things alchemical. CHF's recent acquisition of a trove of 15th-century manuscripts provided the opportunity to highlight the central role of the written word in the alchemical enterprise. Although alchemists did their work in the laboratory using furnaces and crucibles, reading, copying, and taking notes were also essential activities. The recipes and procedures detailed in the manuscripts were often written using coded language and symbols that enabled alchemists to hide their most precious theories from the uninitiated.

The books in the exhibit were chosen not just to showcase the alchemical manuscripts acquired by CHF in September 2013 but also to display printed books from CHF's collection that complement the handwritten manuscripts, both in style and in subject matter. To further illustrate the importance of books in alchemical practice, several carefully selected 17th- to 19th-century Dutch genre paintings showing alchemists reading, jotting notes, and even standing with nose in book while stirring the contents of a crucible hang alongside the rare old manuscripts. These paintings from the Fisher and Eddleman Collections, some never before exhibited at CHF, bridge alchemists' intellectual and practical pursuits.

Also highlighted is the craftsmanship required to create these early manuscripts, from the materials used in their construction to the symbols embedded in the recipes. A section of the exhibit titled "Printing" illustrates

The Alchemist, *17th century; Mattheus van Helmont, Flemish; Gift of Roy Eddleman, Chemical Heritage Foundation Collections; Photograph by Will Brown*

Above: The Bald-Headed Alchemist, *17th cent.; After David Teniers II, Oil on panel; Gift of Fisher Scientific International, Chemical Heritage Foundation Collections; Photograph by Will Brown*
Left: Alchemical miscellany on parchment, showing signs of soot; Northern Italy, ca. 1450–1475; Othmer Library, Chemical Heritage Foundation; Photograph by Les Enluminures
Bottom: Exhibition opening at the Chemical Heritage Foundation, 5 December 2014. Photograph by Conrad Erb

the continuity from manuscript to print traditions. Early printed books mirrored manuscripts in their conventions, such as placing publication information in colophons at the back of the book, and in their evidence of use, with similar marginal annotations in both printed and handwritten texts. CHF's oldest printed book, a Latin Bible from 1478, is included because it closely resembles handmade manuscripts, most specifically Petrus Bonus's *Pretiosa margarita novella* (The Precious New Pearl) in layout, color, and typography.

The paintings, ranging from 17th- to 19th-century works, show the progression of artists' depictions of how alchemists used recipes, manuscripts, and, later, printed books to accomplish their tasks, whether attempting to

transmute metals into gold or preparing dyes and medicines. For example, T*he Bald-Headed Alchemist* by David Teniers II, which presents an alchemist at his furnace stirring a crucible while reading a manuscript, is directly paired with soot-covered alchemical miscellany. This pairing allows visitors to connect the soot stains on the manuscript with the image in the painting. Visitors can also see how artists' views of alchemists changed over time: earlier paintings commonly show alchemists as unkempt fools and quacks, while many later paintings portray them as well-groomed scholars.

Thirty objects from the collections at CHF are on display. Included are nine manuscripts and three illuminated miniatures acquired in 2013, and five printed books, four of which are from the Roy G. Neville Historical Chemical Library, with the fifth, a gift from Alfred Bader, a part of the Othmer Library collection. In addition to the manuscripts, 13 paintings are hung on the Hach Gallery walls. Four are from the Fisher Collection and nine are from the Eddleman Collection.

This exhibit continues CHF's effort to communicate the importance of science and technology to the general public. Not only will regular visitors to CHF be engaged by this exhibit, but those visitors curious about rare books and manuscripts, calligraphy, and paleography will see important objects in their areas of interest. Those particularly interested in fine art, especially Dutch genre painting and material culture, will also get a glimpse of one of the largest collections of alchemical paintings in the world.

Books of Secrets will be on display in CHF's Hach Gallery through 4 September 2015. The Museum at CHF is open from 10:00 a.m. to 5:00 p.m. Monday through Friday and open until 8:00 p.m. on the First Friday of every month. Group tours are available. The museum is often open later for CHF award events and public lectures. If you are attending an event at CHF and would like to visit the museum, please contact the event staff to confirm the museum hours for that event.

www.chemheritage.org/visit/museum/exhibits/books-of-secrets/index.aspx

Neil Gussman <neilg@chemheritage.org> is strategic communications and media relations manager at Chemical Heritage Foundation.

Museumgoers examine the numerous paintings and manuscripts on display at the exhibit opening on Friday, 5 December 2014. Photographs by Conrad Erb

What's in a Name? Quite a Lot, as it Happens!

by Mark I. Borkum and Jeremy G. Frey

Names are essential to data manipulation and data interpretation. IUPAC standardizes the names that chemists use in their scholarly works, which it publishes as a suite of terminology, nomenclature and ontology, the IUPAC colour books. Currently, machine-accessible representations of these publications are not available on the Web. In this article, we argue the case for Web-based, machine-accessible representations of IUPAC publications.

What's in a name? Names are used to identify whole classes of things, or individual things, either uniquely, or within a given context. Scientific disciplines standardise their terminology (sets of names), nomenclature (rules for the selection of names) and ontology (denotation of names and definitions of associated things) to ensure that their scholarly works have unambiguous interpretations. Names are also an essential component of the architecture of the Web, where they are used to identify Web resources.

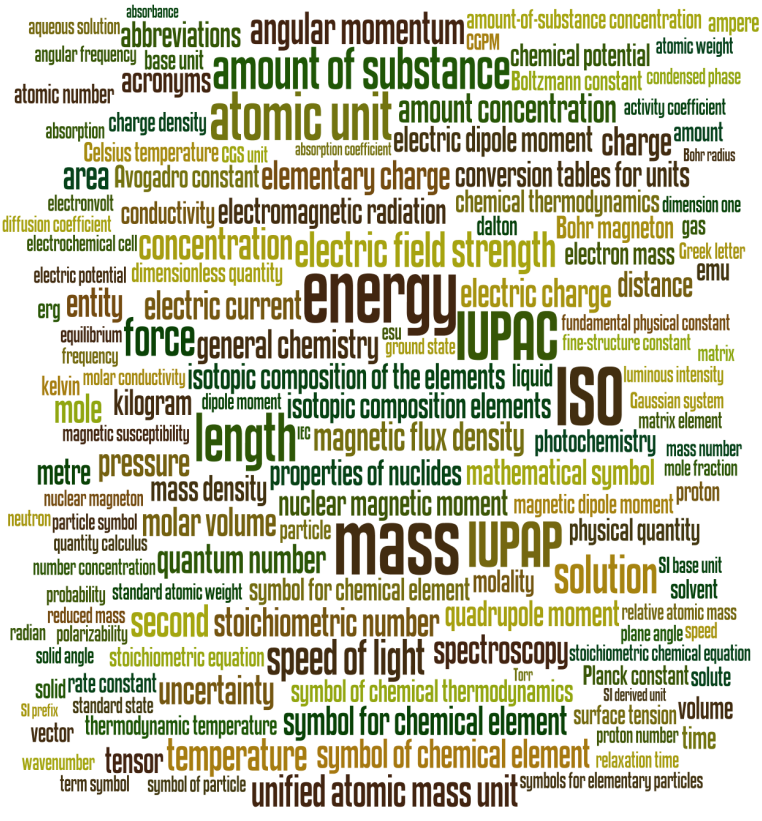
Today, an increasing number of chemists, working around the world, disseminate their scholarly works using the Web. Some, with the assistance of specialist publishers. Unfortunately, instead of being readily available for data integration, much of the world's chemical information is "trapped" inside of vast "data silos", whose contents are accessible to humans, but not machines. The *lingua francas* of the Web (HTML, PDF, e-book, etc.) are rudimentary emulations of paper and ink, designed for data presentation, not data communication. As these data formats do not codify names, it is not possible to delineate and explicate data structure, and hence, the information content of the resultant Web resources is inaccessible to machines.

One of the main roles of IUPAC is to standardise the names that chemists use in their scholarly works. Accordingly, it publishes the IUPAC colour books: a suite of terminology, nomenclature and ontology for chemistry. Currently, only five of these publications are available online [1,2], represented as a mixture of unstructured and semi-structured Web resources that cannot be easily reused by software developers. These projects are *ad hoc* and their outputs mutually incompatible, lacking long-term planning and centralised coordination, as demonstrated by the fact that the only comprehensive list of Web resources is provided by Wikipedia, and not IUPAC's own homepage (which, as a particular example, omits compendia like the Silver book).

But all is not lost! A critical observation is that many, if not all, IUPAC publications are typeset using software-based document preparation systems, meaning that, given some preprocessing, the information content of these publications, such as the subject indices, can, in principle, be made available for data integration.

At the University of Southampton, we are exploring the usage and applications of Semantic Web technologies for chemistry research. In a recent publication [3], we describe the extraction and enrichment of the subject index of the IUPAC Green Book [4]. We note that the subject index is of a particularly high quality. An IUPAC-endorsed, machine-accessible representation would be of considerable interest to software developers. The image [below] is a depiction of the weighted frequency list (or "tag cloud") of the most frequently referenced terms in the subject index of the IUPAC Green Book, rendered using Wordle [5].

"Tag cloud" of the IUPAC Green Book subject index



As a follow-up, and in conjunction with the Royal Society of Chemistry's Chemical Information and Computer Applications Group (RSC CICAG) [6], we organized the one-day meeting, "What's in a name: Terminology and nomenclature, the unsung heroes of open innovation" [7], which was held on 21 October 2014, at Burlington House, London, UK. Presentations covered a wide range of topics of interest to both industry and academia, including: the representation of crystal structures, polymers and chemical reactions; the impact of the Web on the communication of chemical information; and the challenges of managing translational research in an "open" software architecture.

Despite its name, the meeting highlighted the ease with which, from a computer science perspective, many common misunderstandings about names permeate human discussion. For example, it is all too easy to confuse the name of a thing with the thing itself, to ignore the distinction between the processes of identification and resolution, or to forget that the same name can be resolved by more than one identity provider. To paraphrase the Belgian surrealist, René Magritte: "Ceci n'est pas une structure chimique," (ceci est une représentation d'une structure chimique).

In this niche area, chemists risk succumbing to the "curse of knowledge", focusing on the minor details of their own discipline while bypassing the major practicalities of software engineering; an issue that can only be resolved by actively seeking collaboration with computer scientists. There are many fine examples of "chemist-ware" on the Web, but their developers represent an absolutely tiny fraction of the world's chemists, who are presently unable to fully express themselves.

The Web is indispensable to modern chemistry research. It is only a matter of time before the "killer app" for chemistry is successfully developed, "infecting" its end-users with its own potentially problematic interpretation of the discipline. If IUPAC does not take immediate measures [8], leveraging the power of its brand to promote a cohesive vision of chemical terminology, nomenclature and ontology on the Web, then it risks being supplanted as the international authority for chemical sciences.

Semantic Web Technologies

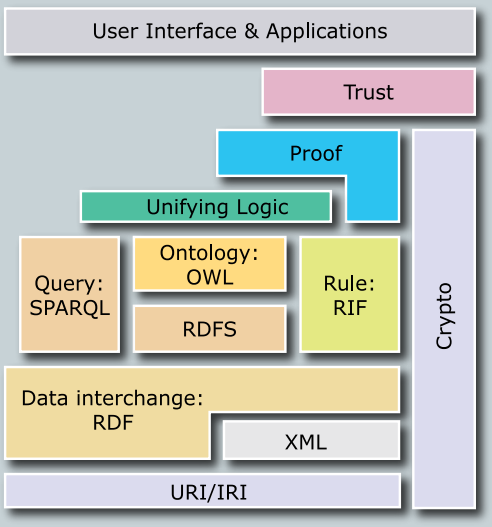
The Semantic Web [a] is a collaborative movement led by the international standards body the World Wide Web Consortium (W3C) [b], whose goal is to transform the human-accessible "Web of documents" into a machine-accessible "Web of data". The Semantic Web is realized as a hierarchy of technologies (see figure), where each successive layer builds upon and extends the capabilities of the preceding layers.

At the base, the fundamental technology of the Semantic Web is the Uniform Resource Identifier (URI) [c], which provides a mechanism to identify the name of a resource. Given identification by one or more URIs, representations of a resource can be exchanged over the network. The most common form of URI on the Web is the URL (the thing that you type into the address bar of your Web browser).

The next layer is the Resource Description Framework (RDF) [d], a family of specifications that collectively define a method for modelling information resources by making assertions about their nature and characteristics. Each assertion takes the form of a "subject-predicate-object" triple, where the subject and predicate are both resources, identified by URIs, and the object is either a resource, identified by a URI, or a literal value, such as a string, number or timestamp.

In RDF, every set of assertions induces a labelled, directed graph, where vertices and edges correspond to resources and assertions respectively. A core capability of RDF is that any two graphs can be added together, to yield a third graph of equal or

Depiction of the stack of technologies underlying the architecture of the Semantic Web (the "layer cake"). Source: www.w3.org



Mark I. Borkum <m.i.borkum@soton.ac.uk> is a Postdoctoral Researcher at the University of Southampton. While his academic background is Computer Science, he is a member of the Chemistry department. His research interests include how the machine-readable representation of chemical, laboratory and health and safety information can support Chemistry-themed use cases. Twitter: @markborkum
LinkedIn: https://uk.linkedin.com/pub/mark-borkum/1b/196/89b/

Jeremy G. Frey <j.g.frey@soton.ac.uk > is a Professor of Physical Chemistry at the University of Southampton. His interests include how e-Science infrastructure can support scientific research, with an emphasis on the way appropriate use of laboratory infrastructure can support the intelligent access to scientific data. Twitter: @profechem
LinkedIn: www.linkedin.com/in/jeremygfrey

References

1. Wikipedia, the free encyclopedia. IUPAC book; available at http://en.wikipedia.org/wiki/IUPAC_book
2. IUPAC. Nomenclature and Terminology (including IUPAC color books); available at www.iupac.org/home/publications/e-resources/nomenclature-and-terminology.html
3. Borkum, M. I. and J. G. Frey. "Usage and applications of Semantic Web techniques and technologies to support chemistry research". *J. Chem. Inf.*, **6**(1):18, 2014; http://dx.doi.org/10.1186/1758-2946-6-18
4. Cohen, E. R., T. Cvitas, J. G. Frey, B. Holmström, K. Kuchitsu, R. Marquardt, I. Mills, F. Pavese, M. Quack, J. Stohner, H. L. Strauss, M. Takami, and A. J. Thor. *Quantities, Unit and Symbols in Physical Chemistry*, 3rd edition, 2nd printing (IUPAC Green Book). Cambridge: IUPAC and RSC Publishing, 2008.
5. Feinberg, J.. Wordle - Beautiful Word Clouds; available at www.wordle.net
6. Royal Society of Chemistry. Chemical Information and Computer Applications Group; available at www.rsc.org/Membership/Networking/InterestGroups/CICAG
7. Royal Society of Chemistry. *What's in a name?* available at www.rsc.org/events/detail/11834
8. Frey, J.G.. "Digital IUPAC: A vision and a necessity for the 21st century". *Chem Int.* **36**(1):14-15, 2014; http://dx.doi.org/10.1515/ci.2014.36.1.14

greater extent, i.e., the addition operation for graphs is monotonic [e]. Consequentially, when using RDF, data integration is always possible.

The interpretation of labels in RDF graphs is formalised by two related technologies, RDF Schema (RDFS) [f] and Web Ontology Language (OWL) [g]. The former is a vocabulary for RDF, which facilitates the description of rudimentary entity-relationship models. The latter is an extension of the former, founded upon description logic, which enables the description of arbitrarily complex data models.

Another core technology is the Simple Knowledge Organisation System (SKOS) [h], a standard built upon RDF and RDFS for the representation of controlled vocabularies, including, but not limited to, thesauruses, classification schemes, subject-heading systems, and taxonomies. SKOS employs a concept-centric model of vocabularies, where the abstract notions of the vocabulary are represented by instances of the SKOS "\concept" class. SKOS concepts are annotated with RDF properties, including: index terms (labels), synonyms and alternative spellings, common misspellings, definitions, notes and notations.

References

a. Berners-Lee, T., J. Hendler, and O. Lassila. The Semantic Web. *Scientific American*, **284**(5):28-37 (2001).
b. World Wide Web Consortium (W3C); available at www.w3.org.
c. Berners-Lee, T., R. Fielding, and L. Masinter. RFC 3986, Uniform Resource Identifier (URI): Generic Syntax (2005).
d. Cyganiak, R., D. Wood, and M. Lanthaler, editors. *RDF 1.1 Concepts and Abstract Syntax*. W3C Recommendation. W3C, February 2014
e. Hayes, P. J. and P. F. Patel-Schneider, editors. RDF 1.1 Semantics. W3C Recommendation. W3C, February 2014
f. Brickley, D. and R. V. Guha, editors. *RDF Schema 1.1.* W3C Recommendation. W3C, February 2014
g. Hitzler, P., M. Krötzsch, B. Parsia, P. F. Patel-Schneider, and S. Rudolph, editors. *OWL 2 Web Ontology Language Primer* (2nd edition). W3C Recommendation. W3C, December 2012
h. Miles, A. and S. Bechhofer, editors. *SKOS Simple Knowledge Organization System Reference*. W3C Recommendation. W3C, August 2009

The History of the IUPAC Nomenclature of Organic Chemistry

by Evan Hepler-Smith

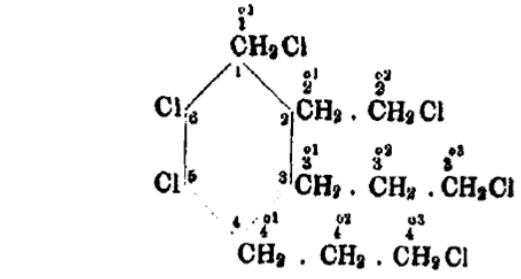
For chemists and chemistry students around the world, "IUPAC" is synonymous with "nomenclature" – especially the nomenclature of organic chemistry. Generations of chemists have learned – sometimes grudgingly – to read and write systematic names for organic compounds using guidelines codified by the International Union of Pure and Applied Chemistry. [1,2,3] The prefixes, suffixes, numbers, and parentheses of IUPAC names put molecules in order: individually, by expressing the network of atoms and bonds that constitutes the structure of an organic compound, and collectively, by situating each compound among the tens of millions of known organic chemical substances. IUPAC names carry this order out of chemical journals and into such sites as patent records, customs lists, and environmental regulatory databases.

The latest IUPAC *Nomenclature of Organic Chemistry* runs to 1,568 pages. [4] A curious reader thumbing through this volume might reasonably assume that systematic nomenclature is made by layering a verbal logic atop the ever-expanding variety of carbon compounds that nature and synthetic chemistry have devised. However, the drive for *rigor*—economical, categorical, logically consistent rules—is only a part of the story of systematic nomenclature. The making of the 1930 Liège Nomenclature, the foundation of official IUPAC organic nomenclature, also required *flexibility*—tolerance for carefully-curated variation and inconsistency among chemical names, in the service of making the nomenclature system easier to adopt and adaptable to a wider range of circumstances. Formed amidst the disordering aftermath of war as well as a disorderly chemical vocabulary, the Liège Nomenclature gained acceptance not only because of how it ordered molecules, but because of how it organized chemists.

The development of an international system of organic nomenclature began nearly three decades before the founding of IUPAC, at the Geneva Nomenclature Congress. During the late nineteenth century, as chemists synthesized more and more novel organic compounds, they often found it expedient to give each new compound a name that expressed their view of its chemical structure. However, since chemists turned to numerous conflicting conventions for doing so, such names threw the already disorderly nomenclature into further disarray. Over four days in April in 1892, thirty-four prominent organic chemists from across Europe gathered in Geneva to develop a system of nomenclature rules to put this confusion in order. [5]

The delegates to the Geneva Congress were presented with a choice between two ideas of how systematic nomenclature should work, each advocated by a leading chemist of the day. Charles Friedel, the Frenchman who organized the Congress, envisioned a flexible system of nomenclature that would allow chemists to use different sorts of trivial and systematic names adapted to their diverse needs and preferences. German luminary Adolf von Baeyer, in contrast, advocated a rigorous system of nomenclature rules. Such a system, Baeyer argued, could be an invaluable aid to chemical editors in the task of sorting an endless stream of organic chemical names into reliable subject indexes. Baeyer's plan won the day: the Geneva Nomenclature would generate a unique name for every organic compound, expressly for use in ordering and searching through the tens of thousands of entries in chemical handbooks and journal indexes.

That was the idea, anyway. In reality, generating unique names that clearly expressed the structure of organic compounds was no easy task. Most compounds of even moderate complexity – for example, anything containing more than one kind of functional group – fell outside of the scope of the rules that the Congress had been able to



Benzenchloromethyl-1-chloro-2-äthyl-2-chloro-3-propyl-3-chloro-4-propyl-4-dichlor-5,6.

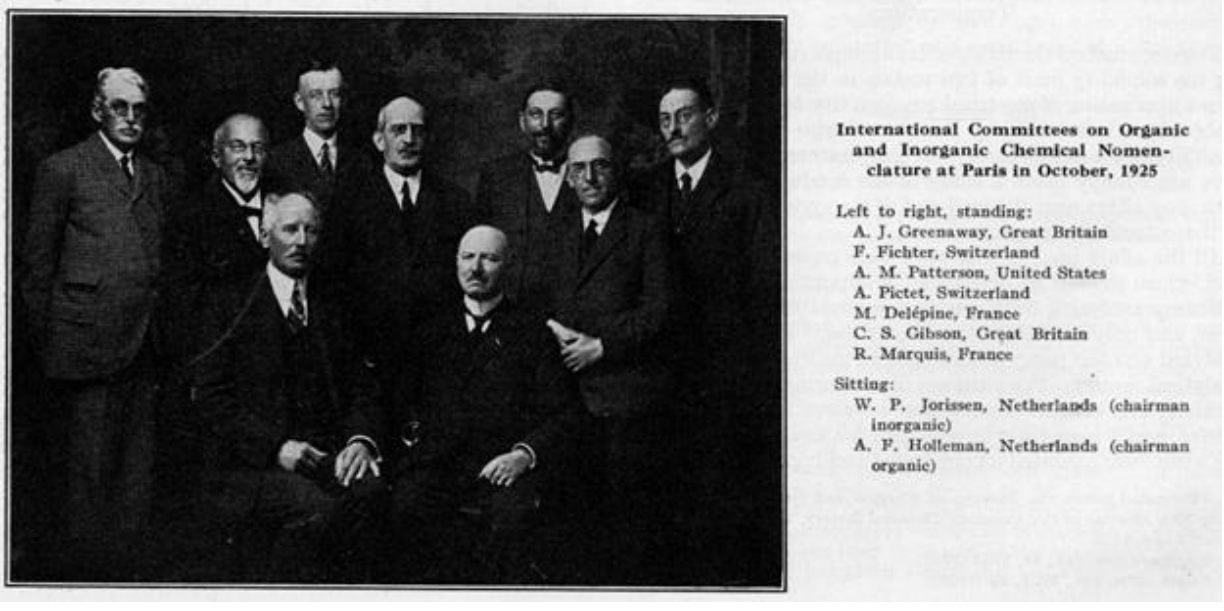
German chemical lexicographer Max Moritz Richter, a colleague of Paul Jacobson, offered this example of the excessive complexity of some Geneva names. [Max Moritz Richter, "Ein Beitrag zur Nomenclatur," Berichte der Deutschen Chemischen Gesellschaft 29, no. 1 (1896): 603.]

agree upon. To other compounds, the Geneva rules assigned names that seemed excessively complicated to chemical readers and authors alike. As a result, some of the editors for whose benefit the Geneva nomenclature had been created felt that they could not make use of it.

Foremost among these editors was Paul Jacobson. A young organic chemist of Jewish heritage, Jacobson had left a junior professorship in Heidelberg to become editor-in-chief of the publications of the German Chemical Society, an expanding collection of periodicals and reference works including the invaluable *Beilstein's Handbuch* [6] Jacobson considered the Geneva nomenclature to be a lost cause. In his publications, he shunned systematic nomenclature and alphabetized lists of names in favor of chemical indexes ordered by empirical formula. For the mammoth undertaking of compiling an entirely reorganized fourth edition of Beilstein, Jacobson and his deputy Bernhard Prager developed the elaborate classification of organic compounds that became known as the "Beilstein system."

Despite, or perhaps because of, his skepticism regarding the rigorous Geneva project, when another international project to reform organic nomenclature began to coalesce, Jacobson seized a leading role. At the first meeting of the International Association of Chemical Societies, held in Paris in 1911, Jacobson took the initiative to present a plan for the nomenclature work that the Association would undertake. [7] His approach was diametrically opposed to that of the Geneva Congress. Instead of prominent chemists, Jacobson advocated that the new nomenclature commission be made up of experienced editors and indexers. Instead of developing a rigorous system of nomenclature rules – or any system of nomenclature rules at all – he proposed that the commission merely evaluate novel nomenclature proposals and address specific instances of confusion among existing chemical names. Some of his fellow commission members had different ideas, but Jacobson managed to secure the chairmanship of the organic nomenclature commission. For an editor in the middle of a project as enormous as the fourth edition of *Beilstein*, it was a savvy move. By taking charge of nomenclature reform and shepherding it in the direction of flexibility, he could stave off any rigorous new rules that might interfere with his work in progress.

Just as Jacobson's commission was beginning to get to work over the summer of 1914, the German army invaded Belgium. Like many other areas of international scientific cooperation, nomenclature reform came to a sudden halt. It remained suspended for the duration of World War I. Though dormant, the project was not forgotten; after the armistice, the members of Jacobson's commission sought to resume their prewar efforts. The conditions of international scientific relations had changed substantially. The International Association of Chemical Societies was dissolved in 1919, and the International Union of Pure and Applied Chemistry founded under the umbrella of the International Research Council (IRC). As with all the member unions of



International Committees on Organic and Inorganic Chemical Nomenclature at Paris in October, 1925

Left to right, standing:
A. J. Greenaway, Great Britain
F. Fichter, Switzerland
A. M. Patterson, United States
A. Pictet, Switzerland
M. Delépine, France
C. S. Gibson, Great Britain
R. Marquis, France

Sitting:
W. P. Jorissen, Netherlands (chairman inorganic)
A. F. Holleman, Netherlands (chairman organic)

*The members of the organic nomenclature working group, along with colleagues on an analogous group dealing with inorganic nomenclature (*Industrial & Engineering Chemistry *17, no. 12 (December 1, 1925): 1245.*

the IRC, a kind of scientific Treaty of Versailles established by representatives of the victorious Entente nations, Germans and German institutions were banned from membership in IUPAC. The landscape of organic nomenclature had changed as well. The initial volumes of the fourth edition of *Beilstein* had been published, as had another authoritative reference work, the first collective index to the American abstract journal *Chemical Abstracts*. Under these challenging conditions, and without the help of the German Jacobson, IUPAC took up the reform of organic nomenclature.

In 1921, the IUPAC Council established a Commission on the Reform of the Nomenclature of Organic Chemistry, composed of one representative from each of the Union's twenty-one member nations. (Parallel IUPAC commissions took up inorganic and biochemical nomenclature; the three commissions operated independently during the 1920s.) Over the following two years, several representatives proposed different starting points for the commission's work. One, for example, suggested picking up precisely where Jacobson's commission had left off; another advised portioning out the entire field of organic compounds and putting each commission member in charge of nomenclature within one such section. The commission met only at the Union's annual conferences, and chronic absenteeism among commission members left these meetings as *ad hoc* affairs offering little opportunity to reconcile the various proposals.

At the encouragement of the Union president, the commission decided upon a different way of advancing its work. The commission assigned responsibility for organic nomenclature reform to a working group made up of six members appointed by the editorial boards of leading American, British, Dutch, French, Italian, and Swiss chemical publications. Cutting through the Gordian knot of commission reports from before and after the war, the commission instructed this working group to base its discussions on the one concrete point of departure that could be identified without further discussion: the Geneva nomenclature.

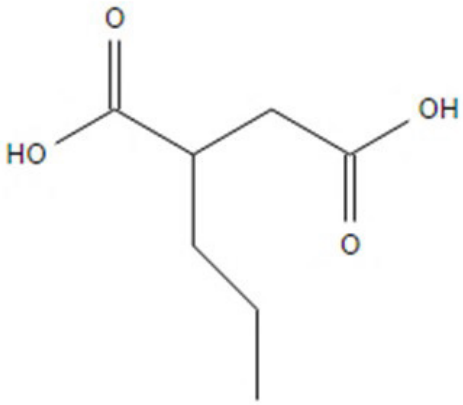
The working group took up this task in 1924, under the presidency of University of Amsterdam professor Arnold Holleman, a respected textbook author fluent in French, German, and English as well as his native Dutch. The American member, Austin Patterson, was regarded as the world's leading authority on organic nomenclature – outside of Germany, at least. Just as importantly, as the architect of the nomenclature used in *Chemical Abstracts*, Patterson could help ensure mutual understanding between the working group and this important publication. In order to establish a similar sort of relationship with Beilstein despite the IRC boycott of Germany, both Holleman and Patterson corresponded unofficially with Prager, the reference work's editor (Jacobson had died in 1923).

The working group faced a conundrum. Under Jacobson's watch, international work on organic nomenclature had shifted decisively in the direction of flexibility, and the further entrenchment of the nomenclature systems used in *Chemical Abstracts* and *Beilstein* seemed to make such flexibility all the more important. At the same time, the working group had been charged with building rules based on the rigorous Geneva nomenclature.

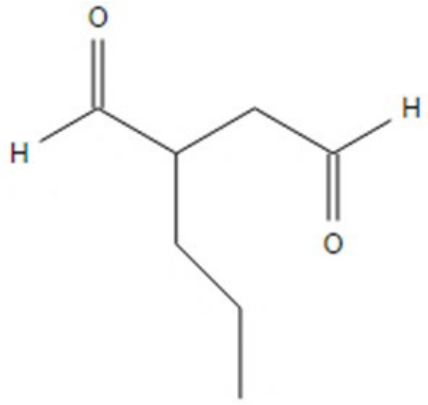
Holleman's solution was to adopt the content and form of the Geneva rules, but to subtly reshape them according to the spirit of Jacobson's flexible approach. During five meetings over the course of two and a half years, Holleman led the working group step by step through the official text of the Geneva nomenclature. By 1927, Holleman's group had agreed upon a set of sixty-eight rules. These rules covered nearly the same ground as the sixty-two Geneva rules, sanctioning most of the same prefixes and suffixes. However, when it came to general matters, the working group took a much more flexible approach, tolerating variation and preserving well-established trivial names where the Geneva rules had assigned exclusively unique, systematic names. Where the Geneva Congress had codified a rigorous approach to organic nomenclature, and Jacobson had resisted the codification of any such system, the working group's nomenclature codified a *systematically flexible* approach to organic nomenclature.

Satisfied that they had discharged their duty, the working group submitted these rules for affirmation by the organic nomenclature commission. One commission member, though, stood ready to defend the rigorous spirit of the Geneva Nomenclature. Victor Grignard, who represented France on the commission, saw the flexible approach embodied in the working group's rules as an abdication of the consistency and logic achieved by the Geneva Congress. His opinion mattered more than most; Grignard was a Nobel laureate and one of the most famous chemists in France. Speaking from a position of scientific prestige akin to that of Friedel and Baeyer in 1892, Grignard advocated instead addressing the shortcomings of the Geneva rules by developing an alternative but no less rigorous system.

At the 1927 IUPAC conference, Grignard laid out this critique for his fellow commission members. His eloquent appeal to the logic of Geneva – and surely also his scientific reputation – convinced the commis-



Geneva: 3-methyl-1,3[1]-hexanedioic acid
WG: 1,2-pentanedicarboxylic acid
propylsuccinic acid



Geneva: 3-methyl-1,3[1]-hexanedial
WG: propylbutanedial
propylsuccinaldehyde

Naming a diacid and its corresponding dialdehyde according to the Geneva rules and the rules proposed by the working group in 1927. The Geneva rules assign systematic names to each compound using a consistent logic. These names are cumbersome, but they express the structural relationship between the two compounds unambiguously. The working group's rules address each compound using a different approach; the resulting names are easier to read, but they do not capture the structural similarity of the compounds as precisely. The working group's approach also permitted the use of the established trivial names* succinic acid *and* succinaldehyde. *(Neither system considered stereochemistry.)

sion to defer its approval of the working group's rules. Over the subsequent year, Grignard had his critiques printed and distributed, seeking to generate enough opposition to the rules to stave off their acceptance once more.

He was perhaps more successful than he intended. When the organic nomenclature commission assembled once again in 1928, Grignard's impassioned campaign and the Union's lax approach to commission participation combined to turn the meeting into a free-for-all. Grignard and his sympathizers once again spoke out against the working group's rules, as curious delegates wandered into and out of the meeting room at will. A few of these visitors volunteered off-the-cuff ideas that had nothing to do with either the rules or Grignard's critiques. With tempers flaring among commission members, Holleman adjourned the meeting early, though not before Grignard had rallied a majority to vote down the working group's rule for naming carboxylic acids. Still, Holleman did not back down from his commitment to flexibility. Instead of replacing the working group's rule with Grignard's preferred approach, he retained the former as an acceptable alternative.

At the insistence of the IUPAC Council, Holleman scheduled his rules for a definitive vote at the 1930 conference in Liège. While Grignard carried on his attempts to rally chemical public opinion, Holleman worked to shore up his support among influential editors. At Patterson's request, Holleman agreed to suppress a rule that might have led to conflicts with the nomenclature used in *Chemical Abstracts*. After revisions in IRC and IUPAC bylaws opened the way for Germany to join the Union, Holleman met with German editors in Berlin. There, he allowed Prager to attach a rider to the working group's rules, stipulating that they were not to be taken to interfere with naming practices in the two preeminent reference works.

Holleman's painstaking revisions made the working group's rules more flexible and less rigorous – a change in the opposite direction as that sought by Grignard and his fellow critics. However, they secured the support of the editors of Beilstein and Chemical Abstracts. Holleman no doubt reminded the commission members of the importance of this support when he solicited their votes – this time, before they assembled at the conference.

The appeal succeeded. Even Grignard conceded the fight, though not the argument, acknowledging that the nomenclature practices of the reference publications presented, in his words, "nearly insurmountable difficulties" for one aiming to bring rigorous no-

menclature into an international setting. [8] When the nomenclature commission met in 1930, the working group's rules were approved without debate, and became the Liège Nomenclature.

In recent years, the focus of IUPAC nomenclature work has turned to the development of unique identifiers for organic compounds, in the form of "preferred" IUPAC names (PINs) and computer-readable notation (InChI). [4,9] Such projects are driven by the demands of a new technological context – the wholesale shift from print to a variety of computer-based resources for handling chemical information. But their fundamental aim is neither entirely new, nor even the next step in a progression of increasingly rigorous ways of naming and ordering chemical compounds. Rather, the InChI and PIN projects are the latest episodes in a long history of competing demands for flexibility and rigor in organic nomenclature, a history whose product is IUPAC nomenclature itself. Today's efforts to develop nomenclature and notation standards are related by both analogy and genealogy to decisions taken in 1892, the 1920s, and since. The more we understand about how chemists have confronted the challenges that the making of systematic nomenclature has presented over the past century and a quarter, the better we can equip those who develop and use chemical information systems to deal with these challenges, now and in the future.

Evan Hepler-Smith <ehepler@princeton.edu> is a doctoral candidate in the Program in History of Science at Princeton University. He spent the year 2013-2014 at the Chemical Heritage Foundation in Philadelphia as Herdegen Fellow in the History of Scientific Information.

Notes, References, and Further Reading

1. Verkade, Pieter Eduard. *A History of the Nomenclature of Organic Chemistry*, trans. S. G. Davies. Boston: Reidel, 1985.
2. Fennell, Roger. *History of IUPAC, 1919-1987.* Boston: Blackwell Science, 1994.
3. For more information on current IUPAC nomenclature activities, see the webpage of the Chemical Nomenclature and Structure Representation Division. www.iupac.org/body/800
4. Favre, Henri A. and Warren H. Powell, eds., *Nomenclature of Organic Chemistry: IUPAC Recommendations and Preferred Names 2013.* Cambridge: Royal Society of Chemistry, 2014.
5. Hepler-Smith, Evan, "'Just as the Structural Formula Does': Names, Diagrams, and the Structure of Organic Chemistry at the 1892 Geneva Nomenclature Congress," *Ambix* **62**(1): 1-28, 2015.
6. Founding editor Friedrich Beilstein transferred responsibility for his *Handbuch* to the German Chemical Society during the late 1890s.
7. Van Tiggelen, Brigitte and Danielle Fauque, "The Formation of the International Association of Chemical Societies," *Chemistry International* **34**(1):9–11, 2012.
8. Grignard, Victor, *Traité de Chimie Organique, vol. 1.*: 1075. Paris: Masson, 1935.
9. Heller, Stephen, et. al., "InChI - the Worldwide Chemical Structure Identifier Standard," *Journal of Cheminformatics* **5**:7 (January 24, 2013).

Election of IUPAC Officers and Bureau Members – Call for Nominations

At its General Assembly in Busan, Korea, on Wednesday 12 and Thursday 13 August 2015, the IUPAC Council will be asked to elect a Vice President, a Secretary General, a Treasurer, and members of the Bureau to fulfill the vacancies created by retiring members. IUPAC National Adhering Organizations are invited to submit nominations no later than 12 June 2015.

On 1 January 2016 Natalia Tarasova (Russia), Vice President and President-Elect of IUPAC, will become President. Mark Cesa (USA), current President, will become Past President and remain an officer and a member of the Bureau for a period of two years, while Kazuyuki Tatsumi (Japan), current Past President, will retire. Acting Secretary General Colin Humphris (UK) was elected by the Bureau in April 2014 to fulfill the vacancy only till the end of the biennium and will retire. Treasurer John Corish (Ireland) will also retire after completing a second and final four-year term.

In addition, there are three vacancies for Elected Members of the Bureau this year. Elected Members serve a four-year term, and are eligible for re-election to a second four-year term. No National Adhering Organization shall have more than one Elected Member on the Bureau, and the principle of fair geographical representation of Members shall be taken into account, as stipulated in the IUPAC Statutes. Elected Members whose terms expire at the end of 2015 are:

- Prof. Christopher M. A. Brett (Portugal) (2012-2015), eligible for nomination
- Prof. Javier García-Martínez (Spain) (2012-2015), eligible for nomination
- Prof. Ram Lamba (Puerto Rico) (2008-2011, 2012-2015)

The following are Members whose terms continue to the end of 2017:

- Prof. Russell J. Boyd (Canada) (2014-2017)
- Prof. Tavarekere K. Chandrashekar (India) (2014-2017)
- Prof. Richard Hartshorn (New Zealand) (2014-2017)
- Mr. Colin Humphris (UK) (2010-2013, 2014-2017)
- Prof. Christopher K. Ober (USA) (2014-2017)
- Prof. Kaoru Yamanouchi (Japan) (2014-2017)
- Prof. Qi-Feng Zhou (China) (2010-2013, 2014-2017)

In addition to the five officers and the ten Elected Members, the Bureau also includes eight Division Presidents (each elected by an individual Division), and five ex officio members representing the following Standing Committees: the Committee on Chemistry Education (CCE), the Committee on Chemistry and Industry (COCI), the Committee on CHEMical Research Applied to World Needs (CHEMRAWN), the Interdivisional Committee on Terminology, Nomenclature and Symbols (ICTNS), and the Committee on Publications and Cheminformatics Data Standards (CPCDS).

IUPAC National Adhering Organizations are invited to submit nominations for Vice President, Secretary General, Treasurer, and Elected Members to the Secretary General <secretariat@iupac.org> no later than **12 June 2015**.

It is important for a vibrant organization that all vacant positions are filled after a fair and vigorous election process, so all nominations are encouraged. To make your voice heard, contact your National Adhering Organization and get involved.

What Is the Bureau?

The Bureau is established by the Council to act for the Union during the intervals between meetings of the Council. It consists of the officers (president, vice president, secretary general, treasurer, immediate past president), the division presidents, and the chairs of the operational standing committees, as well as 10 other members elected by the Council.

What Does the Bureau Do?

The Bureau normally meets once a year, ensuring continutity between Council meetings. The principal duties of the Bureau are as follows:

- to ensure the strict observance of Statutes and Bylaws
- to prepare the agenda for Council meetings and in particular to make provisions for elections
- to make recommendations to the Council and attend Council meetings
- to implement the decisions of the Council and execute the program of the Union as directed by the Council
- to take steps to ensure that international congresses of pure and applied chemistry are held
- to take decisions about the holding of scientific meetings as proposed by the division committees
- to take all other steps necessary for the good conduct of the affairs of the Union

See the Statutes and Bylaws for details.

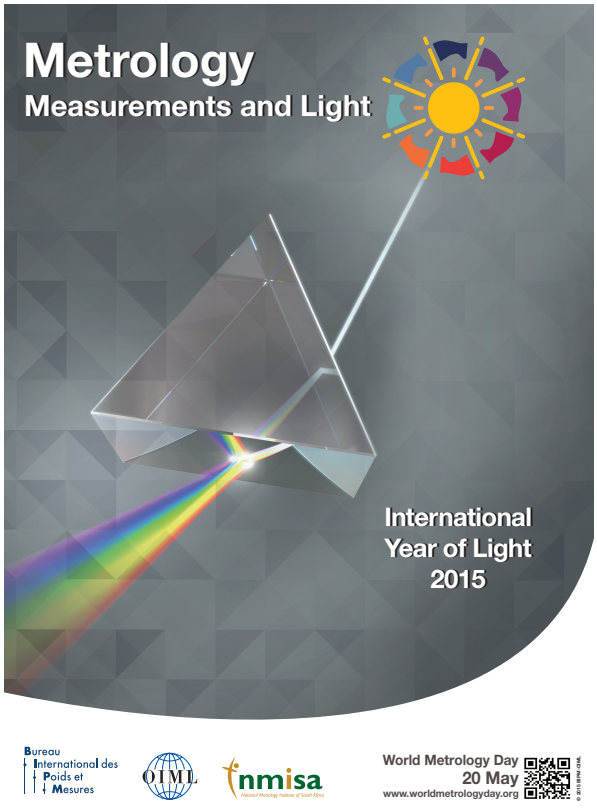
Measurements and Light

On 20 May 2015, World Metrology Day will join the 2015 International Year Light (iyl2015.org), with day-long celebrations on the theme of Measurements and Light.

World Metrology Day celebrates the signature by representatives of seventeen nations of the Metre Convention on 20 May 1875. The Convention set the framework for global collaboration in the science of measurement and in its industrial, commercial and societal application. The original aim of the Metre Convention —the worldwide uniformity of measurement—remains as important today as it was in 1875.

The World Metrology Day project is realized jointly by the Bureau International des poids et Mesures (BIPM) and the International Organization of Legal Metrology (OIML). We hope that you enjoy this site and that your Country or Metrology Organization will join us and participate in this year's event.

www.worldmetrologyday.org



ICSU announces Dr. Heide Hackmann to be Executive Director and Dr. Lucilla Spini to be Head of Science Programmes

Heide Hackmann, a social scientist with extensive experience running international research organizations, will be Executive Director of the International Council for Science (ICSU) Secretariat from March 2015. Lucilla Spini, a biological anthropologist with experience in international science coordination, will take on the newly created role of Head of Science Programmes in early January.

Dr. Heide Hackmann joins ICSU from the International Social Science Council (ISSC), where she has been Executive Director since 2007. During her tenure she strengthened ISSC's activity profile, membership base and financial position, and forged strong links with the International Council for Science through key partnerships. These include the Integrated Research on Disaster Risk program and the Science and Technology Alliance for Global Sustainability, the consortium of international organizations that founded Future Earth, the new global research initiative on global sustainability, and coordinating input from the international scientific community on key policy processes at the United Nations. Hackmann also led the launch of the regular World Social Science Forums and spearheaded the development of a new series of World Social Science Reports. She initiated a new global social science research funding and coordination program on Transformations to Sustainability, which was launched in March 2014 as a major contribution to Future Earth. Hackmann was born in South Africa and completed her PhD in Science and Technology studies at the University of Twente, Netherlands in 2003. From then until 2007 she was Head of the Department of International Relations and National Quality Assurance and Director CO-REACH (an EU-funded multi-lateral initiative for the Coordination of Research between Europe and China) at the Royal Netherlands Academy of Arts and Sciences (KNAW).

On 12 January 2015, Dr. Lucilla Spini took on the newly created post of Head of Science Programmes. In this role, she will manage the development and implementation of ICSU's scientific and science for policy initiatives, as defined in its Strategic Plan. Spini is an Italian national who holds a B.A. in anthropology from New York University, as well as an M.Sc. in human biology and D.Phil. in biological anthropology, both from the University of Oxford. Since 2001, she has worked on science/policy bridging, global environmental change, sustainable development and re-

search coordination for a number of international organizations, including UNESCO, UNU, and the FAO. Prior joining ICSU, she was a Giorgio Ruffolo Research Fellow in the Sustainability Science Program at Harvard's Kennedy School of Government.

www.icsu.org

The 2014 AAAS Award for Science Diplomacy goes to Zafra M. Lerman

Zafra M. Lerman, creator and advocate for the Biennial Malta Conferences, which promote international scientific cooperation and diplomacy by convening scientists from 15 Middle Eastern nations, has been chosen by the American Association for the Advancement of Science (AAAS) to receive the 2014 Award for Science Diplomacy.

Lerman—an accomplished chemist, science educator, and humanitarian—serves as president of the Malta Conferences Foundation. She was honored by AAAS for her efforts to "elevate the use of scientific cooperation as an instrument of peace, and as a pathway to better understand the role of science in addressing major societal challenges in the broader Middle East, despite the political barriers that exist at the official levels."

The Biennial Malta Conferences bring together scientists from Bahrain, Egypt, Iran, Iraq, Israel, Jordan, Kuwait, Lebanon, Libya, the Palestinian Authority, Qatar, Saudi Arabia, Syria, Turkey, and the United Arab Emirates to collaborate on shared science-based concerns such as regional water quality, solar-energy conversion and storage, science curricula, green chemistry, and chemistry safety and security. (Reports on the Malta Conferences have regularly appeared in *Chemistry International* since 2004; a compilation of these references and many others is available at www.maltaconferencesfoundation.org)

AAAS Chief International Officer Vaughan Turekian said: "Many of the scientists who participate in the Malta Conferences could not otherwise meet face-to-face because of tensions between governments. Dr. Lerman has brought together scientists at all levels, from Nobel Prize winners to early-career researchers and students, to build collaborative links that extend beyond scientific interactions."

The AAAS Award for Science Diplomacy dates to 1992. It recognizes an individual or small group working in the scientific and engineering or foreign affairs communities making an outstanding contribution to furthering science diplomacy. Renamed in 2010 by the AAAS Board of Directors, the Award consists of a plaque and an honorarium of $5,000. The AAAS Award for Science Diplomacy was bestowed upon Lerman during the 181st AAAS Annual Meeting in San Jose, California, 12-16 February 2015.

www.aaas.org/news/zafra-m-lerman-receives-2014-aaas-award-science-diplomacy

OPCW-The Hague Award Presented at 19th Conference of States Parties

On 1 December 2014, the opening day of the Nineteenth Session of the Conference of the States Parties of the Organization for the Prohibition of Chemical Weapons at the headquaters of the OPCW in The Hague, Dr. Robert Mathews (Australia) and the Finnish Institute for the Verification of the Chemical Weapons Convention (VERIFIN) were jointly presented with the inaugural OPCW-The Hague Award.

The Award was created by the OPCW as an outcome of its winning the 2013 Nobel Peace Prize. The Award is supported by a financial contribution from the City of The Hague. It is intended "to honour and recognise individuals and organizations that have made an outstanding contribution to achieving a world free of chemical weapons."

Dr. Mathews and VERIFIN have made valuable contributions toward the goal of reducing and eliminating chemical weapons. In keeping with the purpose of the Award, they have been credited with providing "sustained leadership and support to the development of key concepts of the Convention, as well as to initiatives to promote chemical disarmament and non-proliferation around the world."

Dr. Mathews is Head of the Nuclear, Biological and Chemical Arms Control Unit in the Australian Defence Science and Technology Organization. He has dedicated his career to the disarmament and non-proliferation of chemical weapons. He made significant contributions to the final drafting of the Chemical Weapons Convention, as well as to its establishment, implementation and promotion as a unique instrument eliminating an entire category of weapons of mass destruction. He has been involved in several IUPAC projects and is currently part of the task group "Updating, Piloting, and Disseminating Educational Material for Raising Awareness of the

Multiple Uses of Chemicals and the Chemical Weapons Convention" (www.iupac.org/project/2013-020-1-050)

The Finnish Institute for the Verification of the Chemical Weapons Convention (VERIFIN) has been in existence for 40 years. During that time VERIFIN has made a sustained contribution to chemical disarmament by focusing on the development and dissemination of analytical chemistry techniques and tools for the verification of the Chemical Weapons Convention. VERIFIN has been instrumental in efforts to build the capacity of laboratories around the world to provide effective and accurate analysis of CWC-related chemicals.

IUPAC has been privileged to work with the OPCW, both in contributing technical expertise to the Review Conferences of the CWC and in developing educational resources on the multiple uses of chemicals.

www.opcw.org/news/article/opcw-the-hague-award-presented-to-pioneers-of-the-chemical-weapons-convention/

IUPAC Physical Chemistry Cartoon Competition 2015

The Physical and Biophysical Chemistry Division (Division I) together with the Committee on Chemistry Education are pleased to announce the 2015 Physical Chemistry Cartoon Competition. This year's theme is "Light and Chemistry", in recognition of the UN's International Year of Light, and entries should reflect this theme.

Awards of USD 100 will go to four students whose cartoons are chosen as winning entries. Prizes of USD 100 will be given in three age groups to students aged 11 – 14, aged 15 – 18, and over 18, and one overall first-prize winner from all entries submitted.

Judging:
The cartoons will be judged by a panel with members from the IUPAC Division of Physical and Biophysical Chemistry and the Committee on Chemistry Education. Reviewing criteria (from most- to least-weighted) will include:

- Relevance to the theme of Light and Chemistry
- Creation of interest, novelty, entertainment value, etc.
- Clarity and educational content
- Presentation

Submission instructions:
Students currently in secondary (students aged 11-18) or tertiary education (up to first degree level) are invited to submit:

- a one-page (pdf or powerpoint) file containing an original cartoon
- a brief letter of endorsement from a Chemistry teacher or faculty member to verify that they are a currently enrolled student at the closing date for entries and confirming that the work is the student's own.

Entries should be submitted by email to <ChemistryCartoon@iupac.org>

Key dates:
The competition closes on Friday **29 May 2015** at 17:00 Zürich time.

http://www.iupac.org/news/news-detail/article/iupac-physical-chemistry-cartoon-competition-2015.html

IUPAC Office move

The IUPAC Secretariat office has been located in the Research Triangle Park (RTP) since May 1997, following its relocation from Oxford, England after 29 years. The office was housed in a small building right in the center of RTP, which is one of the most prominent high-technology research and development centers in the USA, centrally located near major universities, including Duke University in Durham, the University of North Carolina at Chapel Hill, and North Carolina State University at Raleigh.

This past February, the office headed by the recently appointed Executive Director, Lynn Soby, moved 1 mile north to an improved space that is safer, more secure, and more functional. The smooth relocation included the move of about 300 boxes of paperwork, financial records, historical archives, and IUPAC's servers and equipment. It also included packing over 7000 IUPAC books for relocation to a lower cost warehouse space. The staff, including Linda Tapp and Enid Weatherwax, made the transition quite easily as their work commutes have not really changed. The office mailing address stays the same (PO Box 13757, RTP, NC 27709), but if you plan to drop by for a visit, the new office is located at 79 T.W. Alexander Drive, Research Park Triangle, NC 27709.

While Lynn, Linda, and Enid are very busy setting up the new office space, Fabienne stays put in her remote office in the Chemistry Department at Boston University.

IUPAC Provisional Recommendations

Glossary of Terms Used in Neurotoxicology

The primary objective of this Glossary of Terms Used in Neurotoxicology is to provide clear definitions to readers who contribute to studies relevant to neurotoxicology, or must interpret them, but are not themselves neurotoxicologists, neuroscientists or physicians. This applies especially to chemists who need to understand the literature of neurotoxic effects of substances without recourse to a multiplicity of glossaries or dictionaries. The Glossary includes terms related to basic and clinical neurology as far as they are necessary for a self-contained document, particularly terms related to diagnosing, measuring, and understanding the effects of substances on the central and peripheral nervous systems. The glossary consists of about 750 terms as primary alphabetical entries, including Annexes of common abbreviations and examples of chemicals with known effects on the nervous system. The authors hope that, in addition to chemists, this glossary will be helpful, to groups including toxicologists, pharmacologists, medical practitioners, risk assessors, and regulatory authorities. In particular, it should facilitate the worldwide use of chemistry in relation to occupational and environmental risk assessment.

Comments by **31 May 2015**

Corresponding Author:
Doug Templeton
doug.templeton@utoronto.ca

www.iupac.org/project/2013-001-2-700

Stamps International

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

Otto Wichterle: An Eye for Hydrogels

Soft contact lenses, worn these days by an estimated 125 million people worldwide, were invented in the early 1960s by Otto Wichterle (1913-1998), an ingenious Czech organic chemist. It was in the mid-1950s that he first prepared poly(2-hydroxyethyl methacrylate), a novel polymeric material that was transparent, absorbed up to 40% of its weight in water to form a colloidal gel, and exhibited suitable mechanical properties for further processing. In a seminal paper published in the 9 January 1960 issue of *Nature*, Wichterle and Drahoslav Lím, one of his colleagues at the Institute of Macromolecular Chemistry in Prague, outlined the syntheses and properties of hydrophilic gels based on pHEMA and disclosed their potential use in the fabrication of soft contact lenses and other highly biocompatible products. The polymers used to manufacture soft contact lenses were continuously refined in the ensuing decades, particularly to improve oxygen permeability and comfort. The world market value of contact lenses (80% of which are of the soft variety) is now nearly US$8 billion. Significantly, the development of new hydrogels as drug delivery agents, cell culture platforms, artificial cartilage, and other applications in the healthcare industry has been a very active area of research in chemistry and biomedical engineering in recent years.

The Czech stamp illustrated here was issued in 2013 to commemorate the centennial of Wichterle's birth. In addition to his pioneering work on hydrogels, he studied the polymerization of ε-caprolactam to produce Nylon 6 and investigated the conversion of vinylic halides such as 1,3-dichloro-2-butene to ketones (a variation of the Robinson annulation that now bears his name). He published more than 150 scientific articles and obtained approximately 180 patents for his multiple contributions to chemistry and materials science. In 1967, he became the founder and first president of IUPAC's Macromolecular Division, which became the Polymer Division ("Division IV") in 2004. Shortly after democracy was restored in his homeland at the end of 1989, he was elected President of the Czechoslovak Academy of Sciences, a belated honor for a man who served his country in both the political and scientific arenas. Interestingly, even though Wichterle is universally considered the father of soft contact lenses, he never stopped wearing his own pair of eyeglasses!

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

Immunochemical Recognition and its Diagnostic and Therapeutic Applications

by Douglas Templeton and Michael Schwenk

The October 2014 issue of *Pure and Applied Chemistry* includes several papers arising from an IUPAC project on immunochemistry that describe interactions between molecules of the immune system and their ligands [1,2] and consider how a knowledge of this chemistry is furthering the development of both the analytical applications of immune-based sensors [3], and of better therapies for a variety of human medical conditions [4]. Each paper is structured to provide some historical context, followed by a critical presentation of our current perspective on the role chemistry is playing in the basic understanding of the immune system and its potential for exploitation.

The intricacies of the human immune system represent one of the most complex areas of current biology. In a forum in *Scientific American* (April 2012), Stuart Firestein noted that, as a neurobiologist, he can "understand the questions that drive immunology", but though he "can't grasp much of immunology … the wonderful thing is that most immunologists can't either". The point was, of course, the increasing specialization of all fields of science, but the example was well chosen. It is a challenge to discuss developments in immunology in a narrative that is comprehensible to chemists. Nevertheless, by including information boxes in the first two papers that are intended as a minimal introduction to the immune system, and by setting developments in a historical context, the *PAC* papers attempt to do so.

The immune system manages the body's reactions to invading microbes, allergens, and other foreign substances. It has two subsystems. The first, called "acquired" (or "adaptive") immunity, recognizes non-self-structures (antigens; Ag) of the invader and counteracts them with molecular responses that reflect a memory of previous exposure. This is what happens when, for example, we are vaccinated, become immune to recurrent disease, or develop allergies. This subsystem relies upon immunoglobulin protein antibodies (Ab's) and receptor proteins produced by two classes of specialized blood cells called lymphocytes. B lymphocytes, or "B cells", secrete Ab's that must recognize and combine with the foreign chemical structures into body fluids. T lymphocytes, or "T cells", express the recognition proteins as surface receptors on their cell membranes. Each of these cell types proliferates when the target molecule is detected, expanding to produce a large number of cells of a single clone. The B cell clones express monoclonal Ab's, and the T cell clones express identical copies of the T cell receptor (TCR), in each case recognizing the triggering Ag.

The second subsystem of immunity, described as "innate", recognizes and then counteracts microorganisms and/or viruses based on certain specific chemical structures that do not occur in vertebrates. This involves molecules with names like NOD-like, Toll-like, and RIG-like helicase receptors that are said to serve their function through pattern recognition; they are termed pattern recognition receptors (PRRs). Both subsystems of immunity involve intricate processes of molecular recognition; Ag-Ab and peptide-TCR in the first case, and ligand-receptor in the second. A number of crystal structures have been presented [1,2] to demonstrate how the recognition process occurs at a structural level. Examples have been chosen that reflect current research in the field, recognizing that the focus of much of this research is on infectious and autoimmune diseases and cancer. They also illustrate the beauty in the common themes and subtle variations of these interactions.

Antigen binding

Human immunoglobulins consist of disulfide-bonded dimeric structures with two so-called heavy chains (H chains) and two light chains (L chains) arranged as shown in Fig. 1. Antigen-binding sites are found in the regions between the L chain and the short arm of the H chain. The minimal recognition and binding structure consists of this fragment only, called a Fab fragment. For simplicity of crystallization and analysis, most structures have been determined with Ag-Fab complexes. Complex gene shuffling for coding regions of variable sequence in the binding pocket of Fab gives rise to the vast variety of sequences necessary to recognize seemingly any antigenic sequence the environment can present. These variable amino acid sequences are found in six complementarity-determining regions (CDR), three on each of the H and L chains, that dominate molecular interactions with Ag. In the case of a peptide/protein Ag, interaction occurs with a specific region of the Ag's peptide surface, called an epitope, that may involve several adjacent amino acids or, more commonly, amino acids widely separated in the primary peptide sequence that are in close proxim-

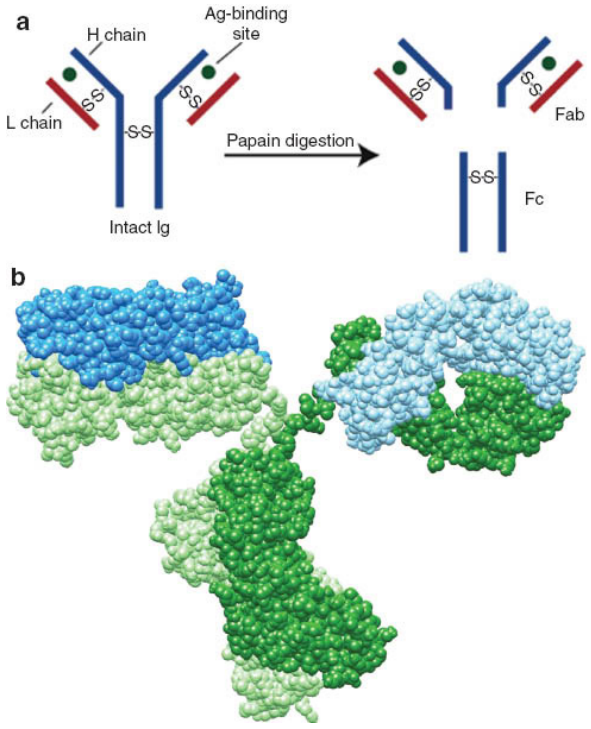


Fig. 1: Depictions of immunoglobulin structure. (a) Conventional schematic of a bivalent immunoglobulin showing disulfide-bonded H chains (blue) and L chains (red), presenting two Ag-binding sites (antigens shown as green circles). Upon digestion with papain, cleavage of the H chains releases two Fab and one Fc fragments. (b) A more realistic depiction based on crystallographic data, showing the two L chains in blue and the H chains in green. [1]

ity in the folded Ag protein.

Initial structural studies with abundant model proteins—hen egg white lysozyme was historically one of the most important—revealed that the Ag-Ab contact surface was relatively flat and reasonably constant in area. Energetic studies suggested that multiple contacts were involved and that the exclusion of water molecules from the contact region could provide a significant entropic contribution to binding. When a refined structure of a lysozyme-Ab complex at 0.20 nm resolution became available in 2000, several generalities were established. First, all six CDRs were in contact with the Ag epitope, and provided multiple hydrogen bonds, salt bridges, and van der Waals contacts. Second, small conformational movements in the CDR loops and flexibility in side chains of amino acids in the interface region enhanced complementarity of binding—an interplay of lock-and-key fit and conformational flexibility provide the required enthalpic and entropic contributions to binding energy. Third, far from excluding water, the interface region included ordered water molecules that were not observed at lower resolution. These water molecules fill gaps in the interface region, improving fit and accommodating unpaired hydrogen-bonding residues.

Since the detailed analysis of the structure of the lysozyme-Ab complex was presented, several thousand Ag-Ab structures have been solved, and a structure is now pretty much expected as part of Ab characterization. The field of greatest activity is in studying viral epitopes, notably of influenza and the human immunodeficiency virus, although many other proteins are of interest. An attractive structure occurs, for example, in an Ab binding to a lethal venom from the scorpion *Androctonus australis hector* (Fig. 2). Less planar than most interactions, the toxin embeds into the Ab in a structure the authors describe as an "egg in a cup". The "cup" consists of a binding pocket 1.3 nm deep and 1.2 nm wide formed by the six CDRs. An extended L-chain CDR1 and an anionic H-chain CDR2, together with the long H-chain CDR3, form a boundary that "clamps" the cationic toxin, with additional anchoring points on the remaining CDRs. Strong complementarity buries about 25 % (10 nm^2) of the venom surface at the interface. A detailed understanding of such Ag-Ab interaction suggests strategies for a molecular approach to both Ab blocking and Ab design.

Homologous to the immunoglobulin H and L chains, the TCR has α and β chains that also use six CDRs for recognition and binding. Here, interaction is not with the complete antigen protein, but with a protein fragment presented to the T cell by another component of the immune system, a cell-bound molecule of the major histocompatibility complex (MHC). Although fewer structures have been presented, in part because of the complexity of crystallization and structural analysis of tertiary complexes of MHC-peptide-TCR, not surprisingly the recognition and binding principles of the TCR resemble those of the immunoglobulin Ab. In addition to studies of viral recognition, the involvement of T cells in autoimmune diseases has stimulated intensive effort to understand binding of TCR to self-molecules.

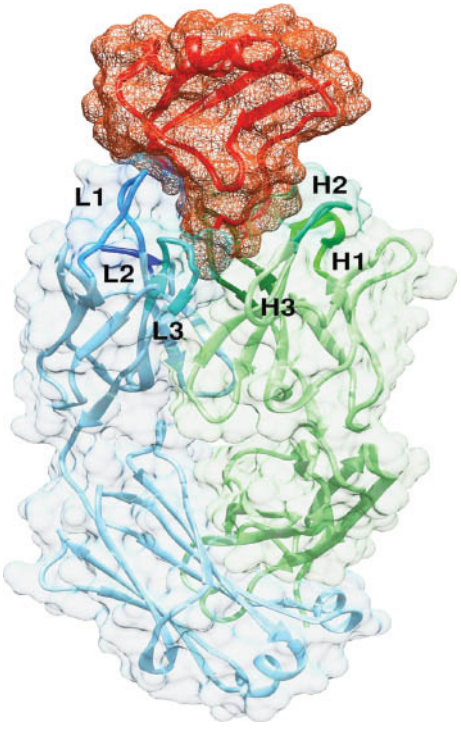


Fig. 2: The fitting of a scorpion toxin (red) into Fab4C1 makes contacts with all six CDR loops of the H chain (green) and the L chain (blue). The authors have described this as "an egg inserted small-end first in the egg cup" (see text for details). The basket around the toxin represents the molecular surface of the protein in mesh style, and the surface around Fab antibody is rendered as a transparent solid. [1]

Interactions with pathogen-associated molecular patterns

The PRRs on cells of the innate immune system, such as dendritic cells, detect a variety of molecular signatures referred to as pathogen-associated molecular patterns (PAMPs) from a broad range of different invading pathogens. A number of PAMPs are known that range in size from relatively small molecules, to molecules of intermediate size such as bacterial lipopolysaccharides, lipopeptides, and oligosaccharides, to macromolecules such as viral DNA, RNA, and pathogen-associated proteins such as flagellin. A major class of PRRs is the Toll-like receptors (TLR) that consist of a large extracellular binding domain, a transmembrane helix, and an intracellular signaling domain. The nucleotide-binding and oligomerization domain (NOD)-like receptors (NLRs) are cytosolic proteins and detect PAMPs that have gained access to the cell. Both NLRs and TLR extracellular domains contain multiple leucine-rich repeats that form crescent structures responsible for PAMP recognition. Upon binding to the PAMP, both types of PRRs initiate signals that ultimately lead to selective expansion and activation of appropriate B- and T-cell populations with specificity for the infectious agent presenting the PAMP. The structure of a mouse TLR3 homodimer binding to viral double-stranded (ds)RNA is shown in Fig. 3. Two other major classes of the PRRs are the C-type lectin receptors that contain lectin-like carbohydrate binding domains, and RIG-like helicase receptors that recognize viral dsRNA. Upon binding to viral DNA, RIG-1 initiates a signaling cascade that induces innate immune defenses. However, aberrant RIG-1 signaling can also lead to apoptosis, inflammation, autoimmune disease, and cancer.

Diagnostic applications

Biochemists have long exploited the specificity of

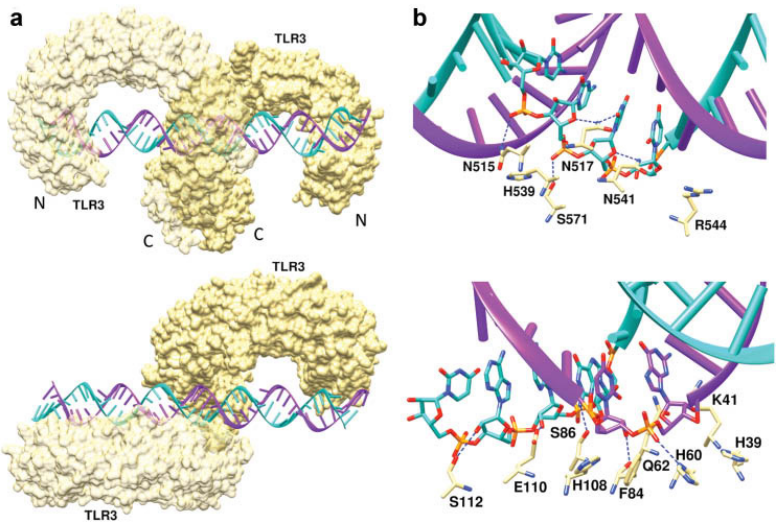


Fig. 3: The double-stranded (ds) RNA:TLR3 signaling complex. (a) Mouse TLR3 ectodomains form a dimer on the dsRNA. (b) The dsRNA binding sites of TLR3. TLR residues within contact distance of the dsRNA include, at the C-terminal site, Asn515, Asn517, His539, Asn541 and Arg544, which are all well conserved in vertebrates. The N-terminal interaction site is formed by His39, His60, Arg64, Phe84, Ser86, His108 and Glu110. [2]

Ag-Ab recognition to design selective separation and detection techniques, and Gubala et al. [3] have surveyed these in the context of recent developments in immunosensor design and diagnostic Ab production and use. Realization that fragments (e.g., Fab noted above) carry the recognition sites means that production of such fragments by a technique called phage display now often replaces the lengthier traditional approaches of animal injections and hybridoma technology. Interest has also focused on camelid Abs, as these naturally lack the L chain; they are quite stable and are themselves of low immunogenicity in humans. Small molecules become antigenic when conjugated to a larger protein, but then conventional means of Ab production yield mixtures of Abs that also react to epitopes on the macromolecular carrier, and purification can be tedious. One direction where small molecule Ab technology is finding increased use is in generating Ab's that can simultaneously measure multiple congeners of a drug or metabolite. Other advances are being made in introducing chemical reactivity into engineered Ab's that facilitate immobilization, and amplification with secondary Ab's against a structure chemically attached to the first. Such recognition or reactive sites may be introduced either by genetic engineering or chemical synthesis.

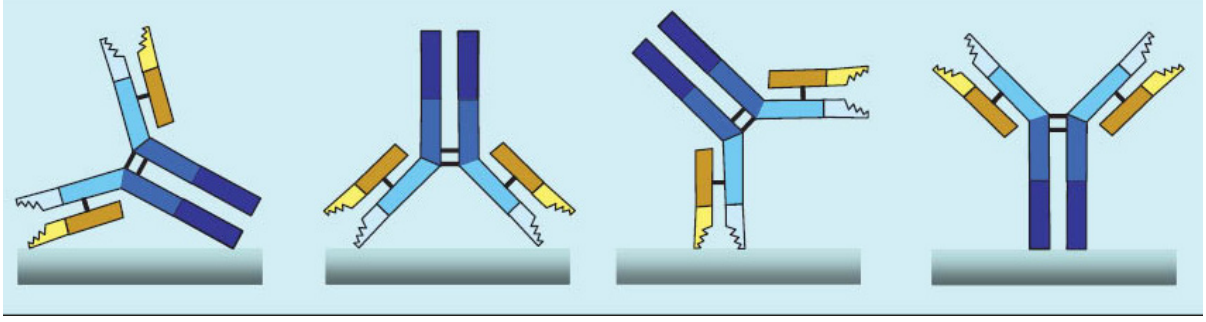
Traditional approaches of immunoseparation and immunodetection have included immunoprecipitation and agglutination, immunodiffusion, immunochromatography and immunoelectrophoresis. These approaches have seen advances from improved chemistries for coupling to substrates, the development of many commercial kits for miniaturized sandwich-based assay systems, and microfluidic chromatography. Improvements in Ab manipulation are also responsible for increased applications of flow cytometry to diagnostic examination of cell populations. Knowledge of how primary structure and conformational flexibility affect Ab affinities and specificities has allowed these advances to come together in immunosensor design and implementation of chip technology. New coupling chemistries are providing more robust surface coverage, as well as optimal Ab orientation and flexibility to maximize affinity to Ag (Fig. 4). The most favourable orientation of the immobilized biomolecules is generally that in which the Ag-binding site is oriented away from the surface itself. Approaches include engineering glycan moieties into the Ab, or metal-binding sites to exploit with metal ion affinity methods. New areas where these advances are being applied include drug monitoring and detection of markers for organ-based diseases, autoimmune diseases, infectious diseases, cancer, food hygiene, and environmental chemical exposures.

Therapeutic applications

Further promise for revolutionary advances in health care by exploiting Ab chemistry comes in the field of vaccinology. Molecular details of how an immune response is triggered in the organism and how an Ab recognizes its target are fertile ground for manipulation. Chemical principles are being applied to enhance immune system activation and Ab effectiveness through a number of strategies [4].

Traditional procedures for vaccination against a virus involve techniques for cultivation of the virus, identification of the infectious principle, selection and purification of appropriate Ag, cloning, animal testing, and vaccine development—a process typically taking 5-15 years. Today, vaccination with a DNA plasmid encoding the Ag is common, and predicting epitopes in silico ("reverse vaccinology") can further reduce the time of vaccine development to 1-2 years. DNA vaccines expressed from plasmids may enter cells for subsequent expression and release of the Ag, which

Fig. 4: Possible orientations of immunoglobulin G on a surface. The schematic shows that some of the orientations will lead to partial or total blocking of the antigen-binding sites of the antibody. Therefore, it is important to be aware of this problem when designing an assay using immobilized antibody. [3]



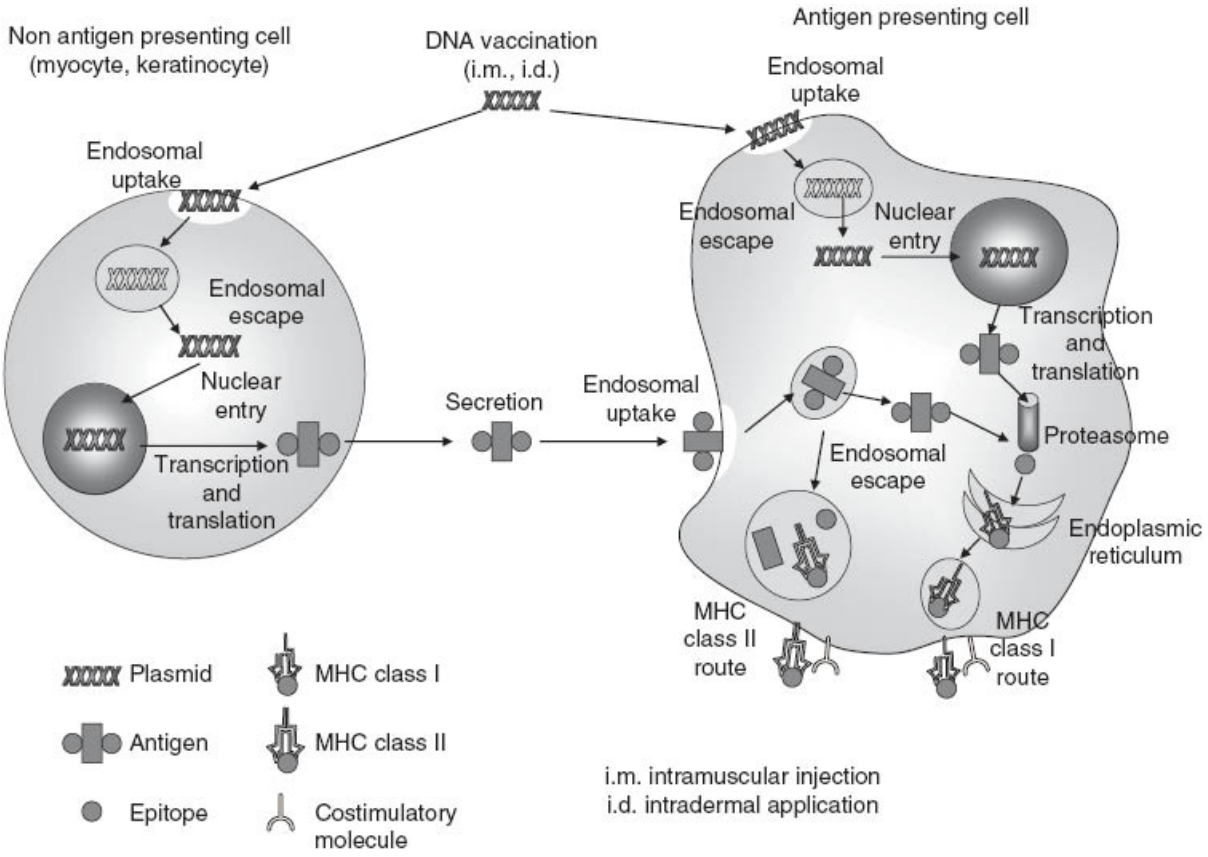


Fig. 5: Mechanisms of antigen expression and presentation upon vaccination with plasmid DNA (pDNA). pDNA is taken up by cells via endocytosis. After endosomal escape, cytosolic trafficking, and nuclear entry, the pDNA can be transcribed into mRNA, followed by intracellular translation of the antigen peptide. For T-lymphocyte activation, antigens must be presented in the context of MHC molecules in the presence of co-stimulatory molecules. Although non-antigen-presenting cells (non-APC) cannot induce T-cell activation, extracellular release or cell death can lead to an uptake of the antigen by APC. Antigens produced by direct transfection of APCs are presented by MHC class I. Antigen present in the cytoplasm of APC probably because of endosomal escape can also enter the MHC class I pathway ("cross presentation"). [4]

may then be taken up by antigen-presenting cells and processed for presentation by MHC molecules to the TCR of T cells (see above) (Fig. 5). Instead of inserting the plasmid into a viral vector, against which some recipients may already have immunity, delivery now is often via particulate carriers, where charge and size can be altered to increase efficiency of delivery (e.g., plasmid DNA binding to carboxylated polystyrene particles via a cationic poly-L-lysine-linker). Rapid progress is also being made using biocompatible, biodegradable nanoparticles such as polycaprolactone (PCL), polyvinylpyrrolidone (PVP), and polyesters—particularly polylactic acid (PLA) and poly(lactic-*co*-glycolic acid) (PLGA)—and those based on a core of iron oxide such as maghemite (γ-Fe_2O_3) or magnetide (Fe_3O_4). Furthermore, encapsulation in nanoparticles not only protects the plasmid DNA from degradation, but controlled DNA delivery systems can be designed to exhibit varying degradation times and release kinetics of DNA for prolonged gene expression. Co-administration of adjuvants enhances the immunogenicity of the Ag. The traditional ajuvant was alum, although its mechanism of action was not really understood. Today, adjuvants are being designed to selectively enhance certain aspects of the immune response by increasing cytokine production, cell recruitment, endocytic pathways, etc., and these may be encoded in the same plasmid that carries the Ag sequence.

Structural and computational chemistry is facilitating the development of epitope mimetics. With knowledge of the receptor for a particular virus on

a cell surface, Ab's can be designed to fit structural epitopes without building the epitope itself. These structural studies have also revealed that many of the protective epitopes of human pathogens contain loop, β-hairpin, or α-helical motifs. Conformationally constrained (e.g., cyclized) synthetic epitope mimetics based on these structures are proving useful in vaccine design. Epitope screening of random peptides can be followed by computational modeling to derive a consensus sequence for the target epitope.

Chemistry is playing a central role in engineering effective Ab's. Structural studies such as those described above [1,2] are proving useful in tailoring designed Ab's for maximum affinity and specificity by site-directed mutagenesis, CDR shuffling, computational approaches to affinity maturation, etc. Engineering is also directed towards improving pharmacokinetics and pharmaceutical properties, increasing thermal and chemical stability with amino acid analogs, improving solubility and viscosity of the delivery system, reducing non-specific and Ag-mediated clearance, modifying protein aggregation, and improving heterogeneity (e.g., with the presence of glycosylation sites in the Ag-binding regions).

Molecular genetics comes into play in reducing antigenicity of mouse-derived monoclonal Ab's by replacing all or part of the Ab with human sequence. In this way, 'humanizing' all but some murine residues in the CDR recognition sequences has produced several therapeutic Ab's now in clinical use, including alemtuzumab (an Ab against a lymphocyte surface Ag, used in treating chronic lymphocytic leukemia), trastuzumab (targeting the HER2 receptor in some breast cancers), and daclizumab (an Ab against a cytokine receptor on T cells used in managing rejection following organ transplant). Fully humanized Ab's are now being produced in mice, as has been achieved with the XenoMouse™ (Fig. 6). This mouse was created by engineering yeast artificial chromosomes (YACs) and then producing chimeric mice by fusion of yeast spheroblasts with mouse embryonic stem cells. These chimeras were then crossed with mice carrying a series of targeted disruptions of mouse heavy and light chain genes. However, even fully humanized Ab's may carry the risk of eliciting an immune response in the recipient, and although several are in clinical trial, they will not represent the final answer to the 'perfect' therapeutic Ab.

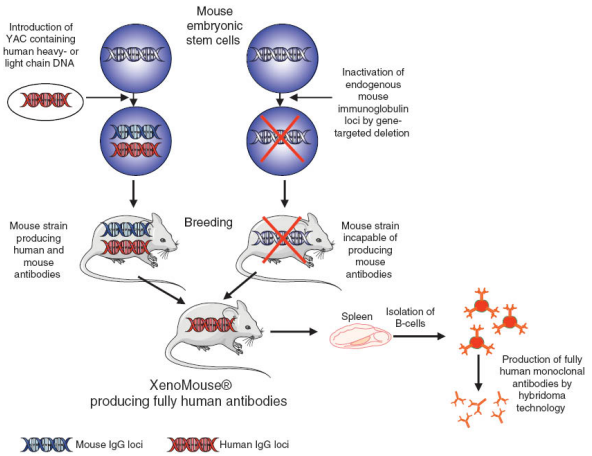


Fig. 6: Steps in the production of fully human monoclonal antibodies using the XenoMouse technology. [4]

Advances in biology and structural chemistry are identifying new targets for vaccine research—not only in infectious diseases but also in cancer, allergies, autoimmune diseases and other chronic inflammatory disorders. A critical question for the development of successful vaccines in the future will be which of many available technologies will elicit the best protective or therapeutic response toward a specific pathogen or antigen.

References

1. Templeton, D.M. and K. Moehle, Structural aspects of molecular recognition in the immune system. Part I: Acquired immunity. *Pure Appl. Chem.* **86**(10):1435-1481, 2014. http://dx.doi.org/10.1515/pac-2013-1020
2. Robinson, J.A. and K. Moehle, Structural aspects of molecular recognition in the immune system. Part II: Pattern recognition receptors. *Pure Appl. Chem.* **86**(10):1483-1538, 2014. http://dx.doi.org/10.1515/pac-2013-1026
3. Gubala, V., R. Klein, D.M. Templeton, and M. Schwenk, Immunodiagnostics and immunosensor design. *Pure Appl. Chem.* **86**(10):1539-1571, 2014. http://dx.doi.org/10.1515/pac-2013-1027
4. Klein, R., D.M. Templeton, and M. Schwenk, Applications of immunochemistry in human health: Advances in vaccinology and antibody design. *Pure Appl. Chem.* **86**(10):1573-1617, 2014. http://dx.doi.org/10.1515/pac-2013-1028

On the Use of Quantity Calculus

by Tomislav Cvitas

Quantity calculus is a system of algebra in which symbols are consistently used to represent physical quantities and not their numerical values expressed in certain units. We always take the values of physical quantities to be the products of a numerical value and a unit, and we manipulate the symbols for physical quantities, numerical values, and units by the ordinary rules of algebra. A more appropriate name for "quantity calculus" might be "algebra of quantities", because the principles of algebra rather than calculus are involved.

Each symbol of a physical quantity (single letter, italic) in an equation stands for the value of the quantity which is

$$\text{(quantity)} = \text{(numerical value)} \times \text{(unit)} \qquad (1)$$

In this way the equations hold for any unit as we believe the laws of nature should. Units are a matter of human choice, and no law in nature should depend on them. For example,

$$\text{force} = \text{mass} \times \text{acceleration}$$

or, with symbols,

$$F = m\,a \qquad (2)$$

irrespective of what units we choose. Equations should therefore be written in a form not implying certain units. In applications with many repetitive calculations, it is often convenient to write equations with numerical values in certain units. Then, however, different symbols should be used. Equation (2) can for a certain purpose be written in the form

$$\{F\}_{\mathrm{N}} = \{m\}_{\mathrm{kg}} \cdot \{a\}_{\mathrm{m\,s^{-2}}}$$

or

$$\frac{F}{\mathrm{N}} = \frac{m}{\mathrm{k\,g}} \cdot \frac{a}{\mathrm{m\,s^{-2}}} \qquad (3)$$

where $\{F\}_{\mathrm{N}} = F/\mathrm{N}$ is the numerical value of the force in newtons, etc. Eq. (3) can be derived from (2) by division of both sides by $\mathrm{N} = \mathrm{kg\ m\ s^{-2}}$.

If we measure the mass in pounds and acceleration in inches per second squared and we are still interested in the force in newtons, we can divide equation (2) by $(\mathrm{lb\ in\ s^{-2}}) = 0.545\ \mathrm{kg} \cdot 0.0254\ \mathrm{m\ s^{-2}} = 0.0115\ \mathrm{N}$, obtaining

$$\frac{F}{0.0115\ \mathrm{N}} = \frac{m}{\mathrm{lb}} \cdot \frac{a}{\mathrm{in\ s^{-2}}}$$

or, in a more convenient form,

$$\frac{F}{\mathrm{N}} = 86.7\ \frac{m}{\mathrm{lb}} \cdot \frac{a}{\mathrm{in\ s^{-2}}} \qquad (4)$$

Quantity calculus is recommended for general use in science and technology. It has particular advantages in facilitating the problems of converting between different units and different systems of units, as exemplified above. Another important advantage of quantity calculus is that equations between quantities are independent of the choice of units, and must always satisfy the rule that the dimensions must be the same for each term on either side of the equal sign. The advantages are illustrated in several examples presented in the IUPAC Green Book (E. R. Cohen, T. Cvitas, J. G. Frey, B. Holmström, K. Kuchitsu, R. Marquardt, I. Mills, F. Pavese, M. Quack, J. Stohner, H. L. Strauss, M. Takami, and A. J. Thor. *Quantities, Unit and Symbols in Physical Chemistry (IUPAC Green Book)*. IUPAC and RSC Publishing, Cambridge, 3rd edition, 2nd printing, 2008, page 131).

Professor Tomislav Cvitas is an emeritus professor from the University of Zagreb, in Croatia. A long time member of IUPAC, he is a former President of the Physical Chemistry Division and a former chair of the Interdivisional Committee on Terminology, Nomenclature and Symbols (ICTNS). He is a co-author of the IUPAC Green Book.

About NOTeS - This series, initiated in January 2014, is coordinated by the Interdivisional Committee on Terminology, Nomenclature and Symbols (ICTNS). Topics presented previously include: "On the Use of Italic and Roman Fonts for Symbols in Scientific Text" by Ian Mills (September 2014, p. 23), "Symbols of the Elements" by Juris Meija (January 2014, p.20), "Part II" (May 2014 issue, p, 18), "Part III" (concluded; July 2014, p. 25); and "The Units ppm, ppb, and ppt" by Ian Mills (March 2014, p. 23).

Pesticide Chemistry

by Kenneth Racke

The 13th IUPAC International Congress of Pesticide Chemistry was held 10-14 August 2014, in San Francisco, USA. The Congress was organized by the AGRO Division of the American Chemical Society under the auspices of the IUPAC Division of Chemistry and the Environment (DCE). Two members of the DCE Committee served as co-organizers for the Congress, DCE President Laura McConnell and past-President Kenneth Racke. The Congress Scientific Committee was chaired by Cathleen Hapeman, AGRO Program Chair.

The theme of the Congress was "Crop, Environment, and Public Health Protection: Technologies for a Changing World". The scientific program was organized into nine main scientific topics and 46 individual symposia. Topics ranged from discovery synthesis to environmental chemistry to residues in food to regulation. Each individual symposium included invited lectures, posters, and an interactive panel discussion or workshop discussion. More than 1000 lecture and poster presentations were included in the symposia. Each day of the Congress began with two plenary lectures that all participants attended, and the rest of the day involved nine concurrent sessions which participants could choose between.

A total of 1216 scientists from 53 countries attended the Congress, with approximately one half originating from outside of North America. There was a strong emphasis on the participation of students and younger scientists as well as experts from scientifically emerging regions. More than 50 student travel grants were awarded and a "new investigator" award competition, open to those within 5 years of their Ph.D., generated a number of applicants from which three finalists were selected. A special graduate student luncheon was organized and included guest speakers who discussed international career opportunities. Based on an IUPAC project grant, a world crop protection chemistry leadership workshop was organized during the first day of the Congress. This workshop focused on identifying opportunities for training the next generation of crop protection chemistry leaders for industry, government, and academia. A report outlining a set of consensus recommendations is being prepared by the DCE's Advisory Committee on Crop Protection Chemistry.

A highlight of the Congress was the presentation of the biennial IUPAC International Award for Harmonized Approaches to Crop Protection Chemistry to Dr. Árpád Ambrus, an IUPAC Fellow and Chief Scientific Advisor for the Hungarian National Food Chain Safety Office. For more than forty years, Dr. Ambrus' research has focused on analytical aspects of pesticide residues in food, elaboration of standardized methods and harmonized global residue standards, and capacity building for pesticide residue analysis and pesticide management in scientifically emerging regions. He presented a plenary lecture titled "International Harmonization of Food Safety Assessment of Pesticide Residues" and received his award during the Congress Gala Banquet.

Several collections of presented papers will be published as special issues of leading scientific journals. Details of the 2014 Congress, including post-Congress publications, will be posted to the Congress website. A detailed report of the scientific and social programs of the 13th IUPAC International Congress of Pesticide Chemistry, including a summary of the scientific topics, a list of plenary lectures, and the tabulation of poster awardees, was published in *Outlooks on Pest Management.* A complimentary copy may be downloaded at the following link: http://dx.doi.org/10.1564/v25_oct_02.

The 14th International Congress of Pesticide Chemistry will be held in Rio de Janeiro, Brazil in 2018. Details are available via the 2018 Congress website at www.abq.org.br/iupac2018.

www.iupac2014.org/

Congress opening ceremony showing (left to right): 2014 Congress Co-Chairs Laura McConnell and Kenneth Racke; ACS President Thomas Barton, IUPAC President Mark Cesa, ACS AGRO Chair Stephen Duke, 1994 Congress Co-Chair Nancy Ragsdale.

Photobiology

by Silvia Braslavsky, Congress Chair

The 16th International Congress of Photobiology was held 8-12 September 2014 in the "Argentina Pavillion" located within the National University of Córdoba, Argentina. This conference was the 16th in a series sponsored by the International Union of Photobiology (IUPB, www.iuphotobiology.com). This was the first time that the IUPB Congress was held in the Southern Hemisphere and also the first time held south of the Rio Grande. The University of Córdoba is the oldest in Argentina (founded 401 years ago) and the City of Córdoba offered a wonderful setting (and great weather) for the Congress.

The International Organizing Committee (www.photobiology2014.com.ar) addressed nearly all areas of photobiology and were from many countries. All areas of the interaction of light with the biosphere were covered, sincluding photosynthesis, photomorphogenesis, photomovement of plants and bacteria, the interaction of UV light with ecosystems (including bacteria, phytoplankton, zooplankton, algae, plants, mammalian cells, and humans), circadian rhythms in plants and animals, vision and light-induced damage to the retina, UV induction of skin cancer, as well as the use of light for the treatment of various illnesses and the photochemistry of xenobiotics and biological molecules. The use of light-based technologies for the study of biological processes was also the subject of various symposia.

The Congress registered 507 participants from 38 Countries. 160 participants were from Argentina, 44 from Brazil, 17 from Chile, 60 from the USA, 50 from Germany, and 20 from Japan. 280 of the registered participants were young fellows (graduate students and young researchers). The Scientific Programme (www.photobiology2014.com.ar/programme) included three plenary lectures: Nathan Nelson (Israel) on the "Evolution of the Photosynthetic Apparatus", Thomas Schwarz (Germany) on "Photoimmunology", and Ernst Bamberg (Germany) on "Channel Rhodopsins and Optogenetics". Nine keynote speakers highlighted the frontiers of research in various areas: Carlos Ballaré (Argentina), Rosalie Crouch (USA), Anderson Garbuglio (Brazil), Mario Guido (Brazil), Hideki Kandori (Japan), Alberto Kornblihtt (Argentina),

IUPAC-supported lecturers Dimitra Markovitsi (Left) and Aba Losi (Right)

Special Historical Lectures were given by Winslow Briggs (Left: between Roberto Bogomolni and Silvia Braslavsky) and Phil Hannawalt (Right)

Dimitra Markovitsi (France), Frank Vollmer (Germany), Horacio Zagarese (Argentina), while 51 Symposia (each comprising 130 minutes and between 4 and 6 participants) were organized by one or two contributors to the symposium. There were also two marvelous special (historical) lectures: Winslow Briggs (USA) on his "Scientific and Life Experience", and Phil Hanawalt (USA) on the "History of Research on the DNA Repair Mechanism". A symposium on photomovement was held in memoriam of Masamitsu Watanabe (deceased in 2013), who played a major role in the discovery of photoreceptors implied in photomovement.

IUPB awarded three Finsen Medals with Lecture: Masamitsu Wada (Japan), Herbert Hönigsmann (Austria), and Douglas Brash (USA); one Finsen Lecture: Roman Ulm (Switzerland); as well as one Edna Roe Lecture: Chikako Nishigori (Japan). Graduate students and young researchers presented 200 posters on all areas of photobiological research. Six poster prizes in the form of book vouchers were awarded on Friday during the closing ceremony: two from Springer Verlag, two from the Royal Society of Chemistry and two from IUPAC.

Most symposia were organized with the strong collaboration of colleagues from Latin-America. Some research areas are strong in Argentina (e.g., plant photomorphogenesis, blue-light-induction of microorganism behaviour, vision and UV damage to retina, circadian rhythms, photoecology, UV influence on the environment) and in Brazil (PDT, DNA photodamage, bioluminescence, biodiesel photoproduction), whereas some others are weaker (e.g., molecular aspects of photomedicine, optogenetics, and areas of research that require complex instrumentation: e.g., ultra fast reactions). All symposia were well attended, especially by younger colleagues.

Many of the subjects treated were directly related to the problems and or peculiarities encountered in Latin America, such as the photobiology of extremophile bacteria at high altitude in the Puna (North of Argentina and Chile, Bolivia and Perú) as well as in Antarctica, the effect of the ozone hole in the ecosystems in Argentina and Chile, the special properties of alga in Chile, and the increase in UV-induced skin diseases in Brazil and others.

The participation of Argentinian Scientists working abroad, including Víctor Batista, Roberto Bogomolni, Gonzalo Cosa, Raquel Galián, Thomas Jovin, Diana Kirilovsky, Maria Andrea Mroginski, Ana Moore, Juan C. (Tito) Scaiano, Graciela Spivak, Cristian Strassert, María Vernet, Matias Zurbriggen, and Silvia Braslavsky was very important for the consolidation of the research ties between Argentinian research groups and groups abroad. This was especially valuable in view of the dramatic "brain drain" Argentina suffered between 1966 and 2001, which has been reverted in the last few years, in particular since the creation of the Ministry of Science, Technology and Innovative Production, MINCyT, in 2011.

The science administration agencies from Argentina strongly supported the Congress with grants from the National Research Council, CONICET, (ca. 10000 USD) and from MINCyT (ca. 12000 USD). This allowed the registration fee of all Argentinian graduate students and several young scientists to be waived. In addition, the MINCYT program Red de Argentinos Investigadores y Científicos en el Exterior (RAICES) financed Congress travel for several Argentinian colleagues working abroad.

There was also important support (both financial and logistic) by German institutions including DAAD, DFG, Fraunhofer, and the Humboldt Foundation, as well as the Max Planck Society. Further financial support came from IUBS (International Union of Biological Societies),

Plenary Lecturers Thomas Schwarz (Left), Nathan Nelson (Center), and Ernst Bamberg (Right)

A panoramic photo of the conference attendees

IUPAC, TWAS (The World Academy of Sciences) as well as ESP, ASP and the French Society of Photobiology, who helped finance the participation of young graduate students. These grants permitted the fees of Latin-American graduate students and young researchers to be waived.

Several International companies and representatives of instrumentation in Argentina supported the Congress. Their logos appear in the Programme Booklet and the web page. Major contributors included L'Oreal in particular for sponsoring the contributors of the symposium on photoprotection, BASF and Johnson&Johnson. Exhibition booths for some sponsoring companies were located in the foyer of the Pavillion.

The abstracts of all plenary, special, and keynote lectures, contributions to the symposia and the posters presented were published online and can be found on the Congress website.

The editors of the journals *Photochemical and Photobiological Sciences* ((PPS), the Journal of the European Society of Photobiology, (ESP) and the European Photochemical Association (EPA)), *Photochemistry and Photobiology* (P&P, the journal of the American Society of Photobiology (ASP)), and *Pure and Applied Chemistry* (PAC, the scientific journal of IUPAC) have agreed to publish, in each journal, some of the lectures and symposia presented during the Congress. All submitted papers will undergo the normal evaluation procedure. The submission deadline for all three Journals will be 31 March 2015, with each of the papers publishing immediately after acceptance. A virtual issue will collect all contributions belonging to the Congress.

A major spin-off of the Congress is the creation of the Argentinian Group of Molecular Photobiologists (GRAFOB in Spanish, http://grupoargentinodefotobiologia.info). This group has held two meetings in preparation for the 16th ICP: first in 2011 in La Plata and the second in 2013 in Córdoba, the same city that hosted the 16th ICP in 2014. Both meetings included approximately 90 participants. Several contacts were established between Latin American research groups, including some that could not participate of the Congress. The Argentinian photobiology group met during the Congress and agreed to organize a third GRAFOB meeting in Tucumán in 2016.

The Executive Board of IUPB had a regular meeting during the Congress and also held a general assembly. The newly elected Executive Board is: President: John Spudich (USA); Secretary: Evelyn Sage (France); Treasurer: Franz Trautinger (Austria); Vice-Presidents: Roberto Bassi (Italy), Carlos Ballaré (Argentina), Gary Halliday (Australia), and Yoshitaka Fukada (Japan); Liason member as organizer of the 16th ICP: Silvia Braslavsky (Germany).

Congress participants had the opportunity to enjoy a tango show during the opening reception on Sunday evening, as well as folk dancing on Thursday evening. They could also witness how several students drank their mate during the lectures.

The 17th ICP will most likely be held in 2018 in the UK.

Solubility Phenomena and Related Equilibrium Processes

by Marcus Altmaier

The 16th International Symposium on Solubility Phenomena and Related Equilibrium Processes (ISSP-16) was held 21-25 July 2014, in Karlsruhe (Germany). The IUPAC-sponsored symposium was organized by the Karlsruhe Institute of Technology's Institute for Nuclear Waste Disposal (KIT-INE), with Dr. Marcus Altmaier acting as conference chair and Dr. Susanne Fanghänel as conference secretary. In conjunction with ISSP-16, the 13th annual meeting of the IUPAC Subcommittee on Solubility and

Equilibrium Data (SSED) was held on 20 July, chaired by Clara Magalhães.

The International Symposium on Solubility Phenomena and Related Equilibrium Processes (ISSP) is an established bi-annual symposium gathering international experts on solubility studies to exchange new research and concepts. ISSP-16 in Karlsruhe successfully followed a series of previous meetings, the most recent being ISSP-15 (2012, Xining, China), ISSP-14 (2010, Leoben, Austria), and ISSP-13 (2008, Dublin, Ireland).

ISSP-16 was a very positive contribution to the ISSP conference series, with 116 participants from 24 countries (Australia, Austria, Bulgaria, Canada, China, Czech Republic, Denmark, Finland, France, Germany, Hungary, Ireland, Israel, Italy, Japan, Poland, Portugal, Russia, Serbia, South Korea, Spain, Sweden, Switzerland and USA), as well as the European Commission.

ISSP-16 addressed the general importance of solubility phenomena in a variety of different settings, ranging from green chemistry to nuclear waste disposal and modern technical applications. The meeting featured a wide agenda of topics, specifically highlighting the importance of chemical thermodynamics and solubility studies both in fundamental and applied science. Invited and contributed oral and poster presentations ranged from basic equilibrium measurements to advanced theoretical predictions. ISSP-16 offered a dedicated scientific platform for presenting, discussing and promoting the study of solubility phenomena and related equilibrium processes, and it received very positive feedback from the attendees.

The conference was divided into specific sessions to allow clear focus on topics of key interest. Session topics were:

- Investigation and analytics of aqueous speciation
- Aqueous solutions at high ionic strength
- Kinetics of phase transformations
- Molten salts and ionic liquids
- Effects of solute-solvent interactions on solubility phenomena
- Solubility phenomena in technical and industrial applications
- Computer assisted equilibrium calculations and related thermodynamic databases

ISSP-16 invited distinguished plenary lecturers to introduce main topics. Lecturers were: (in alphabetical order): M. Filella, University Geneva, Switzerland, “Solubility seen from an environmental chemist’s point of view: caveats and needs”; H. Gamsjäger, University Leoben, Austria, “Thermodynamic properties of molybdate ion: reaction cycles and experiments”; I. Grenthe, KTH, Sweden, “Solid phases, structures and solution chemistry - what type of molecular insights do they provide?”; W. Runde, Los Alamos National Laboratories, USA, “Actinide chemistry in chloride brine solutions”; W. Voigt, Technical University Freiberg, Germany, “What we know and still not know about oceanic salts”.

Within ISSP-16, two Franzosini awards (supported by IUPAC-SSED) were presented, given to M. Bendová, Institute of Chemical Process Fundamentals Prague, Czech Republic, and S. Gadzuric, University Novi Sad, Serbia. The laureates awardees introduced their work with invited talks on “Liquid phase behaviour in systems containing ionic liquids: can ‘old-fashioned‘ experiments enable us to understand their properties and structure?” (Bendová) and “Thermodynamics of lanthanide halide + alkali halide binary mixtures: experimental and chemometric study” (Gadzuric).

Reflecting the specific profile focus of the Institute of Nuclear Waste Disposal at KIT, and highlighting a topic of wide international relevance and importance, a half-day workshop on “Solubility and Speciation in Nuclear Waste Disposal” was held. With a strong emphasis on (geo)chemical concepts in nuclear waste disposal, special attention was given to discuss solubility, speciation and thermodynamic data/geochemical modeling. The application of advanced spectroscopy and analytical techniques was highlighted as a key tool for the definition of accurate chemical models and solubility studies in general.

ISSP-16 was sponsored by IUPAC, the NUSAFE programme of HGF (Germany), and the BASF company.

Selected contributions from the conference will be published in a special volume dedicated to ISSP-16, scheduled to appear in *Pure and Applied Chemistry* in 2015. The 17th ISSP conference is scheduled for July 2016 at the University of Geneve (Switzerland); precise dates still to be confirmed.

More than hundred participants from 24 countries and four continents attended ISSP-16.

Data Sharing for Sustainability

SciDataCon2014, the International Conference on Data Sharing and Integration for Global Sustainability, took place on 2–5 November 2014, in New Delhi, India. It was motivated by the conviction that the most significant research challenges—and in particular the pressing issues relating to global sustainability in the face of ongoing natural and human-induced changes to the planetary system—cannot be properly addressed without paying attention to issues relating to equitable access to quality-assured and interoperable datasets and their long-term management and preservation.

We live in a data- rich world, and this provides the opportunity to investigate societally relevant issues in new ways and to develop evidence-based approaches for planetary management and the formulation of policy. However, managing the vast amounts of data currently being generated poses significant challenges. In particular: How do we assure the continuity of monitoring programmes? How do we assure the quality and reliability of the available data? How do we combine diverse datasets from different scientific disciplines? How can we maximise the use of datasets to answer new questions? How do we assure the long-term preservation of datasets? How do we ensure that data is available to all? By seeking to address these questions, SciDataCon 2014 represented a milestone in the discussions about the use of data management to address the issues of global change and global sustainability. While SciDataCon2014 addressed many important issues, the data battle is not over. There are many areas of science where data sharing and data archiving is not the norm. There is a vast amount of data from the pre-digital era, which could be useful for providing the longer-term perspective on current monitoring programmes, that languishes in the archives of individual researchers and needs to be rescued and made available. There is still no clear model for how to support data archives and services into the future and despite the excitement surrounding 'big data', there is still much to do to develop the conceptual, analytic and management tools required to handle such datasets. The World Data System (WDS) will continue to engage with its members and the wider scientific and policy communities to address these issues, so that scientific data can play a role in transforming our world and moving toward greater equity and sustainability.

SciDataCon2014 was hosted by the Indian National Science Academy (INSA) and co-organized by two bodies of the International Council for Science (ICSU) with responsibilities for data management and policy: the World Data System (WDS) and the Committee on Data for Science and Technology (CODATA). This was the first time that WDS (ICSU-WDS.org) and CODATA (CODATA.org) have joined forces to sponsor an international meeting designed to confront data issues.

www.scidatacon2014.org

Green and Microscale Chemistry

27-29 May 2015, Ciudad de México, Mexico

The Universidad Iberoamericana-Cd. de México is organizing the following joint events:

- 5th Latin American Green Chemistry Workshop
- 8th International Symposium on Microscale Chemistry
- 10th Anniversary of the Mexican Chapter of the Green Chemistry Institute—American Chemical Society
- 25th Anniversary of the Mexican Center for Green and Microscale Chemistry
- 70th Anniversary of the Chemical Sciences and Engineering Department—Ibero

Confirmed international speakers and workshop leaders include:

- John Bradley, UNESCO-Associated Centre
- for Microscience Experiments, University of the Witwatersrand (South Africa)
- Supawan Tantayanon, President, Chemical Society of Thailand, Chulalongkorn University (Thailand)
- Bruce Mattson, Creighton Jesuit University (USA)
- Angela Koehler, Romain-Rolland Gymnasium (Germany)
- Abdulaziz Alnajjar, Kuwait Chemical Society (Kuwait)
- Robert Worley, CLEAPSS-Brunel University (United Kingdom)

For more information, please contact Ibáñez Cornejo Jorge <jorge.ibanez@ibero.mx> or Elizabeth García Pintor <elizabeth.garcia@ibero.mx>; Tel: +52 (55) 59504168

www.ibero-dicq.mx/actividades.php

Functional π-Electron Systems

19-24 July 2015, Seattle, WA, USA

The 12th International Symposium on Functional π-Electron Systems (Fπ-12) will be held in Seattle, Washington, USA on 19-24 July 2015. Fπ-12follows the success of previous Fπ conferences organized in Japan (Osaka in 1989, 1999, and 2006, and Kobe in 1992), USA (Santa Cruz in 1995, Ithaca in 2004, Atlanta in 2009), Europe (Ulm, Germany in 2002, Graz, Austria in 2008, and Arcachon, France in 2013), and China (Beijing in 2011). It was initially started as the "International Symposium on Functional Dyes" in Osaka. In order to broaden the scope of the conference and to adjust to developments in academic and industrial research, the name was changed to the "International Symposium on Functional π-Electron Systems" in 2002.

Fπ-12 is expected to attract 400-500 participants from all over the world to discuss their new achievements in research fields including:

- design and synthesis of new π-conjugated molecules and polymers
- organic and polymeric semiconducting materials for thin film transistors
- organic and polymeric photovoltaic and photodetective materials and devices
- organic light-emitting materials for display and lighting application
- hybrid/perovskite materials and devices
- conjugated polymers and oligomers in chemo/bio-sensors
- bioelectronics

For more information, please contact Christine Luscombe <luscombe@uw.edu>, University of Washington, Seattle.

http://depts.washington.edu/fpi12/

Novel Aromatic Compounds

5-10 July 2015, Madrid, Spain

The 16th International Symposium on Novel Aromatic Compounds (ISNA-16) will be held in Madrid, on 5-10 July 2015. The ISNA was founded in 1970 by Professor T. Nozoe* who discovered the first non-benzenoid aromatic compound, hinokitiol, in Taipei. The name and goals of this symposium series have evolved as aromatic compounds have pervaded all branches of science. Highlighting the most exciting challenges in aromaticity, the ISNA-16 in Madrid will also be an opportunity to celebrate the 150th anniversary of a milestone in aromaticity, the first publication of Kekulè's benzene.

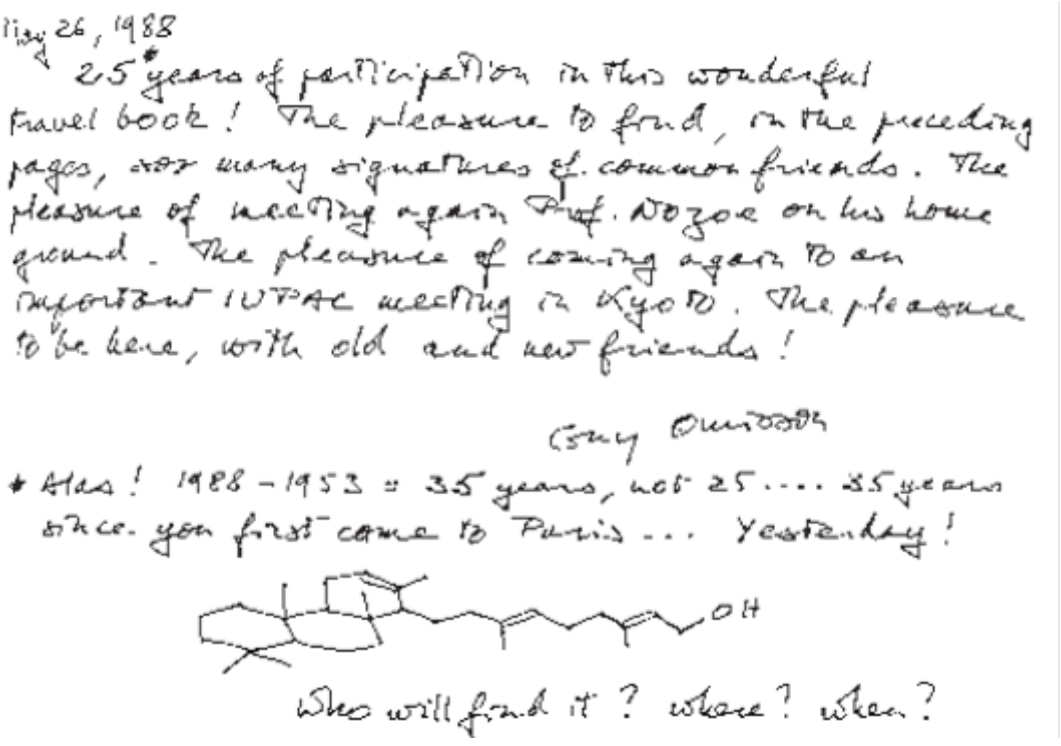
To continue the blossoming tradition of ISNA symposia, ISNA-16 will provide an interactive platform for researchers worldwide to present new findings and exchange innovative ideas on advanced synthesis, structure-property relationship, and applications of novel aromatic compounds for different purposes. The scientific program of this symposium includes the Nozoe memorial lecture, plenary lectures, invited lectures, oral communications, and poster presentations.

* Attendees at the 16th International Symposium on Novel Aromatic Compounds (ISNA-16) in Madrid this summer will have the opportunity to "sign" a new volume of the Tetsuo Nozoe Autograph Books. They, and you, can join Guy Ourisson—Secretary General of IUPAC from 1975–1983—and thousands of others who have added their names and their inscriptions into the Nozoe legacy and a piece of chemical history. The entire 1179 pages of the Nozoe Autograph Books have recently been published in The Chemical Record. A 21st Century volume has an open-door policy and "The Pleasure of Your Company" is called for by Jeffrey I. Seeman and Brian P. Johnson, respectively Guest Editor and Managing Editor of The Chemical Record. All this is highlighted in their recent essay titled The Nozoe Autograph Books: "It Ain't Over 'Til It's Over"; DOI: 10.1002/tcr.201500002 available free at http://www.wiley-vch.de/util/nozoe/online.php.

For more information, please contact Nazario Martín, Symposium Chairman, ISNA-16, Professor of Chemistry, Complutense University, or Ángeles Herranz, Symposium General Secretary, <isna2015@pacifico-meetings.com>

www.isna16.org

Guy Ourisson's entry on page 1003 of the Nozoe Autograph Books dated May 26, 1988. [reprinted with permission]



Mark Your Calendar

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

2015 (After May 1)

5-6 May 2015 • Clinical Laboratory • Barcelona, Spain
8th European Symposium on Clinical Laboratory and In Vitro Diagnostic Industry
Dr. Xavier Fuentes-Arderiu, Hospital L'University de Bellvitge, L'Hospitalet de Llobregat, E-08907 Barcelona, Spain, E-mail: xfa@bellvitgehospital.cat or Program Coordinator Dr. Ariadna Padró-Miquel
E-mail: apadro@bellvitgehospital.cat, www.acclc.cat

10-13 May 2015 • Pesticide Residue • Santiago, Chile
5th Latin American Pesticide Residue Workshop (LAPRW)
Dr. Roberto Becerra, Food Solutions Team, Napoleón 3565, Office 1208, Las Condes, Santiago, Chile, E-mail: info@laprw2015.com, www.laprw2015.com

12-15 May 2015 - Advanced Materials - Lincoln, Nebraska, USA
23rd World Forum on Advanced Materials (POLYCHAR 23)
Prof. Mehrdad Negahban, Department of Mechanical & Materials Engineering, University of Nebraska-Lincoln, Lincoln, NE 68588-0526, E-mail: PolyChar23@unl.edu, http://polychar23.unl.edu

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

21-25 June 2015 • EuroMedLab • Paris, France
21st IFCC-EFLM European Congress on Clinical Chemistry & Laboratory Medicine
Prof. Philippe Gillery, American Memorial Hospital, Laboratoire de Biologie et de Recherche Pédiatriques, CHU du Reims, 47, Rue Cognacq Jay, F-51092 Paris, France, E-mail: pgillery@chu-reims.fr, www.paris2015.org

21-26 June 2015 • Polymeric materials • Dresden, Germany
Congress of the European Polymer Federation (EPF-2015)
Prof. Brigitte Voit, Leibniz Institute of Polymer Research, Division of Macromolecular Chemistry, P.O. Box 120 411, D-01005 Dresden, Germany, E-mail: voit@ipfdd.de, www.epf2015.org

28 June - 2 July 2015 • Organometallic Chemistry • Barcelona, Spain
18th International Conference on Organometallic Chemistry Directed Towards Organic Synthesis (OMCOS-18)
Prof. Antonio M. Echavarren, Institute of Chemical Research of Catalonia, Avenida Paisos Catalans, E-43007 Tarragona, Spain, E-mail: anton.echavarren@uam.es, www.omcos2015.com

5-10 July 2015 • Ionic Polymerization • Bordeaux, France
22nd International Symposium on Ionic Polymerization (IP-2015)
Prof. Stéphane Carlotti, Université de Bordeaux, Laboratoire de Chimie des Polymères Organiques, Avenue Pey Berland, F-33607 Pessac, France, E-mail: carlotti@enscpb.fr, http://ip15.sciencesconf.org

12-15 July 2015 – Polymer – Gold Coast, Australia
35th Australasian Polymer Symposium (35APS)
Nicole Amato, Conference Manager, Leishman Associates, 170 Elgin Street, Carlton VIC 3053, Australia
Email: nicole@leishman-associates.com.au, http://35aps.org.au

9-14 August 2015 • 45th IUPAC World Chemistry Congress • Busan, Korea
Smart Chemistry, Better Life
Hosted by Korean Chemical Society, E-mail: office@iupac2015.org
Prof. Seung Min Park, Program Chair, E-mail: smpark@khu.ac.kr, **www.iupac2015.org**

Mark Your Calendar

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

2015 (continued)

7-10 September 2015 - Macromolecules and Materials - Port Elizabeth, South Africa

13th Annual UNESCO/IUPAC Workshop and Conference on Macromolecules and Materials
Prof AJ van Reenen (Conference Chair), University of Stellenbosch, Department of Chemistry & Polymer Science, Private Bag X1, Matieland 7602, South Africa, E-mail: ajvr@sun.ac.za, http://academic.sun.ac.za/unesco

5-8 October 2015 – Functional Polymers - Kuala Lumpur, Malaysia

Functional Polymers – Advanced Materials for the Future -- 4th Federation of Asian Polymer Societies - International Polymer Congress (4th FAPS-IPC 2105)
4FAPS-IPC 2015 Secretariat, Institut Kimia Malaysia, 127B, Jalan Aminuddin Baki, Taman Tun Dr. Ismail, 60000 Kuala Lumpur, Malaysia, E-mail: 4faps@ikm.org.my, www.4faps-ipc.org.my

18-22 October 2015 • Advanced Polymers • Yokohama, Japan

11th International Conference on Advanced Polymers via Macromolecular Engineering (APME-2015)
Prof. Takeshi Endo, Molecular Engineering Institute Kinki University, 11-6 Kayanomori, Iizuka, Fukuoka 820-8555, Japan, E-mail: tendo@moleng.fuk.kindai.ac.jp, www.apme2015.jp

6-9 November 2015 - ChemRAWN XX- Dhaka, Bangladesh

ChemRAWN XX - Herbal Medicine for Health Care in the 21st Century
Prof Dr Mohammed Mosihuzzaman, International Centre for Natural Product Research (ICNPR), Bangladesh University of Health Sciences (BUHS), 125/1 Darus Salam, Mirpur, Dhaka-1216, E-mail: mmosihuzzaman@yahoo.com

2016

6-10 June 2016 - Mycotoxins and Phycotoxins - Winnipeg, Canada

9th World Mycotoxin Forum & XIVth International Symposium on Mycotoxins and Phycotoxins
Prof. Rudolf Krska (Program co-chair), University of Natural Resources & Life Sciences, Tullin, Austria, E-mail: rudolf.krska@boku.ac.at and Prof. Hans P. van Egmond, Institute of Food Safety, Wageningen, Netherlands, E-mail: hans.vanegmond@wur.nl, Ms. Helena B. Bastiaanse (coordinator), Bastiannse Communication, E-mail: helena@bastiannse-communication.com, www.WMFmeetsIUPAC.org

3-8 July 2016 - Physical Organic Chemistry - Sydney, Australia

23rd International Conference on Physical Organic Chemistry (ICPOC-23)
Prof. Jason Harper, School of Chemistry, University of New South Wales, Sydney, NSW 2052, Australia, E-mail: j.harper@unsw.edu.au, www.icpoc23.unsw.edu.au

Visas

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

How to Apply for IUPAC Sponsorship

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

www.iupac.org

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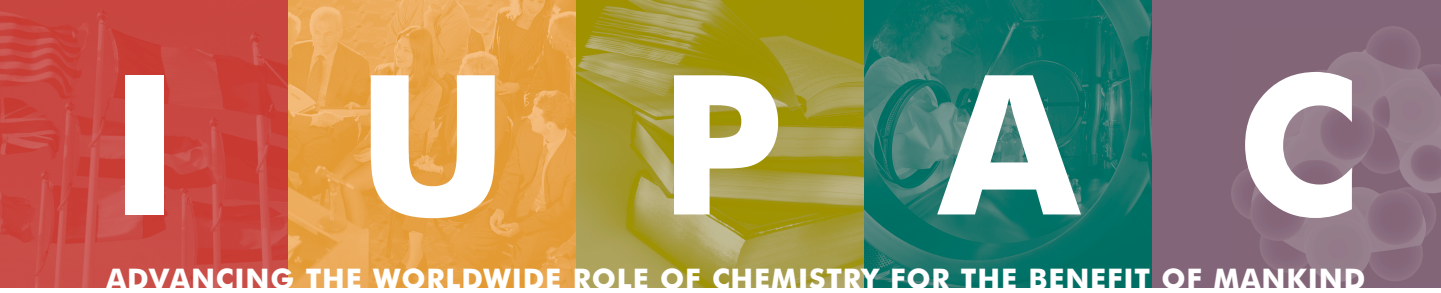

MISSION

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

NATIONAL ADHERING ORGANIZATIONS

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

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