CHEMISTRY International

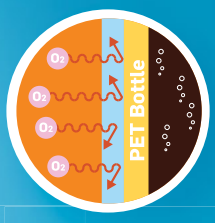
The News Magazine of IUPAC

NANOMATERIALS

April-June 2017
Volume 39 No. 2

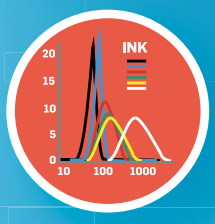
On the brink of revolution? Or the endless pursuit for something unattainable?

01. TiO_2 nanoparticles in sunscreens block dangerous UVB and UVA light.

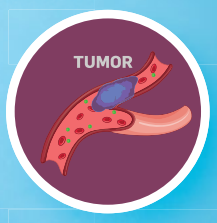


02. SiO_2 nanosheets in PET bottles act as oxygen barrier.

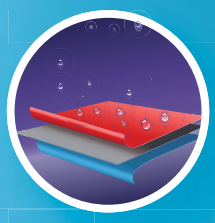
03. Nanomaterials could accumulate in lung alveoli, which can be exploited for a specific treatment or it can be harmful.



04. Composed of almost pure nanoparticles, black and blue tatoo ink are injected into dermis.



05. In nanomedicine, nano-sized drug carriers can be designed to target cells selectively.



06. Nanosilver with antimicrobial properties, SiO_2 and TiO_2 with dirt and water repellent properties are used in textiles.

INTERNATIONAL UNION OF
PURE AND APPLIED CHEMISTRY

CHEMISTRY International

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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: Since the dawning of the new millennium, the unique properties and obscure behaviour exhibited by nanoparticles have captivated research scientists globally. Their versatility has led to an explosion of interest in nanoscience and recognition of its unlimited potential for innovation in modern society. See Gubala 's review on page 10. Cover design: www.lab10.com.

As reported last year (see ***CI*** Nov 2016, p. 16), beginning in 2017, ***CI*** will be published in print format four times a year, ideally at the beginning of each quarter. Meanwhile, the ***CI*** Editorial Board is pleased to report that IUPAC members and ***CI*** subscribers will have access to new and updated content throughout the year via ***Chemistry International: Digital First***, a new electronic version that is in the early stages of development.

The *CI* Editorial Board 's vision is that the Digital First edition of *CI* will provide a preview of what is new since the last print edition was released—news, feature articles, project updates, book reviews—all of the *CI* sections with which you are familiar, plus additional digital-only content and features available exclusively to IUPAC members and *CI* subscribers. The least time-sensitive content, *e.g.* feature articles, book reviews, *etc.*, will ultimately be compiled in the next print edition of *Chemistry International* and will serve as a sort of time capsule for reference.

This digital edition will be accessible to authorized users from the new IUPAC website, allowing IUPAC to stream news and provide timely and perhaps interactive commentary on global scientific issues as they occur and not within the constraints of print production and distribution. It will leverage the features and functionalities of the IUPAC website with which you are by now already familiar and will serve as your portal to the most current information. We are actively working with our publishing partner, De Gruyter, to ensure that there will be seamless "interaction" between their site and the IUPAC site so that authorized users will have access to the new content regardless of their entry point.

The *CI* Editorial Board is excited about *CI Digital First* and continues to meet monthly, not only to focus on the development of the new digital offering, but also to develop the *CI* content pipeline for 2017. Exciting issues are planned, including a special issue on Big Data that will coincide with a symposium on that topic that is being organized for the 2017 IUPAC World Congress in São Paulo, Brazil (www.iupac2017.org). We invite all of our members, Affiliates, National Adhering Organizations (NAOs), Associate National Adhering Organizations (ANAOs), Company Associates, and other Associated Organizations with which we share common goals, to consider the submission of articles that highlight issues you believe will be of interest to the global scientific community, including innovative activities, research developments, and challenges and concerns that you face in your specific geographic region. We are also open to proposals for articles from those outside the chemistry community who have an interest in chemistry and its applications and who are prepared to brief or challenge us with their different perspectives.

In closing, we want to note that *Chemistry International: Digital First* will remain a work in progress and will continue to evolve as we all gain experience in using it. There is a lot of work to be done as we move forward and progress reports will continue to appear in future editions of *CI*. Your comments and suggestions for features and on how *CI* can be used more effectively are most welcome.

Colin Humphris
Chair of the *CI* Editorial Board
chumphris@iupac.org

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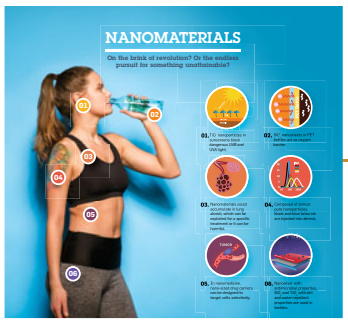

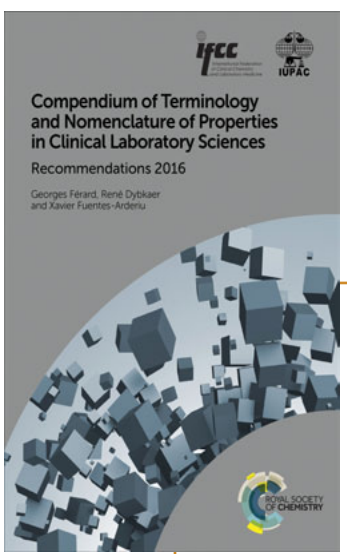

*See Centerfold—A handy 4-page pull-out offers a concise summary of the **Silver Book** and the **NPU Format** for Clinical Laboratory Science Reports Regarding Properties, Units, and Symbols*

The First IUPAC World Chemistry Congress with a Latin Flavor

by Adriano D. Andricopulo

On behalf of the Brazilian Chemical Society (SBQ) and the IUPAC-2017 Organizing Committee, it is our privilege and great pleasure to invite you to join us in Brazil and actively participate in the 46th World Chemistry Congress of the International Union of Pure and Applied Chemistry (IUPAC-2017), to be held in São Paulo, 9-14 July 2017. Held for the first time ever in South America, this Congress represents a unique opportunity for Brazilians to host chemists from countries worldwide.

We are planning a meeting of outstanding scientific interest and quality in the world-famous city of São Paulo. The World Chemistry Congress will be held in the WTC Events Center, which is considered one of the best venues for events in Latin America. São Paulo's diverse cultural and gastronomic attractions can be reached by the city's large public transportation network, including a nearby Metro station.

With the theme, **"Sustainability & Diversity Through Chemistry"**, this wonderful and historic event links all fields of Chemistry. The scientific program has been carefully prepared by the Organizing and Scientific Committees, providing major coverage of the main areas of interest for chemists. The scientific program includes high-level scientific sessions, plenary lectures, and parallel sessions, as well as poster presentations and young scientists' workshops on 12 major topics, including over 100 symposia. The twelve major topics are: Analytical and Food Chemistry; Chemistry

Planning for the IUPAC Congress and General Assembly, on site in São Paulo on 10 March 2017. (From left) Adriano D. Andricopulo, Chairman of the Organizing Committee, Roberto Torresi, Secretary Adjunct; Lynn Soby, IUPAC Executive Director; Luiz F. Silva Jr, Secretary General of the Organizing Committee; and Norberto Peporine Lopes, Coordinator of the Finance Committee for the IUPAC-2017 Congress.

2017 IUPAC General Assembly

7-14 July 2017, São Paulo, Brazil

The IUPAC General Assembly (GA) is the occasion for meetings of the statutory bodies of the Union, specifically of the Council, Bureau, Division Committees, and Standing Committees. The 49th IUPAC General Assembly will take place 7-14 July 2017, in São Paulo, Brazil, running concurrently with the 46th IUPAC World Chemistry Congress. The GA and the Congress will share the same venue and several events, including a joint opening and reception. Detailed information about the Congress is available at www.iupac2017.org, including the program, call for abstracts, and congress registration, as well as information on travel and accommodations.

IUPAC would like to encourage its members to take advantage of their participation in the GA by also attending the Congress. The Congress Organizing Committee has prepared an exciting program with the theme **Sustainability & Diversity through Chemistry**. GA participants (*i.e.* IUPAC Members and Delegates) can register to the Congress at a special discounted rate.

This year, Young Observers are again invited to take part in the activities coordinated around the World Chemistry Leadership Meeting (WCLM) and planned under project 2016-032-2-020. (see page 43)

GA Registration

Access to the GA is free, but registration is required for all IUPAC Members and Delegates planning to attend. Attendees are encouraged to review the Congress website to make their lodging arrangements.

VISA Information

For information regarding VISA requirements, reciprocity treatment, and visa information, visit www.itamaraty.gov.br/en. For information about invitation letters, contact iupac2017@mci-group.com. Invitation letters must come from the Congress organizers in Brazil.

Education; Chemistry for Industry Innovation; Chemical Synthesis; Energy, Water, and Environmental Sciences; Green Chemistry and Biotechnology; Inorganic and Structural Chemistry; Macromolecules and Materials; Medicinal Chemistry and Chemical Biology; Nano Science and Technology; Natural Products and Biodiversity; and Physical, Biophysical, and Computational Chemistry.

During the meeting, scientists will present new multidisciplinary research, listen to the latest information in their areas of professional interest, and network with colleagues from around the world. Nobel laureates and worldwide leaders will share their inspiring stories and experiences on critical topics that have major implications in the world of today and tomorrow. Oral and poster presentations will provide a unique platform for researchers to present their results and to discuss and exchange information with the participants. Particular emphasis will be given to an intensified exchange between academia and industry. The close collaboration with the Brazilian Chemical Industry Association (ABIQUIM) will allow the discussion of themes of interest to companies and broaden the vision of both sides in terms of a deep collaboration. In addition to what is certain to be a stimulating Congress program, participants will also be able to take advantage of exciting social activities.

In 2017, the Brazilian Chemical Society will celebrate its 40th anniversary with the privilege to organize this special event, which will take place together with its 40th annual meeting and the IUPAC 49th General Assembly. The Brazilian Chemical Society is the IUPAC National Adhering Organization (NAO) of Brazil and one of the most representative and important scientific associations in Latin America. With São Paulo hosting the first the IUPAC World Chemistry Congress in South America, we intend to bring an entire region of enthusiastic chemists closer to the global IUPAC community. We will deliver an unforgettable IUPAC Congress, energized by the passion, hospitality, and creativity of the Brazilian people.

Best wishes and we hope to see you all in Brazil in July.

For more information and the latest news, please visit our website: www.iupac2017.org

Adriano D. Andricopulo is Chair of the IUPAC 2017 Congress Organizing Committee

Hotel Information

IUPAC Bureau members will be staying at the Sheraton São Paulo World Trade Center where the General Assembly meetings and Congress will be held. There are many hotels close to the World Trade Center to choose from.

The IUPAC Council meeting and reception will be held at the Hilton hotel, with all other activities taking place at the World Trade Center.

GA Schedule

The schedule outline is identical to 2015, although slightly different than those for previous assemblies. Please review carefully before making your travel plans!

Friday, July 7: early Task Groups
Saturday/Sunday, July 8-9: Division Committees
Sunday/Monday, July 9-10: Standing Committees
Sunday, July 9 (evening): Congress/GA joint Opening and Reception (@ 17:00)
Tuesday, July 11: Bureau Committees (*am*) & Bureau (*pm*)
Wednesday, July 12: World Chemistry Leadership Meeting (WCLM) plenary session (*am*) & Council meeting & evening reception (*pm*)
Thursday, July 13 (am & pm): Council meeting (with elections in the morning)
Thursday, July 13 (evening): Congress Gala Dinner
Friday, July 14: Bureau (am) & Congress Closing (@ *12:30*)

See web site for detailed schedule and updates. We look forward to seeing you in São Paulo, Brazil this July!

https://iupac.org/2017-iupac-general-assembly/

IYCN: A Journey That Has Just Begun

by Christine Dunne and Fernando Gomollón-Bel

International collaboration varies across the world. Your first reaction when hearing those words—international collaboration—may lead you to myriad different thoughts and ideas: research institutions, famous scientists, your own coworkers, or even airports –flying through Tesla International Airport in Serbia, you can't help it! When reading this article, however, IUPAC is probably the first thing that comes to mind. IUPAC has the ability to bring together scientists, crossing nations and borders in the pursuit of knowledge. Early career chemists, however, often do not know how to breach these barriers to start their international scientific journey.

The International Younger Chemists Network (IYCN) is here to educate and mentor young chemists and to help them collaborate and communicate with each other, and, with IUPAC's aid, with the larger community of chemists around the globe. One important aspect of the scientific world is the focus on future generations. What cutting edge ideas can these young chemists bring to the table? What take do they have on established scientific practices and how to improve them? Are we mentoring the next generation properly to become our future global leaders? How can we answer any of these questions without a platform to connect on?

The group of young aspiring chemists who met in August 2015 at the 250th American Chemical Society National Meeting in Boston.

IYCN hopes to become that platform for chemists around the world to truly share ideas in the name of the advancement of science. As young chemists, we cannot start this journey alone. We need support, ideas, and mentorship from established scientists that want to give back by helping educate the future minds of their craft. It is important for you to understand that this was not an idea that came to us overnight. It is one that we have worked tirelessly towards for weeks, months, and even years. Here is our story.

Back in 2015, at the 250th American Chemical Society National Meeting in Boston, a group of young chemists sat around a table with easels, writing with permanent markers in the hopes that they would produce permanent ideas. The participants were inspired by their own international experiences, including many formed during the 2011 International Year of Chemistry at the International Conference for Young Chemists. As the stars would have it, something aligned in the Younger Chemists Crossing Borders (YCCB) Program between the Younger Chemists Committee of the American Chemical Society, the European Younger Chemists Network of European Association for Chemical and Molecular Sciences (EuCheMS), and the German Exchange Program, hosted by the Northeastern Section of the American Chemical Society and the JungChemikerForum of the German Chemical Society. Chemists from 15 countries formulated an idea that would be known as the International Younger Chemists Network (IYCN).

In 2016, some of the founding participants of IYCN had the opportunity to gather at the ACS National Meeting in Philadelphia (USA) and also at the 6th EuCheMS Chemistry Congress (ECC) in Sevilla (Spain). During the 6th ECC, IYCN hosted a soft launch event in collaboration with the participants of the YCCB Exchange Program. Due to the many countries present in Sevilla, IYCN had the opportunity to lay the groundwork for an expansive international network.

As a group of likeminded young scientists, we are aware of the globalization of chemistry within our societies. While many countries were represented in Boston and Sevilla, we know there is so much more of the world that needs representation. That leads us to today, planning for the official launch of IYCN at the 46th IUPAC World Chemistry Congress in São Paulo, Brazil. During this congress, IYCN will collaborate with local organizers, as well as societies around the world, to host two major symposia that discuss issues of great importance to rising stars in chemistry: Green chemistry practices

In September 2016, some of the founding participants of IYCN gathered at the 6th EuCheMS Chemistry Congress in Sevilla (Spain). From L to R: Javier García-Martínez (Spain, IUPAC Member), Christine Dunne (USA), Maarten van Sisseren (Netherlands), Ilya Vorotyntsev (Russia), Michael Linden (Germany) and Fernando Gomollón-Bel (Spain).

and intellectual property rights. Along with these symposia, we will also organize a networking poster session highlighting many countries in attendance to show the true breadth of the ways IYCN can unite early career chemists. At this congress IYCN will not only come together for the first official time with IUPAC members, but we will also elect our first board, who will continue our collaborative, international efforts.

Since the beginning, we have pursued a global and inclusive organization for early career chemists, following the model IUPAC has created in its relationship to our countries and mother societies. We believe our vision strongly correlates with IUPAC's long-range goal to "contribute to the enhancement of chemistry education, the career development of young chemical scientists, and the public appreciation of chemistry". We want to do more than just educate and form working collaborative partnerships. It is our hope that these international connections will allow young chemists to become more well-rounded and versatile scientists and people. With ever-advancing social unrest around the globe, young chemists will have a platform for connection that overcomes this global instability. In conjunction with these ideals, the IYCN could support international education endeavors to promote the advancement of chemistry around the globe.

Chemistry is a universal language. By working together, unity amongst the younger generation of chemists can be established. We look forward to expanding to the rest of the world and creating a truly global network of young chemists in which all feel welcomed. While there is much more work to be done, connections to be made, countries to reach out to, and young chemists to involve, we hope this message will lay the groundwork for people to reach out to us as well. We are confident that chemists throughout the world will benefit from an international networking community for personal, professional, and educational development towards the advancement of chemistry, science, and society.

For more information on IYCN please contact us at IYCN@IUPAC.org. We look forward to seeing you in São Paulo!

Christine Dunne <christine.dunne11@gmail.com> is a member of the Younger Chemists Committee of the American Chemical Society. Fernando Gomollón-Bel <gomobel@gmail.com> is Chair of the European Young Chemists' Network.

IUPAC supports IYCN

IUPAC is very pleased to be involved in the development of the IYCN—we see it as vital for the future of the discipline and also as a key pipeline for future IUPAC projects and people. The IYCN is now formally recognised within IUPAC as an Associated Organisation. It provides another mechanism to involve younger chemists in our projects and activities and to gain a younger chemist's perspective on issues vital to Chemistry. We look forward to collaborating further with IYCN at the 2017 General Assembly and beyond.

Richard Hartshorn
IUPAC Secretary General

IUPAC Facilitating Chemistry Data Exchange in the Digital Era

by Leah Rae McEwen

The scientific community faces an unprecedented communication challenge as larger volumes of research data are published and data storage moves into digital space. Most communication tasks in chemistry involve representing molecules. Traditionally, these have formalized around the need to register, search, view, and publish information about chemicals for human readers. Data collection and analysis are further described by formalized domain vocabularies. In the digital environment, machine-readability, as well as human interpretation of data, is a significant factor in the level of accuracy and completeness of data exchange. More than ever, there is a need for standard and robust protocols that support reliable interoperability: the transfer of depictions and descriptions of chemicals between systems without loss or distortion of information.

IUPAC has long recognized that consistent use of chemical representation and terminology is critical for documenting and reporting chemical data. The former Committee on Printed and Electronic Publications (CPEP) recently re-envisioned part of its remit, becoming the Committee on Publications and Cheminformatics Data Standards (CPCDS). [1] With this shift, the committee aims to leverage IUPAC's deep institutional expertise and authority in chemical nomenclature and representation to support expanding digital applications of chemical data. CPCDS is liaising with the Research Data Alliance (RDA), [2] as well as CODATA (International Council for Science: Committee on Data for Science and Technology), [3] to complement chemical information expertise with international forums for digital data exchange strategies.

In July 2016, IUPAC CPCDS co-sponsored a workshop with the RDA Chemistry Research Data Interest Group (CRDIG), [4] engaging researchers, cheminformatics specialists, educators, publishers, and librarians to identify key opportunities for developing unified approaches to communicating chemical information in the digital environment. Hosted by the United States Environmental Protection Agency (EPA) National Center for Computational Toxicology (NCCT) [5] in Research Triangle Park, NC, the workshop explored the potential of IUPAC scientific definitions to function digitally as machine-readable standards for robust automated processes. Focusing on IUPAC's strengths in developing standards for describing molecules, measurements, and properties, this joint effort aims to support cheminformatics by expanding the reach and impact of IUPAC standards globally.

Interoperability among many sophisticated data software programs in chemistry is key to the accurate publication, re-use, and exchange of data throughout the research cycle. Exchanging information about digital data involves communicating, not just with other chemists, but with computer systems, websites (via APIs), and databases. Computers have different requirements than professional chemists for interpreting meaning; everything must be explicitly captured in the form of rule sets managed by software algorithms. Once codified, these rules can govern the management of astounding numbers of items that meet the criteria, such as tens of millions chemical compounds based on specified parameters of atoms and bonds. The IUPAC InChI (International Chemical Identifier) [6] algorithm is an example of an interoperable and machine-readable rule-set for identifying molecular structure.

For a long time, well-developed practices for the careful documentation of experiments and rigorous systematic nomenclature have been central features of chemistry. [7] Despite these long-established mechanisms for assuring clear communication among (human) chemists, managing the reliable translation of concepts from humans to machines and among computer systems has proved as elusive as consistent depiction of organometallics. Compiling data from multiple published sources into large collections has uncovered hundreds of variations in the representation of enantiomers, ions, salt forms, *etc.* Generating consistent representations of molecular structures for the same compound regardless of the software used is one of the major challenges in chemical information. With emerging machine-readable standards for structure notation and nomenclature, accurate management

and manipulation of large inventories of chemical data is greatly improving. However, there is much inconsistency in defining the input to, and the applications of, these computable standards.

The goal of the joint IUPAC-RDA effort is to facilitate interoperability and the exchange of information at the machine level, as well as among researchers and consumers of data. The workshop participants at EPA identified several key opportunities associated with machine-readable chemical structure representation. These include: 1) augmenting IUPAC graphical representation guidelines to support reliable interpretation by machines, 2) reviewing criteria for file formats conveying information about chemical structures, and 3) standardizing protocols for translation and normalization of variations in chemical depiction. Underpinning these opportunities is a need for engagement with stakeholders in the chemistry community and in the data publishing and reporting industry. The workshop also considered digital applications of standard terminologies, such as those published in the IUPAC Color Books. [8]

Graphical Representation Recommendations were devised and published in *Pure and Applied Chemistry* (*PAC*) in 2006 [9] and 2008 [10] for "the display of two-dimensional chemical structure diagrams." These guidelines are intended to establish conventions to prevent ambiguity in communicating chemical structure information in publications. There are a few alerts to drawing software issues for end users. However, best practices for software encoding are not addressed. Expanding the guidelines to consider machine interpretation of chemical depictions can prevent the corruption of chemists' intentions when converting to computer-defined chemical structures. Harmonizing the guidelines with other structure standardization and nomenclature considerations would improve consistency and reduce translation error in drawing software and databases.

While there are recognized systems for registering characterized chemical substances, there are no officially sanctioned file formats for transferring molecular structure information. A series of file formats originally published by Molecular Design Limited in 1992 has become a *de facto* community standard for representing single molecules (MOLfile), multiple molecules and data (SDfile), and reactions (RXNfile and RDfile). [11] The documentation for these files types is available upon request, and a recent format upgrade greatly expands the potential to encode more complex chemical scenarios. [12] However, these are propriety formats and there are no machine-readable templates or community agreements in place for interpreting these options in practice. Files are re-used, re-parsed, and re-constituted using different conventions for encoding and decoding myriad chemical features of interest beyond basic connectivity. File formats and software for interpreting them are full of idiosyncratic pre-formulated short-cuts devised for different applications that not only vary in their operations but, unknown to downstream users, also obfuscate basic atom-level interpretation.

Machine-readable, parsable structure notations are plagued by the same challenges. SMILES (Simplified Molecular-Input Line-Entry System) and SMARTS (*i.e.*, substructure pattern extensions) are popular chemical notations particularly useful for depicting functional patterns. SMILES rules were published in 1988 in basic form [13] and the copyrighted theory manual is still available for personal use. [14] There has been some community effort to coordinate the development of an open specification. [15] However, numerous diverse extensions and translating schemes persist and there is no formal process or review. The InChI serves a different role as a more formalized structure-based identifier that effectively supports automated structure validation and linking. The standard form of InChI remains limited to small covalent organic molecules, with recent extensions for polymers and reactions and several current projects for organometallics, large molecules, and mixtures. [16] All of these rely on being able to unambiguously represent the chemical structures and systems for which an InChI or other machine-readable notation is desired. The interoperability of chemical data could be improved by standardizing a small number of open chemical file formats.

Normalizing chemical structure is a necessary part of the process to transfer data between systems. Currently, many approaches to normalization exist, usually employed by and for the local needs of the importing system. With an increasing complexity of structures and variability in representation across tens of millions of substances, critical information, such as stereochemical configuration or electron delocalization, can get lost in translation. "Reconstituting" structures in human-readable form is subject to contextual human interpretations and preferences (think of the variety of ways in which chemists draw benzene). When such structures are exported once more, these local preferences can yield a different digital representation than the one that was originally imported. Similar issues may arise when rendering structures most appropriate

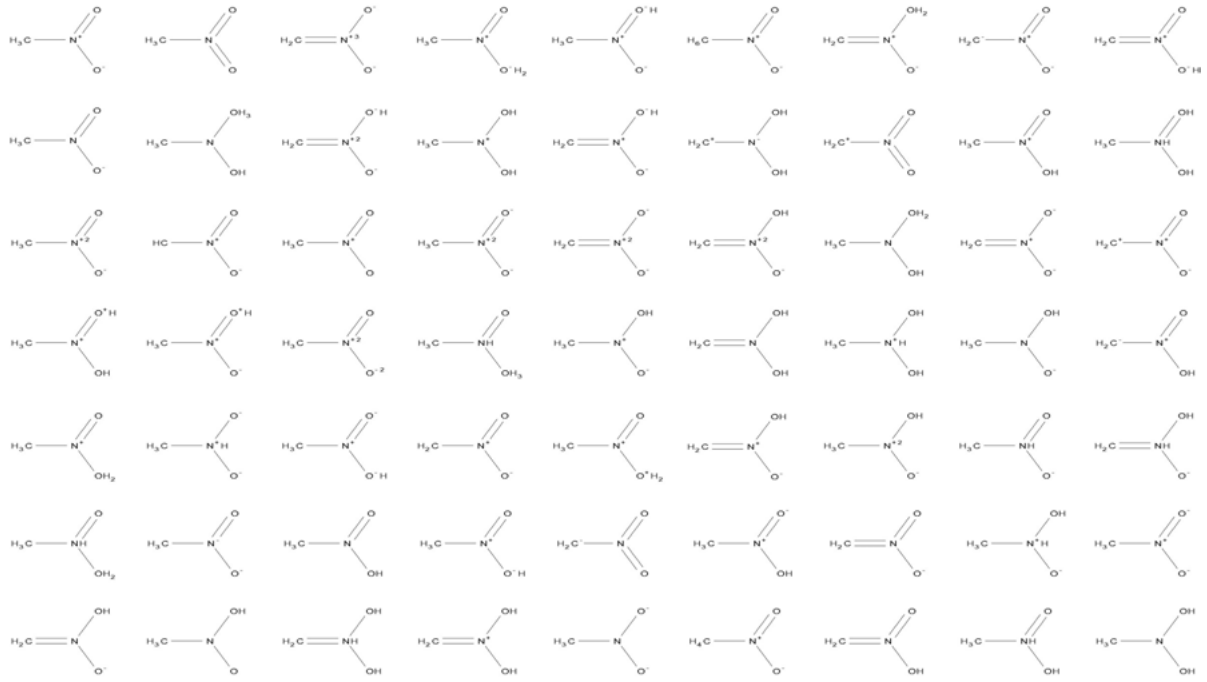

Figure 1. Variations on nitromethane (courtesy of PubChem) [17]

for local conditions, resulting in chemically related but not identical structures, such as tautomers. Iterative interpretations can introduce inaccuracies with implications downstream for the re-use of data by both chemists and computer applications (see Figure 1). Standard protocols for translation, coupled with guidelines for interpreting input and open file formats, could greatly facilitate the accurate exchange of chemical data.

Engaging researchers in the documentation of their research outputs is critical for ensuring integrity in increasingly automated information processes. Outreach efforts can help the chemical information community better understand why chemists draw molecules the ways that they do and where the crucial points exist in communicating chemistry among humans and machines. Targeted standardization of practice can benefit authors, readers, publishers, reviewers, and educators, as well as system and software developers. The research and publishing communities are embracing standard document identifiers such as DOI (Digital Object Identifier), [18] including schema for citing data, [19] and implementing author identifiers, such as ORCID (Open Researcher and Contributor ID). [20] Use of these identifiers is improving the accuracy of citations and cross-linking. [21] Workflows that support further coupling of chemical identifiers, author determined molecular structure, and characterization data files will enhance the chemical record and support research funding mandates to share supporting data. [22] Ideally, standards should operate invisibly, but training the next generation about the positive outcomes from incorporating updated standards in their workflows will result in an improvement in data quality over time.

Engaging researchers in the documentation of their research outputs is critical for ensuring integrity in increasingly automated information processes.

The IUPAC Color Books describe a diversity of measurement methods and properties, as well as molecular nomenclature. [23] Many of these terms, along with others from PAC, are collected in the Gold Book Compendium of Chemical Terminology to facilitate discovery across the corpus of concepts defined by IUPAC. Several IUPAC projects have focused on supporting the Gold Book in an online format, including planning in conjunction with the new IUPAC web presence. Each term in the most recent iteration has a permanent DOI for easier citation and dynamic linking back to IUPAC. [24] However the data are not systematically structured and it is difficult to automatically retrieve linked terms. In order to make the Gold Book reliable and sustainable in the longer term, chemical terms and the scientific relationships that connect them to each other should be drawn dynamically from IUPAC source publications and systematically structured to ensure consistent resolution to the authoritative IUPAC source. Discussions on this point at the EPA workshop fed into a special digital vocabularies session about the Gold

Book at the 8th RDA Plenary in Denver, CO in September 2016. [25]

Formulating the Gold Book for digital use involves the conversion of terms from the current web-display format into a more automated machine-interpretable form. Individual terms can be associated with a URL (or URI – Universal Resource Identifier) pointing to a human-readable form with the term definition and citation. This approach meets requirements for both human and machine access to the information, without compromising functionality. It facilitates both internal and external linking to terms, and additional functionality can be readily incorporated, such as links to provenance. Meaningful relationships among terms could be indicated (*e.g.* synonyms), and feedback and review commentary incorporated into the workflow. Further analysis of the definitions could identify potential overlap among terms, and comparison with the text of the Color Books and PAC could help identify gaps in Gold Book coverage. One use of such a machine-readable compendium of IUPAC terminology could be automated referral from other documentation that incorporates these chemical concepts, such as chemical patents, textbooks, experimental methods, and computational models.

There has been much talk of the potential of Big Data and the Internet of Things, linking measurement instruments to lab notebooks to publication templates. Much of chemical research lies on the long tail of small scale experiments. Although this research may enter the scientific record in countless individual publications, many experimental data files can be classified into a few types that are amenable to substance characterization and property determination. Aggregated across tens of millions of compounds and substances, this is a huge amount of data that should, in principle, be accessible for re-use. If its accessibility and reliability could be assured, this data would become a core resource for chemistry research as a global endeavor, contributing to crucial trans-national impacts in the areas of biomedicine and pharmacology, climate change, pollution, and public health. Opportunities to leverage data and digital technologies in facilitating chemical communication is of utmost interest to the community, and central to IUPAC's mission.

Clearly, there is compelling need for authoritative IUPAC chemical descriptions to be machine-accessible for scalable data processing. As data exchange via the Cloud reaches a global scale, IUPAC is well positioned as an international scientific union to bridge scientific meaning and automated processes with functional elements for data exchange, including open file formats and chemical descriptors. Coordination and collaboration with other international scientific data initiatives, such as CODATA and the RDA, provides exciting opportunities for expanding the impact of IUPAC in the global scientific community. Look for further discussion on this topic in a special issue of *Chemistry International* on Big Data in July 2017 and at a special symposium at the IUPAC World Congress in São Paulo, Brazil. [26]

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Leah Rae McEwen <lrm1@cornell.edu> is chemistry librarian at Cornell University, USA. ORCID.org/0000-0003-2968-1674. She is a member of the IUPAC Committee on Publications and Cheminformatics Data Standards (CPCDS) and co-chair of the CPCDS Subcommittee on Cheminformatics Data Standards.

iupac.org/body/036

Nanomaterials—On the Brink of Revolution? Or the Endless Pursuit of Something Unattainable?

by Emma Perkin and Vladimir Gubala

Since the dawning of the new millennium, the unique properties and obscure behaviour exhibited by nanoparticles have captivated research scientists globally. Their versatility has led to an explosion of interest in nanoscience and recognition of its unlimited potential for innovation in modern society.

Engineered nanomaterials (ENM) are a class of deliberately designed and prepared materials with nanoscale dimensions that have a rapidly expanding range of applications in our every-day life, *e.g.* energy storage, food, cosmetics, sports, and textiles. However, there is now significant interest in more complex nanomaterials, which already have, or are expected to have, an important role as advanced drug delivery systems in nanomedicine, ultra-sensitive reporters in biomedical diagnostics, and as multifunctional probes in environmental management, as well as in advanced electronics, transport, information and communication technology, defense, and manufacturing. But in order to fully appreciate the extent of their potential, it is essential to have at least a rudimentary understanding of these tiny objects.

Nanotechnology—a fashionable trend in research for nearly two decades, but still with unclear terminology

Nanotechnology is a combination of science, engineering, and technology on a 'nanoscale'. To be more precise, it is the manipulation of materials on scale that is 10000 smaller than the width of a hair to achieve desirable outcomes: those characteristics and behaviours useful to daily life. In order to explore this field of science it is important to explain the basic terminology.

The broad applicability of nanotechnology has led to considerable variation in the terms and definitions used by various scientific communities and regulatory authorities. Despite this, it is generally accepted that nanomaterials have two defining characteristics: a size on the nanoscale (between 1 nm to 100 nm) and unique size-dependent properties that are not exhibited by the bulk material, a view endorsed by IUPAC.

Although much initial work on nanomaterials focused on approximately spherical particles, there is now significant interest in high aspect ratio particles and one-dimensional materials. To illustrate the broad range of sizes, shapes and functions of nanoparticles, some scientists provocatively named these materials as 'Nanoparticle ZOO'. It is therefore not surprising that a wide range of terms have been used to describe these materials. Both ISO and IUPAC recognize the terms 'nanoparticle', 'nano-fibre/nano-rod' and 'nanoplate' as nano-objects with either all or at least one dimension in the range of 1 nm – 100 nm. One problem is that the various terms have not been employed systematically in the literature and a variety of other terms have been used. No nano-objects can be seen by the human eye, and they are still too small to be seen even under a normal microscope. Usually, transmission electron microscopy (TEM) is required to view the details of these miniscule nanostructures. The functions of each type of nanostructure is determined by their given shape and size, as well as by the type of material they are made of, and by the chemical/biochemical composition of their surface.

The exact definition of ENM and the variety of terminology used in the literature are not the only problems here, though. Regardless of the size or function of the nanomaterial, every scientist working with the ENM has encountered a problem with clustering of the nano-objects into larger assemblies. The literature is again very much inconsistent. Scientists tend to use terms such as aggregation or agglomeration of nanoparticles/nano-objects. It is possible, however, to distinguish between the strengths of the interactions that lead to clustering of nano-objects, with the term agglomeration used to describe clusters that are held together by weak forces and that can be disrupted with modest energy input and the term aggregation to describe clusters of primary particles that are held together by strong forces and are therefore difficult or impossible to disrupt. Since in most cases it is not clear which type of forces are dominant for specific nano-objects, IUPAC recommends avoiding the use of aggregation/agglomeration and instead using the term association.

Nanoparticles can occur naturally or can be engineered. Scientists' fascination with these tiny devices emanates from the unique behaviours and characteristics they display in contrast to the larger version of themselves and from the limitless potential they may play in our future, particularly in the medical field. Incidental nanomaterials are also generated as an unintentional by-product of manufacturing, biotechnology, or other processes. In short, nanotechnology has taught us to 'expect the unexpected', as the resulting chemical properties can surprise us all. Over the past few decades, we have learnt how to manipulate materials on their atomic scale and how to produce totally new nanoscale materials with various novel features and properties. We have undoubtedly entered a new era of

vast opportunities, where nanotechnology and nanomaterials can be exploited in a huge number of possible applications. Initially, companies and users often consider only the business or the advantages of a new material, but the past has demonstrated that materials and chemicals may also have adverse effects for human health or the environment.

Current applications

A variety of nanoparticles (formed naturally, inadvertently, and/or deliberately) are present in many foodstuffs, however it is those in the form of food additives that have caused some uncertainty and debate over long term usage and the health implications for humans. Titanium dioxide (E171), a colorant, and silicon dioxide (E551), an anti-clumping agent, are just two examples of nanosize additives found in food. Reassuringly, all additives are subjected to stringent testing for safety for human consumption. For example, in 2014 the European Commission (EC) imposed regulations that compel companies to state the inclusion of nano ingredients clearly.

The desire to enhance the durability or appearance of materials used in clothing has seen a growth in the application of nanomaterials in the production of such items as socks and insoles, where silver, known for its anti-bacterial quality, is incorporated. With shoes, the surface is sprayed with 'silica', preventing the water from being absorbed and giving them greater resistance to water and to general wear and tear. Once again, such applications raise concerns as to how safe these materials are if they are in direct contact with the skin.

The cosmetics industry has a huge demand for a variety of ENM; titanium dioxide and zinc oxide have great UV filtering properties, and both are used in sunscreen lotions. Once again, these materials are directly in contact with the skin and, even though they are thought unlikely to reach the bloodstream, there is limited research to support this premise.

Unlike sunscreen, tattoo inks are injected directly into the dermis. Tattoo inks contain a high proportion of nanoparticles; in the most widely used black ink, 99.94% of carbon black consists of nanoparticles. Research on rats suggests that 'carbon black' has been the cause of inflammation and damaged DNA and its carcinogenic properties have been recognised, and yet no direct link between tattoos and cancer has been identified. Nevertheless, there is evidence to show that nanoparticles can be transported in blood to other organs, where they accumulate, bringing their stability into question.

Research papers on the scope and potential of ENM in these fields are plentiful. However, there are few offering a critique of the perceived misconceptions of this emerging science.

Nanomedicine

Nanotechnology was thought to be a new science with the potential to revolutionise healthcare, leading to improvements in therapeutics and diagnostics. The uncertainty suggested by the possibility of a high level of risk to health, with the lack of evidence to prove

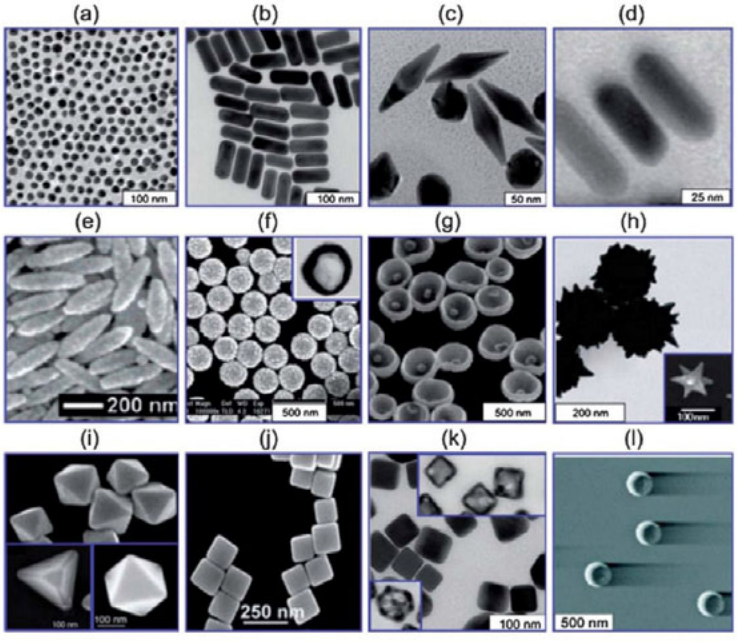


Figure 1. TEM images of various gold nanomaterials; (a) gold nanospheres, (b) gold nanorods, (c) gold bipyramids, (d) gold nanorods with silver shells, (e) nanorice, (f) SiO_2/Au nanoshells (inset is a hollow nanoshell), (g) nanobowl, (h) spikey SiO_2/Au nanoshells (inset is a nanostar), (i) gold tetrahedral, octahedral and cubohedra, (j) gold nanocubes, (k) silver nanocubes (insets are gold nanocages) and (l) gold nanoscrescents. Reprinted with permission from: Jiang, et al., Appl Biochem Biotechnol. *2012 166(6):1533-51.*

otherwise, has restricted their use in advancements in medicine. Indeed, caution is paramount. In sharp contrast, the commercial world has embraced the potential they offer, with companies keen to add them to their products. Production has proceeded on a massive scale with limited knowledge, as yet, of the products' impact on human health or the environment.

The possible uses of ENM in medicine are nearly limitless. Increasingly more sophisticated methods are being developed to create nanostructures with greater complexity to act as nano-drug delivery systems (NDDS). ENM could improve the targeted delivery of medicines in healthcare, such as in the treatment of cancers. They can be formulated to control and sustain the release of the drug until arrival at the location of the target site.

Tumours are surrounded by a rich blood supply, which makes them ideal destinations for drug carriers. When a tumour forms, the uniformity of the blood vessels becomes haphazard and gaps in their surface begin to appear, increasing the likelihood of absorption of the nanomedicines, thus directly attacking the cancer. However, this simple concept hasn't really been demonstrated fully in humans, which is perhaps one of the reasons why so few NDDS products are available on the market. Many scientists have already asked few provocative questions: Has the nanomedicine concept been oversold? Have we simply promised too much?

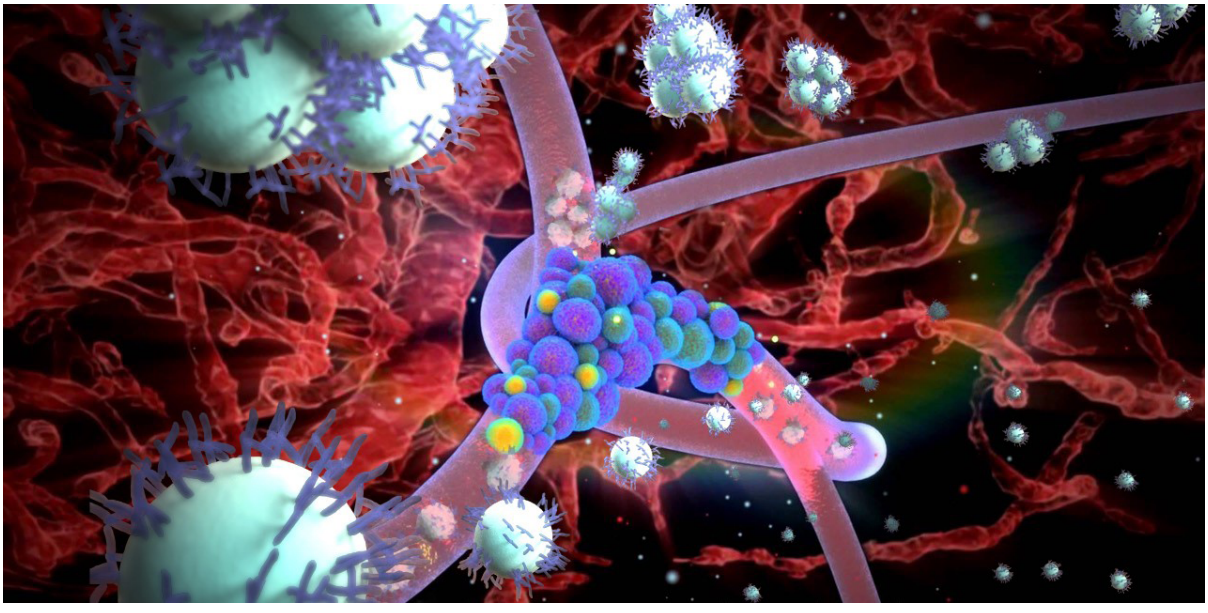
Part of the problem is that to engineer precise nano-scale objects capable of multiple functions in human body, where they are seen by the immune system as foreign intruders, scientists must intensify the desired behaviours through painstaking manipulation of their architecture. Too much effort and specialised equipment is needed in order to add extra features to their surface, increase their targeting capability, and hide them from the natural defence mechanisms of the human body, thus increasing their chance of reaching the target cells/tissues.

Major Limitations of Nanomedicine

In their simplest form, nanomaterials are more robust and easy to produce on an industrial scale. However, with ENM of greater complexity, the techniques used for their creation become more complicated and specialised, making them more difficult and expensive to replicate.

The scalability of such intricate designs can lead to variations and a degree of 'artistic licence' in their preparation and thus variation from the prototype. On an industrial scale, the manufacturing of such medicines would lead to innumerable interpretations of the original version, resulting in further ambiguity on their behaviour when in the human body. An incorrect

Figure 2. Illustration of a tumour being actively targeted with nanomaterial. Nanoparticles are equipped with antibodies on their surface to facilitate specific targeting. This concept was questioned by scientists who suggested that the targeting-antibodies on the surface of the nanomaterial are 'hidden' under a blanket of serum proteins that form so-called protein corona. Passive targeting, on the other hand, counts with accumulation in tumour via leaky vascularisation of the tumour, an effect confirmed on animal models but which is likely to be less prominent in humans. Illustration adapted and modified from: https://www.youtube.com/watch?v=EscII9E785I



attachment or combination of them would reduce specificity and lead to the display of unwanted characteristics by the material, such as incorrect mobility, premature release of the drug, and the possibility of the body rejecting the medicine as 'foreign' to the host organism.

Tests on laboratory-prepared cell cultures and mice are indicative of the actions of NDDS, yet are not a true test of biocompatibility in real fluids and actual living human beings, where an array of cells, plasma, and their substances will come into contact and possibly interact with the nanomedicine. Lack of biocompatibility could be harmful if the NDSS is not removed from the body swiftly. The unpredictability of the associations ENM may make in the body may cause them to accumulate and have toxic effects. Their interactions cannot be observed when in solution (once in the body), therefore the positive and negative effects on the body are largely based on assumption and cannot be fully anticipated, one of many reasons why only a few delivery systems have reached the clinical stage.

One of the key issues facing this field is that, even with the best intentions, unique products engineered to be of use could inadvertently be harmful to us and to the environment at the same time. The relatively young age of this scientific field means there is little evidence of their long-term effects, in particular their toxicity. The increased use of ENM in consumer products will inevitably lead to environmental problems. For example, silver nanoparticles are washed out from silver treated textiles and in turn inhibit the activity of bacterial degradation in water treatment plants.

Nanoethics has emerged from much debate on the future of ENM and exists to assess the benefits and risks of their use, as well as if they surpass the quality and advantages of materials (in particular medicine) that are already in use. Increasing demand for alternative medicines will no doubt result in heightened concerns over animal welfare, as more trials are required: we will still rely on the reaction of animals to a medicine, which provides insight on the likely reaction of the human body.

Conclusion

The ethics of nanotechnology has created a charged atmosphere in the worlds of academia, politics, and industry. The rapid development of ENM has meant their innovation has preceded regulation. Naturally, large companies are resistant to such embargoes. Despite concerns for safety, products are already on the market and are making a difference to people's lives. It is imperative that the regulating authorities catch up with science, ensuring that compelling evidence of toxicity and long-term effects is gained prior to the release of specific ENM on the market.

Although the focus of scientific research has been on cancer therapeutics, NDDS has the potential to accelerate progress in new therapies for neurodegenerative diseases such as Alzheimer's and Parkinson's. Undoubtedly, the main potential of NDDS is that they increase the specificity of a drug, ensuring the correct dosage is administered at the exact time to a specific target area. The versatility and specificity of ENM for drug delivery and diagnostics will benefit increasing numbers of patients, as well as global healthcare.

The question of their validity in our everyday lives still remains, and requires huge financial investment. Researching their biological and environmental behaviours further, as well as developing more sophisticated methods of their mass production, would help eradicate the doubt surrounding ENM, particularly with regards to medicine.

This article is a short extract from two IUPAC Technical Reports recently submitted to *Pure and Applied Chemistry*. Written by an international consortium of scientists, these comprehensive, interconnected reports first summarize the challenges related to the nomenclature and definition of ENM and provide an overview of the best practices for their preparation, surface functionalization, and analytical characterization (DOI 10.1515/pac-2017-0101), while in a second part, the reports focus on ENMs that are used in products that are expected to come in close contact with consumers (DOI 10.1515/pac-2017-0102). Reviewing the nanomaterials used in therapeutics, diagnostics, and consumer goods and summarizing current nanotoxicology challenges as well as the current state of nanomaterial regulation, these reports provide insight on the growing public debate on whether the environmental and social costs of nanotechnology outweigh its potential benefits.

Dr. Vladimir Gubala <V.Gubala@kent.ac.uk> (University of Kent, United Kingdom) is listed as a co-author of this article on behalf of the consortium of the following contributors (in alphabetical order): Dr. Linda J. Johnston (National Research Council Canada), Dr. Ziwei Liu (Cornell University, USA), Prof. Harald Krug (EMPA, Switzerland), Dr. Colin J. Moore (FOCAS Institute, DIT, Ireland), Prof. Christopher K. Ober (Cornell University, USA), Prof. Michael Schwenk (Tuebingen, Germany), and Prof. Michel Vert (University of Montpelier, France).

See iupac.org/project/2013-007-1-700 for more details.

Imitating the Grand Style of R. B. Woodward

by Jeffrey I. Seeman

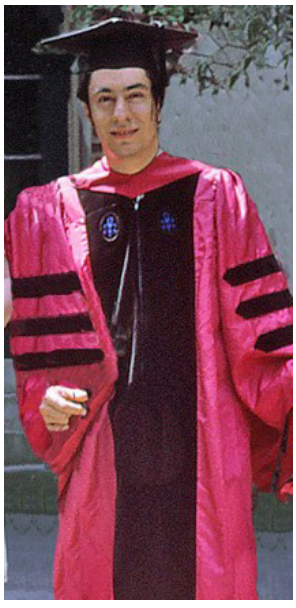
We all are influenced by our heroes, our role models, the individuals who we feel most represent the ideals to which we strive. In the four decades beginning in the early 1940s, the greatest of all organic chemists—certainly one of the greatest of all chemists—was Robert Burns Woodward. Few could replicate his science or his egregious* behaviors, though many tried.

In the previous issue of *Chemistry International*, a paper titled *Taking IUPAC Literally: Woodward's Pure and Applied Chemistry Words* was published. [1] That paper, along with a companion paper published in 2015 in *Angewandte Chemie*, illustrated Woodward's great written communication capabilities. [2] Woodward's grand or high style of writing is found in many of his papers. Woodward's words were, indeed, elegant and commanding. As such, some of his admirers tried their hand at copying Woodward's grand style. To further celebrate the 100th anniversary of Woodward's birth —he arrived on the scene on 10 April 1917—we present several examples of hero worship in words, the imitation of R. B. Woodward.

Subsequent to the publication of *Woodward's Words* in *Angewandte Chemie*, [2] two eminent chemists, Pat N. Confalone and Rick Lane Danheiser, contacted me and shared some of their writing from the early 1970s which emulated Woodward's grand writing style.

Confalone, a former graduate student of Woodward, is a former vice president at DuPont Global R&D and now Chair of the Board of Directors of the American Chemical Society, and an active participant in IUPAC governance. He sent several excerpts from his 1971 Ph.D. thesis, *Synthesis and Photochemistry of 5-Azido-1,3,4-oxadiazoles.* [3]

> "One of the most powerful concepts of synthetic methodology is the effective taming of reactive functional groups by uniting them in a stable molecular array. By thus masking their inherent reactivity, crucial manipulations required elsewhere on the molecule can be carried out under conditions whose relative severity would otherwise prove disastrous. When the desired groups are needed, a single mild reaction serves to dissect their once compelling chemical bondage, and thus unfettered, are made available for their predestined role." [3]



Pat Confalone in Ph.D. regalia, Harvard University, 1971. Photograph courtesy P. N. Confalone.

> "The purity of the recovered starting material woefully indicated that the substance had remained inviolate throughout its many intimate encounters with a host of acylating agents." [3]

> "Hence, in the midst of so exciting a foray, further investigation into the crucial cyclodehydration had to be abandoned, as the emphasis of our assault on the target was radically altered by a fascinating quirk of chemical happenstance." [3]

Rick Danheiser, a former graduate student of E.J. Corey and subsequently professor of chemistry at MIT, sent a Woodwardian-styled excerpt from his 1984 review article, *The Total Synthesis of Gibberellic Acid*. [4]

> "Confident that we had provided for every possible contingency, we believed that the triumphant completion of the total synthesis of gibberellic acid was finally at hand.
>
> That was naïve. We were totally unprepared for the special surprise our foe had held in reserve for the final confrontation . . . All efforts to suppress this translactonization proved futile . . . It was all too clear that our plan for the elaboration of the gibberellin A ring had been undermined by an inopportune exemplification

* "Egregious" typically means shocking or outrageous, and extends to perhaps even more shocking or outrageous definitions. In ancient times, egregious also meant "remarkably good." For the purposes of this paper, the word is a resonance hybrid of all of the above.

Rick Danheiser at Massachusetts Institute of Technology, c. 1985. Photograph courtesy R.L. Danheiser.

> of R. B. Woodward's dictum that 'enforced propinquity often leads to greater intimacy.'[5]" [4]

Finally, from the Woodward papers at the Harvard Archives comes the one page mystery document shown in Figure 1, reproduced on the following page. It is a mystery because we don't know who wrote it or why. The careless typing, including typed-over errors, clearly indicates that this was *not* the work of Woodward's perfectionist secretary, Dolores (Dodie) Dyer, whose name appears as if it were written by her. [6, 7] Nor is the author Woodward himself, as Woodward, ever more the perfectionist, would not have produced a document with so many typist's errors. Likely this document was prepared by one or several of Woodward's students as a playful clownery, a spoof on both Woodward and Dyer. Roald Hoffmann guesses that "they had a goldfish in the office, and one day it disappeared. Dodie accused RBW of doing away with it . . . " [7] Of relevance is the document's clear use of the grand style of writing favored by Woodward. This spoof, very clearly an imitation of Woodward, must surely have amused the grand master, as Woodward kept it permanently in his files, to be found 70 years later by this researcher.

Woodward with Dolores (Dodie) Dyer, ca. 1955. This is a rare picture of Woodward sans *his blue tie. Photograph from the W. Lwowski collection, New Mexico State University, courtesy William Maio.*

As discussed in my earlier paper on Woodward's Words, [2] Woodward did not encourage his students to write in the grand style. Nor, in my opinion, was this an affected style of Woodward, intentionally replacing some other, less grand, style that was his normal manner of communication, in order to impress the reading public. There was no other style for Woodward. That is the way he wrote, in contrast to my conclusion that Woodward intentionally developed and acted a public persona, with the grandeur befitting a nobleman.

In addition to crafting their words to model Woodward's style, according to his one-time graduate student Dan Kemp,

> "Graduate students and postdocs would practice for hours, learning to draw structures sufficiently carefully to be able to make their debut at Woodward's evening seminar—to go to the blackboard in front of the audience and in front of Woodward himself, to pick up the chalk and to draw a proper structure as an answer to one of the problems he had posed." [8]

Coda

Decades ago, Pat Confalone and Rick Danheiser surely had fun in their imitation of Woodward's grand writing style. Today, we join in their fun and also celebrate the wonder that was R. B. Woodward. I am certain that few, if any of us, including myself, could pick out which quotes are imitations and which are true Woodwardian prose, had we been given a randomized mixture of Confalone, Danheiser, and Woodward.

It is appropriate to end this paper with a real Woodward quote. What follows is one of my favorites[†]

[†] I do wince a bit, with the presumptive equivalence of "men" with "chemists" in Woodward's words.

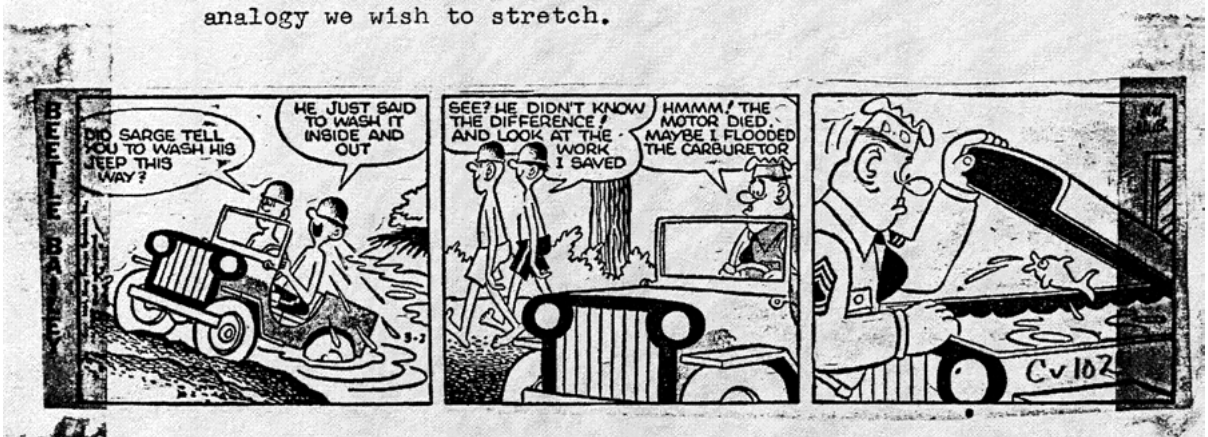
(Contribution from the Chemical Laboratories of Harvard University)

" Hallucinations Related to Genus Pisces " (Part 1)

by Dolores B. Dyer

Recent investigations in these laboratories have indicated the existence of anomalous interbowlular piscine migrations of unknown origin, periodicity and purpose. The details of our work will be published when ancillary experiments are completed. In the sequel we intend to show, skeptic's captious comments notwithstanding, that these ubiquitous rearrangements can be rationalized in terms of more familiar concepts.

The enclosed diagram, reprinted from Bailey[1] without permission, will, mutatis mutandis, indicate the analogy we wish to stretch.



1 Bailey, Beetle, Boston Daily Record, 1 March, 1954, p. 25.

Figure 1. A mystery document found within the Woodward Archives at Harvard University. The cartoon, taped to the typewritten text, is Beetle Bailey*: © 1954 King Features Syndicate, Inc.*

and was independently chosen by Fabienne Meyers, the editor of *Chemistry International*. Enjoy the real Woodward!

> [From *The Total Synthesis of Strychnine,* 1955] "Modern organic chemistry possesses a splendid and powerful armamentarium for the attack on the problems which excite the attention of its devotees. From time to time here mention has been made of some of these weapons, and it is certainly worth emphasizing that this campaign could not have been concluded without constant use of the very great body of principle and mechanism which our theorists have placed at our disposal, and without the beautiful physical tools which we now have. But in one respect, organic chemistry has not changed, nor is it likely to. Its successes depend in the first instance upon the experimental skill and devotion of the men who do the work. DR. MICHAEL P. CAVA spent the better part of a year in the exploratory phases of this work, and was then joined in an intensive effort of another year's duration by DR. W. DAVID OLLIS and DR. ALFRED HUNGER . . . DR. KARL SCHENKER and DR. HANS DAENIKER – the Beresina group; for it was of this gallant band of Swiss, thrown into the breach on a famous and desperate occasion, that DR. SCHENKER thought, when, arriving in the midst of the difficult campaign against Ring VI, he learned his fate for the months ahead. All of these men worked indefatigably, with great skill, and forbearance of a hard taskmaster. It is a very great pleasure to have the opportunity here to point out that the merit in this work is theirs in large measure, and to acknowledge my immeasurable debt to them." [9]

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Dr. Seeman <jseeman@richmond.edu> is at the University of Richmond. His professional activities include research in the history and sociology of science, including responsible conduct of research.

Awardees of the IUPAC 2017 Distinguished Women in Chemistry or Chemical Engineering

To celebrate International Women's Day this March 8th, IUPAC is pleased to announce the awardees of the IUPAC 2017 Distinguished Women in Chemistry or Chemical Engineering:

Prof. Misako Aida, Hiroshima University, Japan
Prof. Lifeng Chi, Soochow University, Suzhou, China
Prof. M. Concepcion Gimeno, University of Zaragoza, Spain
Dr. Jaqueline Kiplinger, Los Alamos National Laboratory, Los Alamos, NM, United States
Prof. Zafra Lerman, Malta Conferences Foundation, Evanston, IL, United States
Prof. Thisbe K. Lindhorst, Universität Kiel, Germany
Prof. Ekaterina Lokteva, M.V.Lomonosov Moscow State University, Moscow, Russia
Prof. Yvonne Mascarenhas, University OF Sap Paulo, Sao Carlos, Brazil
Dr. Veronika Ruth Meyer, Empa St. Gallen (retired), Swiss Federal Laboratories for Materials Science and Technology, Switzerland
Prof. Ingrid Montes-González, University of Puerto Rico, San Juan, Puerto Rico
Prof. Frances Separovic, University of Melbourne, Australia
Prof. Jihong Yu, Jilin University, China

The awards program, initiated as part of the 2011 International Year of Chemistry celebrations, was created to acknowledge and promote the work of women chemists/chemical engineers worldwide. These 12 Awardees have been selected based on excellence in basic or applied research, distinguished accomplishments in teaching or education, or demonstrated leadership or managerial excellence in the chemical sciences. The Awards Committee has been particularly interested in nominees with a history of leadership and/or community service during their careers.

An Award ceremony will take place during the IUPAC World Chemistry Congress in São Paulo, Brazil, coinciding with the special symposium on Women in Chemistry and a reception in honor of the recipients. See www.iupac2017.org for details.

Professor Vanderlan da S. Bolzani, co-chair of the special symposium, remarked: "We are especially pleased with this year's awardees and eager to recognize their contribution in a special session organized for the IUPAC 2017 IUPAC Congress. Each year since 2011, the award has gained more attention in the community. During this year's Congress and with the help of IUPAC leadership, we plan to continue this trend. My hope is to make every day International Women's Day!".

The International Women's Day is a global day celebrating the social, economic, cultural, and political achievements of women. The day also marks a call to action for accelerating gender parity. www.internationalwomensday.com

https://iupac.org/iupac-2017-distinguished-women/

Neil Garg is the Recipient of the 2016 Thieme–IUPAC Prize

We are delighted to announce that the 2016 Thieme–IUPAC Prize has been awarded to Neil Garg of the University of California, Los Angeles (UCLA). The prize includes an award of €5000 and was presented to Neil Garg in January 2017 at the 13th Winter Conference on Medicinal & Bioorganic Chemistry in Steamboat Springs, Colorado/USA following his Thieme–IUPAC lecture.

In his research, Neil Garg has had a major impact on the field of synthetic organic chemistry. He and his coworkers develop new reaction methodologies and synthetic strategies to prepare complex organic molecules. Specific areas of interest include cross-coupling reactions, green chemistry, heterocycle synthesis, and natural product total synthesis.

Sponsored jointly by Georg Thieme Verlag, IUPAC, and the editors of SYNLETT, SYNTHESIS, Science of Synthesis, and Houben–Weyl, the prize is awarded to a scientist under 40 years of age whose research has had a major impact in synthetic organic chemistry. The prize is given on the basis of scientific merit for independent research dealing with synthesis in the broadest context of organic chemistry, including organometallic chemistry, medicinal and biological chemistry, designed molecules, and materials.

www.thieme.de/en/thieme-chemistry/thieme-iupac-prize-55182.htm

The Franzosini Award of 2016

The 2016 Franzosini Award was given to David Fellhauer, in recognition of his contribution to the IUPAC Solubility Data Project, at the 15th Annual Meeting of the IUPAC Subcommittee on Solubility and Equilibrium Data. Held in Geneva, Switzerland on 24 July 2016, the meeting occurred during the 17th International Symposium on Solubility Phenomena and Related Equilibrium Processes.

The recipient of the 2016 Franzosini Award David Fellhauer from KIT-INE with Clara Magalhães, Chair of the Subcommittee on Solubility and Equilibrium Data (SSED), during the conference dinner of the 17th ISSP, held in Geneva, Switzerland.

David Fellhauer is a young investigator working in the radiochemistry division of the Karlsruhe Institute of Technology, Institute for Nuclear Waste Disposal (KIT-INE), Karlsruhe, Germany. He is given this recognition in view of his outstanding scientific contribution to solubility behavior, aqueous speciation, and solid phase formation of actinide elements (especially Np and Pu) in different oxidation states. Based on his work, new comprehensive chemical and thermodynamic models have been derived for dilute to concentrated electrolyte solutions and various pH conditions. The studies provide a significantly improved scientific understanding of actinide solution chemistry and are of high relevance for assessing the long-term safety of nuclear waste repositories.

A Global Approach to the Gender Gap in Mathematical and Natural Sciences: How to Measure It, How to Reduce It?

One of three grants recently awarded by ICSU is to a new joint project led by the International Mathematical Union (IMU) and IUPAC, with the strong involvement of IUPAP. The project will compile evidence worldwide, including on trends on the role of

Who's Who in This New ICSU Project?

Lead Applicant 1

International Mathematical Union (IMU); Committee for Women in Mathematics Chair, Prof. Marie-Françoise Roy

Lead Applicant 2

International Union of Pure and Applied Chemistry (IUPAC); Bureau Member and past chair of the IUPAC Committee on Chemistry Education, Prof. Mei-Hung Chiu

Supporting Applicants

International Union of Pure and Applied Physics (IUPAP); Working Group 5 Chair, Prof. Irvy (Igle) Gledhill

International Astronomical Union (IAU); Women in Astronomy" Chair, Full Astronomer Francesca Primas

International Union of Biological Sciences (IUBS); Executive Director, Dr. Nathalie Fomproix

International Council for Industrial and Applied Mathematics (ICIAM); Past-President of ICIAM and Officer, Prof. Barbara Keyfitz

United Nations Educational, Scientific and Cultural Organization (UNESCO); Chief of the Section on Science Policy and Partnerships and member of the SAGA Steering Committee, Dr. Ernesto Fernández-Polcuch

Gender in Science, Innovation, Technology and Engineering (GenderInSite); Director, Prof. Alice Abreu

Support

ICSU Regional Offices in Africa and Latin America and the Caribbean

Observer

International Union of Theoretical and Applied Mechanics (IUTAM)

women in science, to support informed decisions and provide easy access to materials proven to be useful in encouraging girls and young women to study and work in scientific fields. With the involvement of six scientific unions, UNESCO, and GenderInSite, this project constitutes a large international and multidisciplinary collaboration.

Mathematical and natural sciences have long and honorable traditions of participation by highly creative women contributors. However, the percentages of scientists who are women remain shockingly low and there is a significant gender gap at all levels between women and men. Barriers to achievement by women persist, especially in developing countries. This project will produce sound data to support the choices of interventions that ICSU and member unions can feasibly undertake. Evidence will include trends, since the situation for women continues to change around the world, with some negative developments. Regional information about careers, jobs and salaries will also be provided. The Joint global survey is planned to reach respondents in more than 130 countries, using at least 10 languages, while the Joint study on publication patterns will analyze comprehensive metadata sources corresponding to the publications of more than 500,000 scientists since 1970. Contrasts and common ground across regions and cultures, less developed and highly developed countries, men and women, mathematical and natural sciences, will be highlighted.

The new ICSU grants, each worth 300,000 Euros across 3 years, created three international initiatives led by ICSU Unions. Through this program, ICSU's intent is to foster membership engagement by addressing long-standing priorities for ICSU Members in developing **science education, outreach and public engagement activities**, and by mobilizing resources for international scientific collaboration. In addition to the IMU/IUPAC grant described above, the following projects were awarded this year:

IUPAP-IUCr: Utilisation of Light Source and Crystallographic Sciences to Facilitate the Enhancement of Knowledge and Improve the Economic and Social Conditions in Targeted Regions of the World

IUBS-INQUA: Trans-disciplinary Research Oriented Pedagogy for Improving Climate Studies and Understanding (TROP-ICSU)

www.icsu.org/what-we-do/projects-activities/icsu-grants-programme/grants-2016-2019

New InChI Software Release

The latest version of the InChI software, v1.05, has been released and is now available from http://www.inchi-trust.org/downloads/

In this version, the following features were added:

- Support for chemical element numbers 113-118
- Experimental support of InChI/InChIKey for simple regular single-strand polymers
- Experimental support of large molecules containing up to 32767 atoms
- Ability to read necessary for large molecules input files in Molfile V3000 format
- Provisional support for extended features of Molfile V3000
- Updated InChI API Library, including a novel API procedure for direct conversion of Molfile input to InChI and a whole new set of API procedures for both low and high-level operations (InChI extensible interface, IXA)
- Revised source code to ensure multi-thread execution safety of the InChI Library; several minor bugfixes/changes were made, and several convenience options were added to the inchi-1 executable.

The release is the first update since 2011 and the extended functionality is based on the outputs of IUPAC working groups.

While InChI provides a unique descriptor of molecular structures, the **Reaction-InChI** (RInChI) extends this idea towards reactions. Prototype versions of the RInChI have been available since 2011 (Grethe, Goodman and Allen, *Journal of Cheminformatics* 2013, 5, 45. DOI: 10.1186/1758-2946-5-45). The first official release (RInChI-V1.00) is also now available for download. This release defines the format and generates hashed representations (RInChIKeys) suitable for database and web operations. The RInChI provides a concise description of the key data in chemical processes, and facilitates the manipulation and analysis of reaction data.

Interested in learning more about InChI?
Consider attending the 2017 InChI meeting, 16-18 August 2017, in Bethesda, MD, USA. See more at https://iupac.org/event/chemical-identifier/

http://www.inchi-trust.org/

Database on Molecular Compositions of Natural Organic Matter and Humic Substances as Measured by High Resolution Mass Spectrometry

The investigation of non-living organic matter at the molecular level is a chief focus of modern environmental chemistry. Fourier transform ion cyclotron resonance mass spectrometry (FTICR MS) is a method of choice due to its unprecedented resolution capacity (Hertkorn *et al.* 2007; https://dx.doi.org/10.1007/s00216-007-1589-0). It resolves millions of carbon atoms with distinct chemical environments, both in terrestrial and extraterrestrial organic matter. The data on the molecular diversity of non-living organic matter, coupled to numerous data on biomarkers, can be used to draw conclusions on various biogeochemical processes, past and present. Further progress in this field is conditional on the development of a publicly accessible electronic database containing information about detected compounds and their concentration in non-living organic matter, defined as natural organic matter (NOM) in waters and humic substances (HS) in solid systems (*e.g.* soils, coals, peats, or bottom sediments).

A recently approved project supported by the Chemistry and the Environment Division (Division VI), the Organic and Biomolecular Chemistry Division (III), and the Analytical Chemistry Division (V), have the following specific objectives:

- develop a database architecture for storage, visualization, and classification of large datasets of molecular constituents of non-living organic matter
- compile initial data on molecular compositions of HS and NOM from different environments, with fully annotated protocols of their isolation, FTICR MS data acquisition, and data treatment and upload them into the developed database.

This will enable the elaboration of criteria for further evaluation of data on the molecular composition of NOM and HS. To achieve the formulated tasks, the project brings together researchers with long-term experience in FTICR MS data acquisition and treatment who work with HS and NOM of various origin (water, soil, coal, peat, and bottom sediments) in different geographic regions, using different isolation techniques and data treatment approaches. In addition, the task

group includes professionals in the fields of geostatistics, information technologies, and big data treatment.

The combination of diverse expertise and rich FTICR MS data pools available to task group members is a key prerequisite for the compilation of initial data on molecular constituents of NOM/HS into a user-friendly database. The task group will use the existing Biogeochemistry Database architecture developed by the task group members of the Lomonosov MSU, adapt it to the project needs, and distribute upload tasks among other TG members in accordance with their specific expertise (freshwater NOM, marine DOM, terrestrial HS from different sources) to come up with the demonstration database at the end of the project.

For more information and comments, contact Task Group Chair Irina V. Perminova <iperm@med.chem.msu.ru>
www.iupac.org/project/2016-015-2-600

Integrating Green Chemistry and Socio-Sustainability in Higher Education: Successful Experiences Contributing to Transform Our World

More than ever, Green Chemistry can be considered a powerful tool to modify unsustainable practices in chemistry, engineering, and correlated areas all over the world. It is well known that the contextualized insertion of Green Chemistry principles into the curricula of higher education institutions (HEI) can contribute to a better professional education, engaging students to learn conceptual content associated with procedural and attitudinal subjects.

In order to promote Chemistry Education and Education for Socio-sustainable Development in Latin America and Africa, the project 2013-041-3-300 has

From left to right Prof. Liliana Mammino, Prof. Paul Anastas and Prof. Vânia Zuin

been developed to study, adapt, and create new contents for HEI. Coordinated by Prof. Zuin (Brazil) and Prof. Mammino (South Africa), the project involves researchers, lecturers, professors, students, and related HEI representatives from 14 different countries. The resulting webpage, available in Portuguese, Spanish, and English, can be seen at **http://greenchemed.iupac.ufscar.br/**

At the Federal University of São Carlos (UFSCar), São Paulo, Brazil, for instance, a number of teaching experiments and related didactic initiatives have been conducted at the undergraduate and post-graduate levels since 2013, considering locally important topics, mostly associated with sustainable agriculture, agro-resilience, green chemistry, and socio-environmental technologies, especially for the bio-rational control of plagues. As an example, multifactorial mechanisms to repel, control, or eliminate *Aedes aegypti* have been studied, since they are the main type of mosquito that spreads Zika, dengue, chikungunya, and other viruses. Such scientific approaches have been transformed and adapted to make them suitable to be used as learning objects at UFSCar [1-3].

As a consequence of multiple actions in the Chemistry Department, another collective initiative was the elaboration and implementation of a new curriculum for teaching education at UFSCar at the beginning of 2017, emphasising Green Chemistry principles in several theoretical and practical subjects, including one dedicated exclusively to green chemistry and sustainability projects.

At the University of Venda, South Africa, the Chemical/science education at the tertiary level is a type of educational research fully integrated within tertiary-level science teaching. Its aims are the continuous enhancement of the quality of teaching through the investigation of students' difficulties, through general-character reflections on contents and approaches, and through active participation in international meetings and debates. Particular attention is given to crucial issues, like the language-related difficulties encountered by science students studying in a second language, or the exploration of approaches to suitably and effectively incorporate education for sustainable development into course activities, and to the educational aspects of advanced chemistry courses.

The courses provide a firm foundation in chemical ideas, processes, applications, and the context of chemistry in society. The full picture, from raw materials

Participation by Member Organizations Worldwide

The Pontificia Universidad Católica del Perú

Currently, in Peru, the state is implementing a policy to support the development of science and technology. Among other strategies, it is providing financial support to graduate schools, specifically to the master's programs showing the best conditions for the formation of new researchers. Our master's program is one of the winners of this subsidy program, so the conditions to promote research in Green Chemistry are favorable. We focus particularly on the following objectives of the project:

- Proposing general modules for up-to-date university Green Chemistry curricula for chemistry courses, and developing of Green Chemistry contents for the theoretical and experimental components of such courses.
- Contributing to the establishment of Green Chemistry as a component in the training of professionals and promoting the public understanding of Green Chemistry principles.

In 2013, a new curriculum for the Master's program in Chemistry was implemented, including a Green Chemistry course as one of the elective courses. In this course, the fundamental concepts of green chemistry are presented and the application of its principles is discussed by means of a review and critical analysis of the research reported in the relevant scientific literature.

The Universidad Nacional de La Plata, Argentina; Universidad Pedagógica y Tecnológica de Colombia, Universidad del Cauca, Colombia;

A number of short courses on green chemistry for the undergraduate level, as well as outreach activities (school, communities), are being developed.

through beneficiation to research, including management aspects, is presented. Experimental and field work form an integral part of all courses and self-initiated research is encouraged at the postgraduate level.

Apart from the current courses, several main meetings and workshops have been organised by the coordinators, as is the case for:

- *Green Chemistry Education session on the 4th, 5th, and 6th International IUPAC Conference on Green Chemistry (2012-2016)* [4-5]: www.ufscar.br/icgc4,www.saci.co.za/greenchem2014 and www.greeniupac2016.eu
- *Green Chemistry session in the Brazilian Chemical Society Annual meeting, Brazil (2013-2016)*: www.sbq.org.br/36ra/workshops.php#hiddenDiv6, www.sbq.org.br/37ra/coordenadas-qve.php,www.sbq.org.br/37ra/workshops.php, www.sbq.org.br/38ra/programacao-completa/conferencias-convidadas, www.sbq.org.br/38ra/programacao-completa/sessoes-coordenadas
- 2nd African Conference on Research in Chemical Education: https://sites.google.com/site/acrice2015/

Material about the project has been prepared and disseminated by magazine articles, web pages, scientific papers, and a didactic book published by the Royal Society of Chemistry in 2015 (Worldwide Trends in Green Chemistry Education, http://pubs.rsc.org/en/content/ebook/978-1-84973-949-8)

Another book focusing on the topic will be published by UFSCar, involving many members of the project. It is important to emphasise that we aim to mobilise efforts to achieve the United Nations 2030 Agenda for Sustainable Development and its 17 Sustainable Development Goals. These objectives are discussed together with industries and governmental/non-governmental organisations, as well as with schools.

Some members are actively participating: see box included below and continued on the following page.

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For more information and comments, contact Task Group Chair Vânia Zuin <vaniaz@ufscar.br>

www.iupac.org/project/2013-041-3-300

The Brazilian Green Chemistry School, Brazi

The Brazilian Green Chemistry School is based at the School of Chemistry of the Federal University of Rio de Janeiro (UFRJ), which offers undergraduate courses in chemical engineering, industrial chemistry, food engineering, and bioprocess engineering, as well as a graduate program in Technology of Chemical and Biochemical Processes. The Green Chemistry School has access to a staff made up of professors from UFRJ and other universities, as well as researchers from technology centers and companies. It conducts surveys on the state of the art in bio-based chemicals from raw materials abundant in Brazil; organises courses, workshops and meetings on green chemistry and related topics; and develops materials, experiments, and demonstrations for students at a high school level that can also be used for outreach activities.

The Faculty of Sciences and Technology, Portugal

A four-year doctoral programme was established in the largest Centre of Excellence / Laboratório Associado para a Química Verde (LAQV) at REQUIMTE and has been hosted by three Portuguese Universities (NOVA Lisbon, Porto, and Aveiro) since 2014. During the first year of the course, the students attend mandatory and optional courses offered by the three Universities. During the 2nd, 3rd, and 4th years, the students develop projects covering different fields of Sustainable Chemistry, taken from a very wide view of the research agenda of the SusChem platform (the European Technology Platform for Sustainable Chemistry).

FCT-NOVA is highly committed to the dissemination of Green Chemistry to the general public, hosting different activities for high school students. The students have the opportunity to do research together with Master and PhD students in projects focused on the development of sustainable processes for the production of novel products for different applications. The training period starts with a lecture introducing the Principles of Green Chemistry and Sustainable

Engineering. Special effort is made to give practical examples of the applicability of concepts to the real world. On-going research activities foster a new philosophy in the industry, instilled alongside chemical reactions and processes. The methodology includes the co-supervision of Masters and PhD students developing collaborative projects with national companies.

The Green Chemistry Centre of Excellence, University of York, UK

In addition to the successful Masters course in Green Chemistry & Sustainable Industrial Technology that has been running at the University of York for the past 15+ years, green chemistry will now be incorporated in the undergraduate chemistry curriculum at York, in both taught and practical material.

The Greener Reagents and Sustainable Processes (GRASP) project has been running for the past 2 years with the aim of addressing the use of hazardous/unsustainable chemicals in teaching labs and providing chemistry undergraduates with the requisite skills and knowledge to prepare them for future careers in the chemical industry.

The The Green Chemistry Centre of Excellence (GCCE) recently launched the RenewChem initiative, which incorporates graduate training as one of its core activities. The training will be specifically aimed at equipping future employees of the chemical industry with the requisite skills and knowledge to make an immediate impact on the transition to green manufacturing and circular economy within the chemical industries.

A bespoke e-learning platform has been developed with the aim of promoting the uptake of green and sustainable methodologies, with a particular focus on the synthesis of pharmaceuticals. The CHEM21* online learning platform comprises a range of free, shareable, and interactive educational and training materials that have been created in collaboration with industry.

Also via the CHEM21* project, the GCCE, in collaboration with other CHEM21* academic and industry partners, have organised a series of face-to-face training workshops aimed at graduates, PhDs, and post-docs covering topics such as metrics, route selection, safety, and biocatalysis, to name but a few.

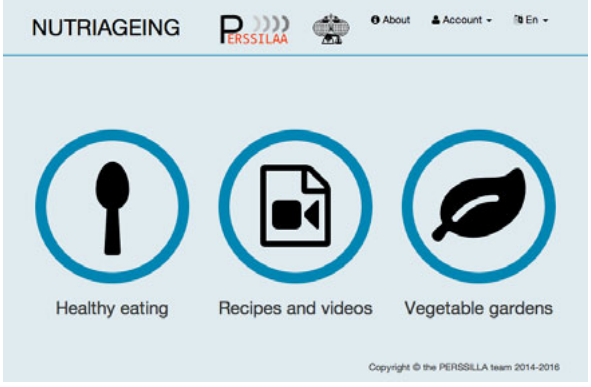
We continue to engage Masters-level students and provide them with hands-on experience organising and delivering public engagement activities to a wide range of audiences, from primary school children to members of the general public. Many of the experiments and exhibitions have focused on obtaining chemicals from food waste in order toof introduce green chemistry principles in a way that is directly relevant to a non-technical audience. The GCCE also continues to engage with our international partners to share knowledge and examples of best practice, in particular through the Global Green Chemistry Centres or G2C2 network (http://g2c2.greenchemistrynetwork.org).

NUTRIAGEING: Combining Chemistry, Cooking, and Agriculture

The website NUTRIAGEING was created to bring chemistry to the general public by demonstrating how chemistry offers unique solutions for society's needs in terms of healthy living and better ageing. It is now open to academic partners and the general public at **http://nutriageing.fc.ul.pt**. Offering modules to promote healthier nutrition, and showing the contribution of food chemistry to health, the website educates, not only on how to improve eating habits, but also on how to grow vegetables and condiments, demonstrating the added value of their chemical activity. In addition, games on the site offer entertainment and allow the user to confirm the knowledge acquired.

Developed within the scope of the IUPAC project "Healthy life and active ageing–the contribution of functional food ingredients" (2013-054-2-300) and the EU Project "Personalized ICT Supported Service for Independent Living and Active Ageing" (GA 610359), this new platform was built for the transfer of scientific knowledge into usable personal advice, with a clean, easy-to-use, "app-like" interface with minimal menus. The responsive layout ensures device-independent accessibility and a good viewing experience for the user.

The website is structured around three major themes: (1) Healthy eating, (2) Recipes and videos, and (3) Vegetable gardens.



The Silver Book and the NPU Format for Clinical Laboratory Science Reports Regarding Properties, Units, and Symbols

Georges Férard[1,*] **René Dybkaer**[2] and **Xavier Fuentes-Arderiu**[3] on behalf of
the joint IFCC and IUPAC Committee-Subcommittee on Nomenclature for Properties and Units (C-SC-NPU);
IFCC-IUPAC project #2007-033-3-700

[1,*]georges.ferard@noos.fr ,[2] Dept of Standardization in Laboratory Medicine, Region H Frederiksberg Hospital, Denmark, and
[3] 2461xfa@gmail.com

Standardized terminology was presented by IUPAC and by IFCC in 1967 [1] and is now updated by the second edition of the Silver Book 2017 [2] which gives recommendations for the clinical laboratory requests and reports, thus ensuring clear meaning and accuracy. The Nomenclature for Properties and Units (NPU) adheres to international standards of metrology and of terminology, in particular the International System of Quantities (ISQ) and International System of Units (SI) [3], the International vocabulary of metrology – basic and general concepts and associated terms (VIM) [4], and also to an outline for a vocabulary of nominal properties and examinations [5]. The NPU format applies to multiple disciplines, including clinical allergology, clinical chemistry, clinical haematology, clinical immunology and blood banking, clinical microbiology, clinical pharmacology, molecular biology and genetics, reproduction and fertility, thrombosis and haemostasis, and toxicology [2]. The present Leaflet recalls the definitions of the concepts used to express a property of a person. The aim of this comprehensive summary is to promote the proper NPU terminology for reliable exchange of person examination data, thus improving person information, comparative and epidemiological studies, and interoperability in the eHealth domain [6].

Basic Concepts in the NPU Format

The terminography used in the examples below adheres to the NPU format, where each of the three main elements of a property term may be augmented by an immediately following parenthetic specification:

System(specification)—Component(specification); kind-of-property(specification)
= nominal property value, ordinal quantity value, or quantity value and unit as appropriate

system: part or phenomenon of the perceivable or conceivable world consisting of a demarcated arrangement of a set of components and a set of relations or processes between these components [modified from 7]. In human biology, it may be a person or a body part of a person or the immediate surroundings; *e.g*. Person, Blood, Urine, Kidney, Beta cells of the pancreas, Exhaled air. The initial letter of the term for a system is a capital letter. The term (and any specification) is followed by a long dash.

component: part of a system [7]. The component may be a physical part of the system, a chemical or biochemical compound, or a process; *e.g*. Calculus, Glucose, Intestinal absorption, Cortisol secretion. The initial letter of the term for a component is a capital letter. The term (and any specification) is followed by a semicolon.

kind-of-property: common defining aspect of mutually comparable properties [7]. The term of this concept is hyphenated to emphasize that it is a single term. Examples are number concentration (C), volume (V), amount-of-substance (n), substance concentration (c), catalytic-activity concentration (b_E), taxon, sequence variation. The initial letter of the term is lower case.

dedicated kind-of-property: kind-of-property with given sort of system and any pertinent sorts of component [7]; *e.g*.
Patient—; mass
Patient—Glucose; substance concentration(procedure).

property: state- or process-descriptive feature of a system including any pertinent components [modified from 7]; *e.g*. Patient(Urine)—Glucose; substance rate(procedure) = 8 $mmol \cdot d^{-1}$. The modifier "procedure" refers to the examination procedure. As the set of possible values will depend on the local procedure, this procedure should be indicated in the report, *e.g*. Plasma—Lactate dehydrogenase; catalytic-activity concentration(IFCC 2002) = 3.2 $\mu kat \cdot L^{-1}$.

First efforts at the standardization of data transmission in clinical laboratories concerned quantities, *i.e*. those properties that have a magnitude, mostly expressed by a number and a unit [1]. However, many important properties of a classificatory nature such as species of microbes or genetic structure are inherently devoid of magnitude. In such cases, the superordinate concept 'property' can be generically divided in four types of property according to algebraic characteristics [7]:

- nominal property: property, defined by an examination procedure, that can be compared for equivalence with another property of the same kind-of-property, but has no magnitude [modified from 7] ; *e.g*. Urine—Neuroleptic drug; taxon(procedure) = chlorpromazine.

- ordinal property, ordinal quantity: property, defined by an examination procedure, having a magnitude and that can be stated only to be lesser than, equal to, or greater than another property of the same kind-of-property [7]; *e.g.* Urine—Bilirubins; arbitrary concentration({0, 1, 2, 4}; procedure) = 2.

- differential property, differential quantity: property having a magnitude and that can be subtracted from, but cannot be divided by another property of the same kind-of-property [7]; *e.g.* Patient—Rectum; Celsius temperature = 36.5 °C. **Logarithmic differential property** is used when the measurement scale consists of logarithmic values; *e.g.* Urine—; pH = 6.1.

- rational property, rational quantity: property having a magnitude and that can be divided by another property of the same kind-of-property [7]; *e.g.* Blood—Erythrocytes; volume fraction = 0.41 or as per cent 41 %.

quantity: property of a phenomenon, body, or substance, where the property has a magnitude that can be expressed by a number and a reference [4]. A reference may be a measurement unit, a measurement procedure, a reference material, or a combination of such.

kind-of-quantity: aspect common to mutually comparable quantities [4, but without hyphens in the term]. Each kind-of-quantity may be designated by a term or a symbol, *e.g.* length (l), and mass concentration (ρ). A given kind-of-quantity may have synonyms; *e.g.* relative molecular mass and molecular weight (deprecated by the ISO [8]), and also synonymous symbols; *e.g.* A and S for area. A given symbol is sometimes used for different kinds-of-quantity; *e.g.* A is the recognized symbol for area, nucleon number, Helmholtz energy, affinity of chemical reaction, and absorbance. The concepts here termed "kinds-of-quantity" are generally termed "quantity" by CGPM [3] and ISO/IEC 80000-1 [8].

quantity of dimension one, also termed dimensionless quantity: quantity for which all the exponents of the factors corresponding to the base quantities in its quantity dimension are zero [4]: $\mathsf{L}^0\mathsf{M}^0\mathsf{T}^0\mathsf{I}^0\Theta^0\mathsf{N}^0\mathsf{J}^0 = 1$. Quantities of dimension one may be divided according to their kinds-of-quantity into fractions, ratios, and relative kinds-of-quantity:

- fraction: quotient of two identical kinds-of-quantity, for which the numerator kind-of-quantity relates to a component B and the denominator kind-of-quantity relates to the given system; *e.g.* Erythrocytes(Blood)—Reticulocytes; number fraction $= 6 \times 10^{-3}$ or 0.6 % or 6 ‰. ISO/IEC 80000-1 accepts per cent with the symbol % for the submultiple unit 0.01, and per mille with the symbol ‰ for the submultiple unit 0.001 [8].

- ratio: quotient of two identical kinds-of-quantity, for which the numerator kind-of-quantity relates to a component B and the denominator kind-of-quantity to another component of the same system, commonly treated as a reference component; *e.g.* Sweat(specification)—Sodium ion/Potassium ion; substance ratio = 3.80 or as 380 %.

- relative kind-of-quantity: quotient of two identical kinds-of-quantity, commonly two kinds-of-quantity related to different systems, the second being a reference system; *e.g.* Plasma—Coagulation factor XI; relative substance concentration(immunological; actual/norm; procedure) = 0.80 or as 80 %.

arbitrary kind-of-quantity: kind-of-quantity outside the ISQ. There is no dimension or SI unit involved; *e.g.* Thrombocytes(Blood)—Aggregation, collagen-induced; arbitrary activity({normal, lightly weakened, weakened, utmost weakened}; procedure) = lightly weakened. This example is also an ordinal quantity [2].

Generalities Concerning Kinds-of-Quantity and Units

'Kinds-of-quantity' are used to classify quantities of the same kind. Quantities of the same kind within a given system of quantities have the same dimension. Different kinds-of-quantity can also have the same dimension; *e.g.* substance content (n_B/m_{system}) and molality ($n_B/m_{solvent}$) both have the dimension $\mathsf{N}\mathsf{M}^{-1}$ and the coherent SI unit mol kg^{-1}.

Base Kinds-of-Quantity in the ISQ, their Dimensions, and their Units in the SI

A base kind-of-quantity is one that is conventionally accepted as being independent of other base kinds-of-quantity in a system of kinds-of-quantity. The remaining kinds-of-quantity are derived and are related to base or derived units. To each base kind-of-quantity of the ISQ is assigned a dimension represented by a sans-serif capital-letter symbol (except for number of entities). For example, the dimension of amount-of-substance is represented by N.

Base kind-of-quantity		Base unit		Dimension
Term	Symbol	Term	Symbol	Symbol
number (of entities)	N	one	1	$\mathsf{1}$
length	l	metre	m	L
mass	m	kilogram	kg	M
time	t	second	s	T
electrical current	I	ampere	A	I
thermodynamic temperature	T	kelvin	K	Θ
amount-of-substance	n	mole	mol	N
luminous intensity	I_v	candela	cd	J

Number of entities can be regarded as a base kind-of-quantity [ref. 4, § 1.4 note 3; ref. 8, part 1, § 3.4 note 3] and the number one (symbol $\mathsf{1}$) as a base unit [ref. 4, § 1.10 note 3].

The kind-of-quantity amount-of-substance is proportional to the number of specified entities that may be atoms, molecules, ions, electrons, other particles, or specified groups of such particles [3]; *e.g.* Urine—Nitrogen(N); amount-of-substance(procedure) = 360 mmol.
The relationship is governed by the Avogadro constant (symbol N_A or L): $n_B = N_B/N_A = N_B/L$.

Symbols of Derived Kinds-of-Quantity, Coherent Derived SI Units, and Quantity Dimensions

Striving for monosemy, *i.e.* one symbol only relates to one concept, single-letters are sometimes modified by subscripts, superscripts, or different fonts**,** *e.g.* A_r is the symbol for relative atomic mass (atomic weight), and A_m is that for molar radioactivity. N is the dimensional symbol of amount-of-substance and N is the symbol of the unit newton. The unit for Celsius temperature, *i.e.* the degree Celsius (symbol °C), is equal in magnitude to the kelvin (symbol K), the unit of thermodynamic temperature. A Celsius temperature is given, *e.g.* as 37 °C (not 37, not 37° C, not 37°C, and not 37C).

The term "katal" and symbol "kat" for the 'SI coherent derived unit for catalytic activity' have been recognized by IUPAC, IFCC, International Union of Biochemistry and Molecular Biology (IUBMB), World Health Organization (WHO), and General Conference on Weights and Measures (CGPM) [3]. IUPAC & IFCC [9] recommended that the enzyme unit, international unit U be progressively replaced by submultiples of the katal, where 1 U = 1 μmol·min^{-1} ≈ 16.67 nkat; *e.g.* Plasma—Aspartate transaminase; catalytic-activity concentration(IFCC 2002) = 2.2 × 10^{-6} kat·L^{-1} or 2.2 μkat L^{-1}.

A specification regarding the measurement procedure used is necessary when catalytic activity is involved, here "IFCC 2002". If the symbol U is used, it must not be confused with the symbol IU (meaning International Unit, also abbreviated int.unit), which is the symbol used by the WHO and mentioned in the SI Brochure [3] in expressing biological activity of certain substances that cannot yet be defined in terms of the SI; *e.g.* Plasma—Insulin; arbitrary substance concentration(IRP 66/304; procedure) = 120 × 10^{-3} IU·L^{-1} , where IRP stands for International reference preparation of the WHO.

Non-SI Units

Several non-SI units are widely used in clinical laboratory sciences and have corresponding values in SI units.

Kind-of-quantity	Term for unit	Symbol for unit	Expression in terms of SI coherent unit
length	ångström	Å	= 0.1 × 10^{-9} m
volume	litre*	L, l	= 10^{-3} m^3
mass	dalton*	Da	= 1.660 538 921(73) × 10^{-27} kg
time	minute*	min	= 60 s
	hour*	h	= 3 600 s
	day*	d	= 86.4 × 10^3 s
	week	wk	= 604.8 × 10^3 s
	year	a	≈ 31.556 952 × 10^6 s
pressure	millimetre of water	mmH_2O	= 9.806 65 Pa
	millimetre of mercury	mmHg	≈ 133.322 Pa
	bar	bar	= 10^5 Pa

*Non-SI unit accepted by CGPM for use with the International System of Units [3]. The unmarked entries of the second column and their corresponding symbols have no official sanction from CGPM [3].

The symbol for litre is either L or l. ISO and IEC prefer l, because the term "litre" is not derived from the proper name of a person. L is preferred here to avoid confusion with the numeral 1 [2, 3]. Dalton is also termed unified atomic mass unit (symbol u); its standard uncertainty is indicated in the table parentheses.

Prefixes for Multiples and Submultiples of Units

Prefixes denoting decimal factors 10^n have been defined [3]. For convenience, the Commission on Clinical Chemistry of IUPAC and IFCC recommended a preference in the clinical laboratory for decimal factors with decimal prefixes in steps of a factor 1000 [1]. This selection of a decimal prefix often permits numerical results to be reported with a numerical value in the recommended interval between 0.1 and 999. For most purposes, the prefixes hecto, deca, deci, and centi can be avoided, though they have equal legal standing.
The prefix symbol and the unit symbol are combined without any space; a second prefix should be avoided in units already containing a prefix; *e.g.* for picogram use pg, not p g or μμg. In units, with a numerator and a denominator, multiple and submultiple shall be in the numerator; *e.g.* the number concentration of thrombocytes in blood should be expressed as 215 × 10^9 L^{-1} (not 215 × 10^6 mL^{-1}) and the substance concentration of arsenic in urine should be expressed as 41 nmol L^{-1} (not 0.041 nmol mL^{-1}).
Capital letters are used for the positive powers equal to or greater than mega. This avoids the confusion between mega (symbol M) and milli (symbol m), between peta (symbol P) and pico (symbol p), and between zetta (symbol Z) and zepto (symbol z).

Prefix with $n \geq 1$			Prefix with $n \leq -1$		
Term	Symbol	n*	Term	Symbol	n*
yotta	Y	24	deci	d	–1
zetta	Z	21	centi	c	–2
exa	E	18	milli	m	–3
peta	P	15	micro	μ	–6
tera	T	12	nano	n	–9
giga	G	9	pico	p	–12
mega	M	6	femto	f	–15
kilo	k	3	atto	a	–18
hecto	h	2	zepto	z	–21
deca	da	1	yocto	y	–24

*The variable n is the decimal exponent of the factor.

Terminological Rules of the NPU

To avoid misunderstandings, a set of rules is needed for transmission of data about properties:

- The symbol for a **kind-of-quantity** is a single letter (Greek or Latin), printed in italic, with very few exceptions, *e.g.* pH. For each kind-of-quantity, there is only one coherent SI unit. However, the same SI unit may be used to express the values of quantities with different kinds-of-quantity. Therefore, a unit cannot identify the kind-of-quantity; *e.g.* volumic mass and mass concentration use $kg \cdot L^{-1}$, so both the unit and the kind-of-quantity must be stated.

The **kind-of-quantity** and any modifiers may be abbreviated; *e.g.* conc., cont., num., pr., temp., arb., cat., rel., sat. for concentration, content, number, pressure, temperature, arbitrary, catalytic, relative, saturation, respectively [2].

- The symbol for a **unit** is represented by one, two, or three upright lower-case letters, except if the unit is termed after a person; *e.g.* A and K for ampere and kelvin, respectively, and the special case of L for litre. Each term is still written with an initial lower-case letter. In the clinical laboratory, in expressions of volume, the litre and its submultiples are preferred to cubic metre and its submultiples.

- The systematic term for a **component** should not be abbreviated, because abbreviations are not internationally accepted. In the NPU format, the initial letter of the component is a capital letter, except for some prefixes; *e.g.* T4 should be replaced by Thyroxine and α–Amylase is correct. Bacteria, viruses, fungi, plants, and animals including parasites should be designated by their taxonomic term. Terms for genera, species, and subspecies are printed in italic; terms for orders and families, and for strains or races are printed in roman script, but the IFCC data bank of dedicated kinds-of-property uses roman script throughout [10].

Urine(catheter)—Bacterium, nitrite producing; number concentration(procedure) = $2.3 \times 10^6\ L^{-1}$.

Expectorate—Bacterium; taxon = *Mycobacterium tuberculosis*.

- The **system** and any modifiers may be abbreviated; *e.g.* Pt, B, P, U, a, f, v for patient, blood, plasma, urine, arterial, fasting, and venous, respectively [2].

A specific NPU code NPUXXXXX is assigned to each of the 16 000 entries in the NPU data bank [10, 11]. This code is well-adapted to electronic health records or laboratory administrative systems; *e.g.* NPU10547 Pt—Insulin(administered); substance content(i.v.; amount-of-substance/body mass) = 0.3 $\mu mol \cdot kg^{-1}$.

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11. Danish release center http://www.labterm.dk/Enterprise%20Portal/NPU_download.aspx (acc. 2016-09).

The **Healthy eating** section, developed by chemists, biochemists, and nutritionists, is mainly focused on nutritional literacy, supported by chemical and biochemical science. The How much should I eat subsection covers macronutrients and micronutrients, but also answers questions, such as "what type of fat should I choose for eating and cooking", "what about fiber", and "how much water should I drink". Further information covers calcium and salt intake, antioxidants, and functional ingredients, the latter also reporting findings that are the outcome of lab work to illustrate the importance of chemistry for the discovery of the active principles isolated from natural resources. Clinical nutrition focuses on the importance of an integrated approach for the nutritional evaluation of subjects. Nutritional risk factors, clinical nutrition evaluation, nutritional intake, anthropometric measurements, and nutritional status classification, and dietary plans are included in this subsection. Nutritional labelling, another subsection, aims to give the user concepts for informed choices when buying food products, covering the type of information available on the package, mandatory food information, how to understand it, reference intakes, *etc.* Finally, the Enjoy subsection is interactive, with quizzes that allow the user to evaluate if he/she knows how to make a balanced diet and word puzzles. Gaining knowledge with pleasure!

A **Recipes and videos** section is an innovation of this website. It includes 15 videos of recipes developed by the famous Portuguese chef, Hélio Loureiro. While cooking a recipe, he chats with two experts and a young researcher, discussing the chemical principles of recipe components and their benefits. Overall, about 23 experts in various areas of chemistry (*e.g.* organic, analytical, food chemistry, *etc.*) and biochemistry participated in the videos. Scientific discussions were conveyed to the public in a simple and understandable manner.

Finally, the **Vegetable gardens** section is another innovative area. The user may wish to produce some of the recipe ingredients in his/her garden. A landscape architect teaches users how to plan a vegetable garden in a variety of settings, from the backyard to the balcony or even small pots on the kitchen window. By accessing the recipe, *e.g.* one with peppermint, and clicking on the icon that appears on the word "peppermint", the user is taken to the vegetable garden section, where the information on how to grow this herb is given.

Enjoy, learn, cook, and eat with Nutriageing, and take part in some of the great pleasures of a healthy life!

Lívia Sarkadi (Department of Food Chemistry and Nutrition, Szent István University) and Amelia Pilar Rauter (Universidade de Lisboa) (left) in the session dedicated to functional ingredients

Chef Hélio Loureiro, cooking and talking....

The Portuguese team standing on the periodic table at DQB-FCUL. From left to right: Antonio Ferreira, Marta Sousa Silva (FCUL), Helena Soares da Costa (INSA), Amelia Pilar Rauter, Antonia Turkman, Marília Antunes, Feridun Turkman (FCUL), and Tania Albuquerque (INSA). Absent: Alice Martins

For more information and comments, contact Task Grup Chair Amélia Pilar Rauter <aprauter@fc.ul.pt>
www.iupac.org/project/2013-054-2-300

Safety Training Program

Safety is our first priority. We often hear that statement in industrial settings. But it isn't universally practiced. Several years ago, the IUPAC Committee on Chemistry and Industry (COCI), with support from UNESCO and UNIDO, developed a program to enable the development of stronger safety cultures in developing countries. The IUPAC Safety Training Program offers chemical professionals the opportunity to visit an industrial host with strong environmental, health, and safety (EH&S) programs and to observe first-hand what is required to create and sustain that culture. Once they have completed the training, the STP Fellows develop an implementation plan that describes how they will realize the value of the training by driving improvements back home. STP Fellows are typically invited to share updates at the IUPAC Congress/General Assembly STP Workshops. These presentations illustrate the impact of the program, as Fellows describe the improvements in the use of personal proactive equipment, safety devices, waste handling methods, pre-task analysis, *etc.* These sessions also inspire the workshop attendees to investigate opportunities for hosting STP trainees.

The biggest challenge to sustaining this program has been identifying host institutions that are willing to share their EH&S expertise with the STP trainees. After attending the STP workshop in 2011 in Puerto Rico, Dr. Al Ribes contacted the Responsible Care Leader at Dow Chemical, Terneuzen, Netherlands, to determine if Dow would be willing to participate in this program. Dow had provided similar learning experiences to fellows from OPCW and was very willing to host two trainees. A team then initiated discussions with COCI to identify the trainees and schedule the training.

In February 2013, two STP trainees from Africa arrived at Dow. Jonathan Babalola, Sub-Dean of Sciences and a Reader in Physical Chemistry, University of Ibadan, Nigeria, had been waiting for a training opportunity for almost 10 years. John Mumbo, Compliance and Enforcement Officer, National Environmental Management Authority, Kenya, had learned about the program while working on a UNIDO funded project on Cleaner Production. Upon their arrival at Dow, they were required to view a safety video and complete a test before they could enter the site.

During the training, John and Jonathan met with a number of EH&S professionals and laboratory staff members who covered topics such as safety equipment, management system requirements, compliance to regulations, emergency preparedness and response, training programs, hazardous materials, strategic planning, process safety, reactive chemicals, and industrial hygiene. Tours were provided of the manufacturing site, as well as R&D laboratories. Throughout the visit, they asked probing questions to understand the underlying objectives of each program, as well as its effectiveness. While the training sessions were lead by EH&S professionals, they also had the opportunity to talk with other employees to understand the safety culture: that each person has a responsibility and a role to play. The trainees learned the expression, "zero accidents, zero injuries, zero excuses".

They each developed a plan of action to be implemented in their own institution upon their return. The actions were classified as immediate, medium-term, or long-term. Here are some highlights:

- Redesign their approach to training with an emphasis on behavioral change and intrinsic values
- Review the environmental impact assessments and audit to prioritize safety
- Improve laboratory safety standards, including installation of safety devices and equipment and guidelines for inspections of laboratories
- Include EH&S in the departmental strategic plan
- Integrate an emergency security services (ESS) within EH&S
- Include remediation of contaminated sites as an activity under rehabilitation of degraded sites
- Develop policies on safety
- Include safety practices into curricula at University level and implement safety education before the first-year practical exam

Jonathan Babalola and John Mumbo Review Laboratory Safety Practices and Equipment at Dow Chemical, Terneuzen, Netherlands

In April 2015, Bayer CropScience, in Research Triangle Park (RTP), North Carolina, hosted Dr. Ahmed Fahmy A.

Youssef, Associate Professor of Chemistry, Cairo University. Dr. Youseff is a professor of analytical chemistry who also works on numerous projects in his home country of Egypt to address problems related to chemical waste management, environmental protection, and air pollution monitoring. His goal was to increase his practical knowledge of environmental process safety management programs.

Dr. Youssef with Bayer CropScience hosts. Left to right: Laura McConnell, Lennie Scott, Bob Lockemer, Ahmed Youssef, Rehan Baig, and Darren Deonarine

In advance of his visit, members of the Bayer CropScience Quality, Health, Safety and Environment (QHSE) team, Patrick Ragan, Rehan Baig, and Lennie Scott, developed a detailed agenda with a variety of training sessions and off-site visits, including a Bayer production facility in West Virginia, a local landfill waste disposal facility, and the chemical waste handling facility at North Carolina State University. Dr. Youssef was invited to attend the Global QHSE North America Spring Community Meeting, where he gave a brief presentation about his work, and he attended the 11th Global Congress on Process Safety in Austin, Texas. He also paid a visit to the IUPAC Secretariat office in RTP.

Overall, the STP was quite positive and beneficial for both the host team and fellows, leading to increased global communication on chemical safety. Dr Youseff's training was financially sponsored by the Civilian Research and Development Fund (CRDF) and the Chemical Security Program (CSP) of the US.

COCI continues to maintain contact and provide support for STP Fellows. Safety Training Program workshops are held in conjunction with each IUPAC General Assembly/World Chemistry Congress (A workshop is being planned for the coming GA in São Paulo). Speakers represent industrial, academic, and governmental institutions. Fellows provide updates on the improvements they have made in their home institutions and within their region or country. Jonathan Babalola has

IUPAC Safety Training Project Fellows 2000-2015

August 2015: Ms. Christine Ashaolu (Nigerian Government Regulatory Agency, Abuja, Nigeria) trained at National Silicates, a PQ Company, Toronto, Canada

April 2015: Prof. Ahmed Youssef (University of Cairo, Egypt) trained at Bayer Crop Science, Research Triangle Park, NC, USA

May 2014: Eng. Noha Zenhom (FEI-ECO, Cairo, Egypt) trained at Woodbridge Group, Mississauga, Toronto Canada

February 2013: Jonathan O Babalola (University of Ibadan, Nigeria) and John O Mumbo (National Environment Management Authority, Kenya) received training at Dow Benelux BV, Terneuzen, The Netherlands

June 2008: Dr. Gursharn Singh Grover (National Chemical Laboratory, India) trained at Novozymes, Denmark

January 2007: Prof. Fabian Benzo (Universidad de la República, Montevideo, Uruguay) and Dr. Godfred Ansah Nyarko (Tema Lube Oil Company Ltd., Ghana) visited Mitsui Chemicals (Japan)

November 2005: Prof. Said Mohamed Mahmoud Bayomi (Mansoura University, Egypt) received training at the facilities of the pharmaceutical company AstraZeneca in the UK

October 2004: Mr. Isiaka O. Bakare (Rubber Research Institute of Nigeria) visited Mitsui Chemicals Co. sites in Japan

October 2003: Ms. Jane B. Nyakang'o (UNIDO Kenya National Cleaner Production Centre) and Ms. Ana Luisa Arocena (CEMPRE Uruguay) trained at the BP Chemicals Technology Center in Naperville, Illinois, USA and the acrylonitrile production plant in Lima, OH, USA

September 2002: Mr. Zhang GuoHong (Sinopec, China) received training at BP Chemicals Inc. USA research facilities in Naperville, IL and production facilities in Lima, OH

August 2002: Mr. Kelvin Khisa (UNIDO Kenya National Cleaner Production Centre) trained at Sankyo Co., Ltd production and research facilities in Japan

June 2002: Mr. Tersoo Charles Gwaza (Shell Petrochemical Development Co, Nigeria) received training at Sasol Chemical Industries, South Africa

August 2000: Prof. Ali El-Emam (Mansoura University, Egypt) trained at Bristol-Myers Squibb in the USA

April 2000: Ms. Esma Toprak (Bogazici University, Turkey) trained at BP Chemicals Inc in Naperville, IL, USA; a side visit was arranged to the Illinois Institute of Technology

shared examples of improvements he drove in Nigeria, including improved waste disposal, safety training and behavior, and emergency response. Several STP Fellows are now collaborating on initiatives to develop Regional Safety Training Centers to expand the reach of this program. The first Regional Safety Training was organized by Professor Fabian Benzo, an STP Fellow from Uruguay. It was held in Spanish at the University of Montevideo in October 2016 (see www.iupac.org/project/2016-021-1-022). A proposal is now being developed to stage a regional STP in India in 2017 and work is starting on regional training in Africa. Efforts like these promise to drive improvements in EH&S practices, policies, and behaviors, and should reduce the number and severity of incidents.

COCI has a list of qualified applicants who are seeking this training. Applicants for the program should be trained scientific or chemistry professionals who are working in industrial, academic, or government institutions. They should have already achieved a position that enables them to drive changes in their organization, so that the benefits of the training can best be realized. A letter of support from their home institution is required. COCI handles the vetting of the applications to ensure that requirements are met. Anyone interested in hosting STP trainees is encouraged to contact COCI.

COCI and the STP Fellows appreciate the support of host companies, trainers, and sponsors of the Safety Training Program. Their dedication and efforts are making a difference and improving environmental, health, and safety practices. Together, we are driving behavioral and cultural changes to achieve the program's vision: zero accidents, zero injuries, and zero excuses.

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For more information and comments, contact COCI chair Bernard West <bernard.west@sympatico.ca>
www.iupac.org/body/022

Bookworm

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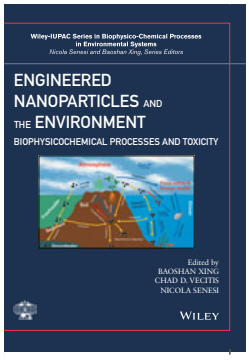
Engineered Nanoparticles and the Environment: Biophysicochemical Processes and Toxicity

Baoshan Xing, Chad D. Vecitis, and Nicola Senesi (Eds)
Wiley 2016, ISBN: 978-1-119-27582-4



Engineered nanoparticles (ENP, 1-100 nm) are found in an increasing number of consumer and food products (such as shampoos, paints, chewing gums) and applications (*e.g.*, biomedical, electronic, industrial, and environmental) due to the rapid development and implementation of nanotechnology. This technology is one of the most promising new research areas of the 21st century and will have dramatic impacts across all scientific fields. Due to their anticipated high-volume production and widespread use, ENP will be unavoidably introduced into the environment during the intentional application, accidental release, and end of life-cycle disposal of ENP-enabled products. For example, ENP have already been reported to enter the environment as a result of ENP-containing paint. Recent toxicological data raises concern over the environmental and health impact of ENP, which will largely be determined by their fate, distribution, and bioavailability. However, there is also a great deal of potential benefit to society and the world in the discovery, synthesis, and application of nanomaterials. There is a need to systematically collect, integrate, and disseminate the latest information, data, and knowledge on all the aspects related to ENP and the environment (*e.g.*, detection, toxicity, transformation, modeling, application). This interdisciplinary book uses a systematic approach, bringing together world-renowned international scientists on the subject matter in order to integrate the latest discoveries and developments in, as well as the future prospects for,

research of ENP in the environment and ecosystems. We envision this book will be useful for the sustainable development of nanotechnology.

There are 22 chapters in this book, divided into three parts. Part I has 5 chapters, focusing on the synthesis, application, detection, and characterization of engineered nanoparticles. Part II has 9 chapters, focusing on the environmental release, fate, distribution, and modeling of engineered nanoparticles. Part III has 8 chapters, focusing on the toxicity and risk assessment of engineered nanoparticles under different scenarios. The combination of these 22 chapters provides a comprehensive overview of the characterization, application, environmental processing, modeling, toxicity, and risk assessment of engineered nanoparticles.

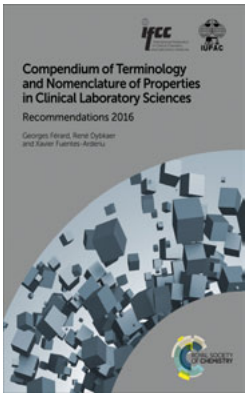
This book is a critical and useful reference book for scientists, engineers, professionals, policy makers, and government regulators who are interested in the biophysico-chemical processes and applications of engineered nanomaterials. This book is also an important addition to the existing literature on the subject matter. Further, this book can be used by undergraduate and graduate students, as well as instructors and professors in environmental, aquatic, soil, agricultural, nano, marine, atmospheric, geological, ecological, biological, and chemical science and engineering. The book chapter authors are recognized as leading authorities in their field of research and each chapter was rigorously peer reviewed, similar to refereed journal articles.

This book is Volume IV of the Wiley-IUPAC series in Biophysico-Chemical Processes in Environmental Systems, and is the outcome of IUPAC project 2011-019-1-600, sponsored by Division VI-Chemistry and the Environment. It was published by Wiley in October 2016 with a total of 484+XIII pages. The book is available in both electronic (ISBN: 9781119275824) and print (ISBN: 9781119275848) versions.

www.wiley.com/WileyCDA/WileyTitle/productCd-1119275822.html
https://iupac.org/project/2011-019-1-600

Compendium of Terminology and Nomenclature of Properties in Clinical Laboratory Sciences

Georges Férard, René Dybkaer, and Xavier Fuentes-Arderiu
RSC 2017, Print ISBN: 978-1-78262-107-2



There has been significant expansion and development in clinical laboratory sciences, particularly in metrological concepts, definitions, and terms, since the previous edition of this —also known as the IUPAC Silver book— was published in 1995. It is of prime importance to standardize laboratory reports for the reliable exchange of patient examination data without loss of meaning or accuracy. New disciplines have appeared and the interrelationships between different disciplines within clinical laboratory sciences demand a common structure and language for data exchange, in the laboratory and with the clinicians, necessitating additional coverage in this book. These new sections are based upon recommendations published by various national, regional, and international bodies, especially IUPAC and IFCC. This book groups and updates the recommendations and will be appropriate for laboratory scientists, medical professionals, and students in this area.

This second edition of the Compendium of Terminology and Nomenclature of Properties in Clinical Laboratory Sciences was discussed in an IFCC and IUPAC joint Working Group: Rene Dybkaer (Frederiksberg); Georges Ferard (Strasbourg, Chair); Francoise Pontet (Paris, co-Chair); Xavier Fuentes-Arderiu (Barcelona); Dongchon Kang (Kyushu); Gilbert Hill (Toronto); Clement Mc Donald (Indianapolis); and Anders J. Thor (Stockholm).

https://iupac.org/project/2007-033-3-700
https://doi.org/10.1039/9781782622451

Isotope-Abundance Variations and Atomic Weights of Selected Elements: 2016 (IUPAC Technical Report)

Tyler B. Coplen and Yesha Shrestha
Pure and Applied Chemistry, 2016
Volume 88, Issue 12, pp. 1203-1224

There are 63 chemical elements that have two or more isotopes that are used to determine their standard atomic weights. The isotopic abundances and atomic weights of these elements can vary in normal materials due to physical and chemical fractionation processes (not due to radioactive decay). These variations are well known for 12 elements (hydrogen, lithium, boron, carbon, nitrogen, oxygen, magnesium, silicon, sulfur, chlorine, bromine, and thallium), and the standard atomic weight of each of these elements is given by IUPAC as an interval with lower and upper bounds. Graphical plots of selected materials and compounds of each of these elements have been published previously. This report provides isotopic abundances, isotope-delta values, and atomic weights for each of the upper and lower bounds of these materials and compounds.

https://doi.org/10.1515/pac-2016-0302

Names and Symbols of the Elements with Atomic Numbers 113, 115, 117 and 118 (IUPAC Recommendations 2016)

Lars Öhrström and Jan Reedijk
Pure and Applied Chemistry, 2016
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A joint IUPAC/IUPAP Working Party (JWP) has confirmed the discovery of the elements with atomic numbers (Z) 113, 115, 117 and 118. In accordance with the 2016 IUPAC guideline for naming new elements, the discoverers were invited to propose names and symbols for the elements. Claims have been assigned to them and the following are proposed: (a) nihonium and symbol Nh, for the element with Z=113, (b) moscovium with the symbol Mc, for the element with Z=115, (c) tennessine with the symbol Ts, for the element with Z=117, and oganesson with the symbol Og, for the element with Z=118. After careful deliberation on these names and symbols, considering the 2016 rules and a public review period, the Inorganic Chemistry Division recommended these proposals for acceptance by the IUPAC Council.

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On the Naming of Recently Discovered Chemical Elements—the 2016 Experience

by Jan Reedijk

In the period of 8 June to 8 November 2016, the "general" public was invited to comment on the draft document in which names and symbols for four new chemical elements were presented. In this short article, I want to sum up a few highlights illustrating that the possibility to comment on the proposed new names was widely used and has been an exciting process.

In the final document on the new names and symbols, [1] we could only acknowledge in general terms the input of so many people, varying from scientist to layman, from school kid to journalist, and from single person up to petitions of over 150 000 signatures. In this article, I would like to present some specific highlights.

According to the current practice, the President of the Inorganic Chemistry Division, in consultation with the members of the Division, considered each comment received during the five months of public review. In addition to regular email correspondence, the Division had the opportunity to debate all pertinent issues during the Division's annual meeting. The process is summarized below.

Reactions from the public

Initially, it appeared that many people and groups of people—in petitions—were proposing alternatives to the names submitted by the discoverers. This resulted from misreading the invitation to comment, or simply not liking the proposed names. Several people did not realize, or were not aware of, the fact that ONLY the discoverers can propose names and symbols; they were also unaware of the fact that the proposed names had to meet specific criteria. [2, 3] So, in responding to proposers of "alternative names", we explained that the right to propose the name of a new element is afforded to the discoverers, largely because of the enormous effort required to produce and verify the existence of a new element. Given that there are few benefits to the discoverers from this sort of science, at the very least

they can be provided the right to propose a name for the new element! This approach is fairly consistent across many areas of science, such as in the discovery of new biological species or astronomical objects.

Some of the proposed names by persons and organisations are nevertheless worth mentioning here, for historic reasons. I have classified them in a few groups:

1. Famous chemists from the past who have no element named after them, for instance Berzelius, Davy, Lavoisier, Levi, Liebig, Moseley and Ramsay. In one case, Levi, the suggestion was even accompanied by an internet petition with over 3000 professional chemists/supporters.
2. Famous musicians, like Lemmy Kilmister and David Bowie, who had passed away recently. An internet petition in favour of "Lemmium" had over 160000 "likes".
3. Famous scientists from ancient civilisations, like Razi, Biruni.
4. More general names like Luciferium, Octarine, named after a mythological concept (with an internet petition of over 50000 "likes"), or in same cases (semi) jokingly proposing names like Taxpayeron, Lazarus, Tattooine.

In addition to comments on the names for the four elements, questions were also received regarding the proper pronunciation of the names of group 17 and group 18, tennessine and oganesson. These questions could not be answered in detail given, for instance, the often-heard differences in pronunciation between American, Australian, and UK English. Additional questions were received on how to convert/translate the name tennessine into other languages and how to derive roots from it, to name their derivatives: many elements of group 17 have truncated names in other languages than English and roots are therefore not always easy to generate. Indeed, unlike elements with a name ending in "ium", the name "tennessine" cannot be automatically transferred into some other languages, since the ending –ine is not kept in these languages and is instead truncated. This was not a problem for chlorine and bromine in the past, but non-straightforward conversions have been used for iodine and astatine in some languages. In the case of tennessine, similar conversion problems and possible solutions have been brought to our attention. Some explanation may be useful; this is given in the next paragraph.

The roots of the names of the halogens are fluere (Latin) and chloros, bromos, and astatos (Greek), which in English have become fluorine, chlorine, bromine, iodine, and astatine, whereas these elements have been given shorter names in many other languages, like cloro in Spanish and Italian, Chlor in German, and chlore in French. Thus, the regular endings of group 17 elements in English are definitely not a rule in all languages. The name Tennessee, on the other hand, derives from Cherokee and the name of the village Tanasi, as explained in the literature. [4] Each language is, of course, independent in performing conversions or translations, but it is hoped that these etymological comments will be of some help when a name is to be produced, *e.g.* in Spanish, German, or French. As a matter of fact, perhaps guidelines from IUPAC could/should be offered when names and roots in non-English languages for tennessine are being asked for. That should help prevent the mistakes made in the past in some languages by incorrectly using, for example, "astatium" for the conversion of astatine.

Argumentation used in the discussion of some received comments

Not all argumentation could be included in the official recommendation for the names and symbols of the 4 new elements published in *Pure and Applied Chemistry*. [1] In fact, a few comments from the public required some discussion within IUPAC. This is particularly the case for comments on tennessine, despite the fact that the name meets all criteria. However, for this element only two straightforward 2-letter symbols were available, as Ti is already used for titanium and Te for tellurium. One was Tn. However, this symbol has been used for Thoron for decades, and is up till now still in use, in particular in the field of the *Journal of Environmental Radioactivity*, so this formerly agreed IUPAC symbol could not be used. The second and only remaining possibility for the symbol was "Ts", which as such is perfect, but as some respondents indicated, is also one of the two commonly used abbreviations for the tosyl (4-methylphenyl)sulfonyl, or p-toluenesulfonyl) group. The abbreviation Ts is, for example, mentioned in a 1996 IUPAC recommendation for carbohydrates. [5] The other abbreviation in use for tosyl is Tos, which was introduced even earlier, and used in IUPAC recommendations for nucleic acid abbreviations [6] and for amino acids. [7] The Handbook of Common Acronyms used in Synthetic Chemistry [8] has for several years mentioned both Ts and Tos as full equivalents.

Given the fact that almost any abbreviation or symbol of two letters has multiple meanings, and as this occurs often inside chemistry itself (*e.g.*, Ac as the symbol

for actinium and the abbreviations for acetyl and likewise Pr for praseodymium and propyl), the conclusion has been drawn that the context in which the element symbols are used will always make clear what the meaning is. Therefore, the chances for any confusion with abbreviations will be extremely small. The alternative, to ask the discoverers to suggest a completely new name and symbol, was considered unrealistic and undesired, and even impolite.

The Inorganic Chemistry Division was extremely pleased to receive so many different reactions from all kinds of people, groups, and countries, illustrating the great interest worldwide in the Periodic Table. It was good and pleasing to receive many reactions of agreement, but also responses that were more critical. Each respondent has received an acknowledgement of receipt, sometimes explaining the current protocol. After the final decision by IUPAC, they also received a final summary of the kind of reactions I have reported above.

Examples of Interested Youngsters

A brief summary from what two school teachers wrote is worth mentioning here. One of them wrote: "My classes read about the naming of the four newest elements to be added to the periodic table and are excited to participate in the public review process. We consider this opportunity to be a once-in-a-lifetime event. We acknowledge that the scientists that discovered the elements and the scientists at IUPAC are far more qualified to offer significant input on the names of the elements, but we wanted to convey our excitement to be part of the public review portion of the naming process. Thank you for allowing my students to contribute."

A second, most heart-warming reaction came from another school teacher, whose class of 75 students wrote individual essays. The teacher asked the students to share the name they would choose if they were allowed to name an element, and to comment on at least two of the four newly proposed names. All 75 essays were scanned, merged, and submitted as a (very large) pdf file. This has delivered me a delightful weekend's reading. Needless to say, I was pleased to learn that many of the students mentioned how proud they were to have been able to participate in these discussions. Congratulations also to their teachers!

Final remarks and Future

In closing, I want to spend some words on the future, dealing with the discovery, claiming, recognition, and naming of newly discovered elements after 2016. In the research field where the new elements are generated, no doubt nowadays the nuclear physicists do the final discoveries. However, as nicely illustrated by the discovery story of tennessine, the importance of the mutual dependence of chemistry and physics is clearly visible and emphasized. Beautiful and painstaking physics is preceded by equally beautiful and painstaking chemistry to synthesize and separate the unique target materials. So, while discovery and claiming is done in the laboratories of physicists, collaboration with chemists preparing and purifying target materials is often necessary, and thus the recognition of new elements needs to be authorized jointly by IUPAP and IUPAC. I look forward to seeing a new joint panel appointed in the not too distant future. The Periodic Table has 7 periods full of known elements. Up to the 8th period!

Finally a sentence about the naming process. Perhaps now is the time to consider offering the discoverers the many suggested names generated in the 2016 process (and from earlier/later processes) as options to consider. They could judge whether appropriate names are amongst those suggested and determine how they can serve as proposals to future discoverers. As the Periodic Table is a brand of IUPAC, the checking of names and symbols will remain an IUPAC duty, but providing a database of suggestions to those who may propose names would do no harm.

References:

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2. W. H. Koppenol, J. Corish, J. Garcia-Martinez, J. Meija, and J. Reedijk. *Pure Appl. Chem*. **88**:401-405 (2016). DOI: 10.1515/pac-2015-0802
3. J. Corish. *Chem. Int*. **38**(2):9-11 (2016)
4. Tennessee, in Encyclopaedia Britannica, 2016
5. Joint IUPAC-IUBMB Commission on Biochemical Nomenclature, Nomenclature of Carbohydrates, *Pure Appl. Chem*. **68**:1919-2008 (1996)
6. Abbreviations and Symbols for Nucleic Acids, Polynucleotides and Their Constituents, Joint IUPAC-IUBMB Commission on Biochemical Nomenclature; (1974)
7. Nomenclature and Symbolism for Amino Acids and Peptides Joint IUPAC-IUB Commission on Biochemical Nomenclature (Recommendations 1983), *Pure Appl. Chem.* **56**:595-624 (1984)
8. www.cheminform.com/acronyms

Jan Reedijk <Reedijk@chem.leidenuniv.nl; orcid.org/0000-0002-6739-8514> is President of the Inorganic Chemistry Division of IUPAC since January 2014. He is a retired Professor of Chemistry from the Leiden Institute of Chemistry, Leiden University, The Netherlands.

IUPAC Provisional Recommendations

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

Terminology of Bioanalytical Methods

Recommendations are given concerning the terminology for methods of bioanalytical chemistry. With respect to dynamic development, particularly in the analysis and investigation of biomacromolecules, terms related to bioanalytical samples, enzymatic methods, immunoanalytical methods, methods used in genomics and nucleic acid analysis, proteomics, metabolomics, glycomics, lipidomics, and biomolecules interaction studies are introduced.

Comments by 30 April 2017
Corresponding author: Jan Labuda <jan.labuda@stuba.sk>
https://iupac.org/project/2011-047-1-500

Nomenclature and Terminology for Dendrimers with Regular Dendrons and for Hyperbranched Polymers

This document provides recommendations for (i) definitions of terms related to dendrimers with regular dendrons and to hyperbranched polymers and (ii) nomenclature for naming these compounds on the basis of structure-based nomenclature for regular and irregular organic polymers, including adjustments for specifying dendritic and hyperbranched macromolecular structures. These recommendations and the examples given deal with organic chemical structures only, but the general principles described in this document can be applied to inorganic and to hybrid organic-inorganic dendrimers and hyperbranched macromolecules as well.

Comments by 31 May 2017
Corresponding author: Alain Fradet <alain.fradet@upmc.fr>
https://iupac.org/project/2001-081-1-800

Definition of the Mole

In 2011, the General Conference on Weights and Measures (CGPM) noted the intention of the International Committee of Weights and Measures (CIPM) to revise the entire International System of Units (SI) by linking all seven base units to seven fundamental physical constants. Of particular interest to chemists, new definitions for the kilogram and the mole have been proposed. A recent IUPAC Technical Report [1] discussed these new definitions in relation to the immediate consequences for the chemical community. This IUPAC Recommendation on the preferred definition of the mole follows from this Technical Report. It supports a definition of the mole based on a specified number of elementary entities in contrast to the present 1971 definition.

1. Marquardt, R., J. Meija, Z. Mester, M. Towns, R. Weir, R. Davis, and J. Stohner (2017): "A critical review of the proposed definitions of fundamental chemical quantities and their impact on chemical communities (IUPAC Technical Report)," *Pure Appl. Chem.* (in press); http://dx.doi.org/10.1515/pac-2016-0808

Comments by 30 June 2017
Corresponding author: Jürgen Stohner <sthj@zhaw.ch>
https://iupac.org/project/2013-048-1-100

Terminology of Separation Methods

Recommendations are given concerning the terminology of methods of separation in analytical chemistry, including chromatography, electromigration techniques, and field-flow fractionation and related techniques. Most of the terms have been drawn from papers published in *Pure and Applied Chemistry*. A number of new sections and terms have been included, using terms proposed as definitions in the literature. To complete these areas a number of new terms have been proposed for acceptance.

The capitalization of previously accepted terms has been corrected to bring them up to date with current practice and terms have also been amended in certain cases to link the definitions specifically to chromatography "(in chromatography)". In a few cases, minor changes have been made to include both LC and GC in a term, or to reflect significant changes in practice, such as the universal change from chart recorders to electronic integration.

This Recommendation will be the basis for a chapter in the forthcoming fourth edition of the Orange Book (https://iupac.org/project/2012-005-1-500).

Comments by 30 June 2017
Corresponding Author: Tatiana Maryutina <tatiana@maryutina.com>
https://iupac.org/project/2011-046-1-500

IUPAC Standards and Recommendations*

by Ron Weir

In 1919, the year of the birth of IUPAC, international science was in its infancy. Modern instantaneous communication as we know it had not been born, but a number of scientists foresaw the need for an international organisation with a focus on chemistry to serve as a catalyst, to promote standards, and to facilitate clear, unambiguous communication throughout the world in the rapidly growing discipline. The early founders of the organisation could not have foreseen the explosion of knowledge and instant communication networks available today. However, they did understand the serious ramifications of not having clear, unambiguous communication in science and engineering.

For those individuals who cling to the notion that historic national practices trump safety, practicality, and international trade, please read the following.

Definitions of terms, standard values of quantities, procedures, rules for naming compounds and materials, standardised units, names and properties of elements in the periodic table—all constitute standards that facilitate communication and set international norms. These IUPAC standards and recommendations are internationally binding for scientists in industry and academia, patent lawyers, toxicologists, environmental scientists, legislation, and others working in or for the chemical enterprise. In this column we briefly review the reasons why standards are necessary, how they are created, and how they are updated as new information becomes available.

Q. What purpose is served by the creation of standards and recommendations?

There is more than a single purpose fulfilled by the creation of IUPAC standards and formal Recommendations. All are relevant to society. These are (i) saving resources, (ii) saving money, and (iii) saving lives. Below are three illustrative examples.

Example 1: The American NASA Mars Climate Orbiter in 1999. NASA lost the orbiter due to an incorrect conversion between metric and English (USA) units. While the financial loss amounted to about 150 million US dollars, a price cannot be placed on the loss of scientific data and associated work.

Example 2: Construction of the Laufenburg Bridge over the Rhine between Switzerland and Germany in 2003. Germany used the North Sea level as its standard reference while Switzerland used the Mediterranean Sea as its reference level. The difference in levels is 27 cm. To make matters worse, when the adjustment was made, the signs were applied incorrectly. The total difference applied to the two ends of the bridge was 54 cm, resulting in a costly error.

Example 3: Toxicology and health care. In a patient, blood glucose levels were read on the glucose meter (made in the USA) as 42 $mmol{\cdot}L^{-1}$ (not S.I. approved units) that was assumed by staff to be 42 $mg{\cdot}dL^{-1}$ (approved S.I. units), when it is in fact equivalent to 758 $mg{\cdot}dL^{-1}$! The drastic ramification was a diagnosis of hypoglycaemia, rather than hyperglycemia, nearly costing the patient his life. The problem arose because the glucose meter used did not conform to IUPAC international standards. The USA is one of a few hold-out countries against adopting the metric or S.I. system, even in medical equipment. The International Committee of Medical Journal Editors has demanded that all measurements associated with medicine be reported in metric units, with temperatures given in degrees Celsius. This example emphasises the importance of the adoption of an internationally agreed-upon standard scientific language around the world. For details, see the editorial "S.I. for Dummies" by Dr. Tomaszewski in the *Journal of Medical Toxicology*. [1]

Q. How are the standards and recommendations developed? What level of global consensus is achieved and how is it achieved? Are other scientific bodies involved? What about the general public?

Experts in the various fields of science throughout the world, working together in the IUPAC Divisions and Commissions, develop standards and recommendations. Global consensus is reached through partici-

* An earlier version of this document was first prepared as an introduction to the *IUPAC Standards Online* database developed by DeGruyter (publisher of *Pure and Applied Chemistry* (*PAC*) and *Chemistry International* (*CI*)). The *IUPAC Standard Online* database follows a compilation of the standards and recommendations published by IUPAC in *PAC*. (www.degruyter.com/view/db/iupac).

pation by international representatives serving on the IUPAC Divisions and Commissions; representatives from the IUPAC National Adhering Organisations (including national chemical societies), representatives from six other scientific organisations serving on IUPAC (the International Union of Crystallography, the International Union of Nutritional Science, the International Union of Pure and Applied Physics, the International Union of Biochemistry and Molecular Biology, the International Bureau of Weights and Measures, and the International Union of Pharmacology), and through a public review period of several months.

Following this extensive consultation, approved feedback, and approved scientific review, it is assumed that each respective community supports the consensus.

The general public is not usually directly involved aside from the public review of Provisional Recommendations, during which time the public can submit comments and suggestions.

National newspaper articles often highlight relevant IUPAC work, such as the discovery of new elements and how they are named. A case in point is the recent announcement by IUPAC of the discovery and naming of four new elements in the periodic table.

Q. What is the usual timeline from start to finish?

After extensive consultation as noted above, an IUPAC Division approves the final text of the proposed standard or recommendation and the manuscript is sent to the IUPAC Interdivisional Committee on Terminology, Nomenclature and Symbols (ICTNS) for further review. In the case of formal Recommendations, the manuscript is posted publically for five months to invite and encourage comments from the general public. In parallel, the manuscript is sent to as many as twenty-five additional expert reviewers. The time to publication in the IUPAC journal *Pure and Applied Chemistry* (*PAC*) is about twenty-four months.

In the case of a Technical Report, which is not a policy document of IUPAC but rather a report on the subject of a specific study, such as critical assessments of methods and techniques, the total time elapsed between Division approval and ICTNS review is about fifteen months. For any changes to the International System of Units (S.I.) itself, the International Bureau of Weights and Measures (BIPM) and its hierarchical structure outside of IUPAC may take several years to achieve consensus. A current example is the ongoing discussion to realign the definition of the mole.

Q. How are the Standards and Recommendations used and valued?

The guidelines for good practice with respect to nomenclature, terminology, units, and symbols are embodied in the IUPAC Green Book, along with other IUPAC Colour Books (see www.iupac.org/what-we-do/books/color-books/). In general, the vast majority of scientists and most scientific journals adhere to the IUPAC Recommendations for international practice. There are some exceptions, usually associated with individuals who cannot adjust to change and with some countries whose political history appears to shun international consensus. The potential impact of not following the standards and recommendations was noted earlier.

In terms of value, a number of peer-reviewed journals will only accept papers that follow IUPAC policy. In addition, UNESCO and EU Customs Union recognise the IUPAC system as their official policy.

Q. How often are the Standards and Recommendations updated?

There is no single simple answer. Whenever an IUPAC Division or Commission believes that an update is required to a Recommendation or a Technical Report, then the changes are made *via* the process described above. As an example, the atomic masses of the elements are updated every one or two years. However, the frequency of the discovery of a new element is rare, but when a discovery is verified, such as was announced at the end of 2015, the update is put in place. For the Colour Books, because sophisticated work is involved, the updates may be done at intervals of five or six years, or even longer.

Q. Other thoughts on what should be communicated?

All the work of IUPAC is done, almost entirely on a volunteer basis, by more than a thousand scientists from around the world, who serve on IUPAC Divisions, Commissions, Standing Committees, and Task Groups.

Reference

1. Tomaszewski, C. *J. Med. Toxicol.* **3**(3):87-88. 2007. http://doi.org/10.1007/BF03160915

Ron Weir <weir-r@rmc.ca> is Chair of the Interdivisional Committee on Terminology, Nomenclature and Symbols (ICTNS) of IUPAC and an editor of *Pure and Applied Chemistry.*

Chemical Industry of Sustainable Development

by Zaiku Xie

The IUPAC Committee on Chemistry and Industry (COCI) has held regional workshops in the past. The 5th and latest was held in Beijing on 12 September 2016. The workshop was planned and hosted by Dr. Zaiku Xie and members of his team. Dr. Xie is Director of the Science & Technology Department at SINOPEC and a Titular Member of COCI. COCI members are grateful to Dr. Xie and SINOPEC for hosting an excellent Workshop. The following is a summary of the meeting, which was well attended and praised by the attendees in the discussion session at the end of the meeting.

We were also honoured to have the Vice-President of IUPAC, Professor Qi-Feng Zhouof Peking University, to open the workshop. He participated throughout the day and entertained us at the Peking Duck banquet, which was kindly hosted by SINOPEC.

The COCI Regional Workshop in Beijing was the 5th such workshop organised by members of the committee and held in different global regions and with relevant topical agendas. This workshop brought together speakers from China, Korea, India, and Switzerland. The focus of the meeting was Sustainability and how industry is working towards this goal.

In addition to Prof. Qi-Feng Zhou, the Workshop was opened with welcoming remarks by Dr. Zaiku Xie, the host of the Workshop, and Dr. Bernard West, the Chair of COCI. There were also several local speakers, as well as members of COCI from Canada, USA/Netherlands, Japan, Belgium, Switzerland, Korea, and Russia.

The workshop was divided into three sessions, with Q&A, including the following presentations. A fourth open session was held to enable broader questions.

- Sustainable Development of Refining and Chemical Industry in China, by Dingyi Hong
- Process Intensification: Higee Technology as an Example, by Jian-Feng Chen
- Vehicle Fuel Upgrading Technologies in China, by Mingfeng Li
- Methanol to Olefins Technologies Developed by SINOPEC, by Jiawei Teng
- Development and Prospect of Biomass Energy, by Kai Qiao
- Status of Safety, Environment and Health in Indian Chemical Industry, by Dr. B. Saha
- Responsible Care in China, by Housheng Xu
- Safety Engineering Technology and Response Care for petrochemical industry, by Wei Xu

The agenda and summaries of the presentations, and discussion points are available from the COCI webpage.

www.iupac.org/body/022 or www.iupac.org/project/ 2016-020-1-022

Bioinspired and Biobased Chemistry & Materials

by Frédéric Guittard

The 3rd International Conference on Bioinspired and Biobased Chemistry & Materials (NICE-2016) took place in Nice, France, 16-19 October 2016 and was co-sponsored by IUPAC, MRS, and E-MRS. The meeting took stock of the current state of biobased and bioinspired chemistry and materials. This meeting was the third in the series, following successful meetings held on a similar topic in 2014 and 2012. This edition was also supported by most of the relevant organizations in the field of biomimetics, such as Biomimicry Germany, Biomimicry Switzerland, Biomimicry UK, Institut Biomimetisme Francophone, Biomimicry.be, and CEEBIOS. The acronym of the conference is N.I.C.E: "Nature Inspires, Chemistry Engineers" and the aim of the conference is to share new developments in the growing field of bionspired chemistry and materials. Among the topics discussed were: green chemistry, nanomaterials, renewable energy, stimuli-responsive, adhesive/anti-adhesive, functional polymers, and biobased chemistry and materials, grouped in three

sessions: SmarTech, NanoTech and BioTech.

The opening session started on Sunday, 16 October at the Mediterranean University Center, a fascinating old structure on the Promenade des Anglais. The lecture hall, including theatre-style seating with a magnificent ceiling, hosted the plenary session. The conference opened with short welcoming remarks by the chairman of the conference, Prof. F. Guittard, who also presented an overview of IUPAC activities. The first part of the session focused on the theme, "Biomimetics and Innovation: how learning from nature can solve technological problems in a more sustainable way". This topic was illustrated by Dr. Kristina Wanieeck (Germany) and Dr. Prateep Beed (Germany). The session continued after the coffee break with three compelling plenary talks delivered by Prof. Bushan (USA) on superhydrophobic, self-cleaning and low drag surfaces; Prof. Messersmith (USA) on bioinspired coating from polyphenols; and Prof. Sanchez (France) on bionspired approaches to advanced nanostructured materials.

The conference continued from 17-19 October at the Negresco Hotel, the legendary palace overlooking the Promenade des Anglais. The conference included 5 parallel sessions during 3 days, with over 55 keynote presentations (25 minutes), 164 oral presentations (15 minutes), and 106 poster presentations. The conference welcomed over 400 attendees, who came from 48 countries and from all continents. This edition also included two workshops on how to implement biomimetics in R&D strategies and opportunities for polymers and biobased materials. These workshops were organized in collaboration with the European Center of Excellence in Biomimicry of Senlis (CEEBIOS) and the competitiveness clusters Industries & Agro-Resources (IAR) and TRIMATEC.

The conference social event consisted of a sightseeing tour of Monaco, the smallest country in the world after the Vatican State. We first visited the old town, with the Prince's Palace, the institutional building, the renowned Oceanographic Museum, the Cathedral, and more. We also strolled through the surroundings of the Casino, a mythical place with fabulous architecture, the Café de Paris, the gardens, and the fountains. The visit ended with a dinner at the A'Trego restaurant in Cap D'Ail, at the Monaco border, a trendy restaurant on the sea designed by Philippe Starck.

International Carbohydrate Symposium

by Al D. French

The 28th International Carbohydrate Symposium (ICS, www.ics-2016.org) was held in New Orleans, Louisiana, USA, 17-21 July 2016. The meeting followed a traditional format, starting on Sunday afternoon with the technical program closing on Thursday evening. The technical program was followed by a banquet at Mardi Gras World, a business that creates the floats used in Mardi Gras parades, that educates about this major event in New Orleans, and that provides a venue for receptions and banquets. With the excep-

tion of the banquet, a Tuesday evening Cultural Night held in the nearby St. Louis Cathedral, and a dinner for the country representatives to the International Carbohydrate Organization at a nearby restaurant, all of the meeting was held in the Marriott Hotel. As usual, Wednesday afternoon was free from technical programming, giving the participants time for tours of various destinations in and around New Orleans. The social program included a Sunday evening reception, while the Cultural Night included a jazz quartet and gospel choir. The banquet also included a jazz trio.

The meeting had the endorsement of IUPAC and the sponsorship of the American Chemical Society's Division of Carbohydrate Chemistry and its Division of Cellulose and Renewable Materials, as well as its Louisiana Section. Sponsorship was also received from a number of commercial and university interests.

The meeting was organized under the auspices of the U.S. Advisory Committee for International Carbohydrate Symposia, with membership from the above two ACS Divisions. This committee is the designated organization in the USA to determine the location of ICS. Although the ICS Scientific Committee was otherwise dominated by members from the Carbohydrate Division, the Program Chair, Dr. Sheila Murphy, was the then-current chair of the Cellulose Division, while the Meeting Chair, Dr. Alfred French, has served as Chair of both Divisions at different times. The Scientific Committee was very involved in the selection of Plenary, Keynote, and Contributed Oral Lectures. The functions of registration, receiving abstracts, contract negotiation, etc. were provided by the American Chemical Society's Conference Management Services.

The conference's 505 attendees came from 39 different countries, with the largest contingent from the USA and the second largest from Japan. Visa problems were few in number and caused by very late application.

The program included three award addresses with presentations and a surprise award. The International Carbohydrate Organization's $25,000 R. L. Whistler Award was presented to Benjamin Davis of Oxford University and its Young Researcher Award was presented to Benjamin Swarts of Central Michigan University.

Ben Davis spoke on "Sugars and Proteins", delineating mechanisms of carbohydrate processing systems and their ligands to provide an understanding of their fundamental role in Biology and Immunology, as well as the use of molecules to modulate and manipulate such processes, with a strong associated potential for diagnosis, therapy, and application and interven-

Benjamin G. Davis (left), Oxford University, is presented with the R.L. Whistler Award in Carbohydrate Chemistry by N. Jayaraman, President of the International Carbohydrate Organization. All photos in this report by Michael Santiago Cintrón

Benjamin Swarts (left), Central Michigan University, winner of the ICO Young Researcher Award, with Zbigniew Witczak, incoming President, International Carbohydrate Organization

Left to Right: Dr. Koichi Kato, National Institutes of Natural Sciences, Japan; Serge Perez, former Scientific Director of the European Synchrotron Radiation Facility; Pamela Marino, National Institutes of Health, and Geert-Jan Boons, winner of the Claude S. Hudson Award

Carolyn Bertozzi, Stanford University, giving the Opening Plenary Lecture of the Symposium

From left: Victoria Smith, Angelika Trujillo, and Jessica Causey, Lindenwood University, with H.N. Cheng, USDA, presenting a Poster Award

tion in medicine and other biotechnologies. In the final minutes, he described the possibility that the application of trehalose could help to substantially increase agricultural production.

Ben Swarts' title was "Marking the mycomembrane: Chemical tools for studying and targeting glycolipids of the mycobacterial outer membrane." The lecture focused on the development and applications of probes based on trehalose, a disaccharide that is central to mycomembrane biosynthesis but absent from humans. Mycomembranes are composed of arrays of distinctive glycolipids, including the trehalose- and arabinogalactan-linked mycolates that are important to mycobacterial physiology and pathogenesis. The award was sponsored by TCI America.

The Carbohydrate Division presented its Claude S. Hudson Award to Geert-Jan Boons, who described "An integrated approach to uncover ligands for heparan sulfate binding proteins". The methodology has been employed to identify ligands for the ROBO-1, a protein involved in cell signaling and development. Furthermore, the synthetic HSoligosaccharides have been used for the development of a microarray and screening efforts have uncovered novel aspect of heparin sulfate-protein binding.

Megazyme's Bruce Stone Award for Excellence in Plant Polysaccharide Biochemistry went to Harry Brumer, University of British Columbia. The Bruce Stone Award is presented as a surprise at appropriate international scientific conferences, in this case right after the contributed lecture "The evolution of carbohydrate-active enzyme specificity in genomes." Brumer covered Glycoside Hydrolase family 16 (GH16) which comprises a large diverse group of enzyme specificities encoded by microbial and plant genomes. The specific biological role(s) of GH16 members remains enigmatic, but the present biochemical and structural characterization provides new insight into plant cell wall enzyme evolution, which will continue to inform genomic analyses and functional studies across species.

The eight plenary lectures and their titles were:

- Carolyn R. Bertozzi, "Glycocalyx engineering toward probing cancer glycome evolution"
- James C. Paulson, "Sialic acids as determinants of self"
- Muthiah Manoharan, "GalNAc-conjugated oligonucleotides as a new paradigm in RNAi therapeutics for human diseases"
- Soledad Penadés, "Glycans and glyconanotechnology"
- Koichi Kato, "Structural views of glycan-dependent determination of glycoprotein fates in cells"
- Stephen Withers, "Accessing new and improved CAZymes through metagenomics, synthesis and directed evolution"
- Vincent Bulone, "A journey into the world of Eukaryotic cell walls: structure and biosynthesis of essential polysaccharides"
- Bruce Hamaker, "Carbohydrate quality and how the concept may relate to healthier foods."

The 32 invited keynote lectures headlined most of the five parallel sessions, which were completed by 203 contributed oral papers. A wide range of topics were covered in both the plenary lectures and oral papers. There were 200 posters on display throughout the meeting in the same area as the exhibits and coffee breaks. Poster prizes were awarded based on voting by meeting participants. Interest in the sessions was high, despite the location of the meeting at the edge of the French Quarter, a famous entertainment district.

There were several innovations at this meeting, with excellent participation. A special Sunday morn-

ing panel discussion on Directions in Glycoscience was presented. It was chaired by Geert-Jan Boons (University of Georgia), with panelists Pamela Marino, NIH (USA); Serge Perez, European Union ; and Koichi Kato, National Institutes of Natural Sciences (Japan). A session on new technology for characterization of carbohydrates was presented by representatives of instrument manufacturers. The sustainability of processes and products at DuPont were described in another organized session. Both of those sessions were keynoted by university faculty members, however. The program was available in printed form, except for the abstracts of the contributed papers, which were available in the full program presented in various electronic formats, including a smart device app.

Nikolay Nifantiev and Amelia Rauter have volunteered to shepherd the various lectures to publication in *Pure and Applied Chemistry*. Peer review is currently underway. The next International Carbohydrate Symposium XXIX ICS (2018) will be held in Lisbon, Portugal, 15-19 July 2018, organized by Professor A. Rauter.

Validation of Test Methods, Human Errors and Measurement Uncertainty of Results

by Ilya Kuselman

The 3rd biannual international IUPAC/CITAC workshop on quality and metrology of chemical analytical results, organized with the participation of the Israel Analytical Chemistry Society (IACS) and the Israel Laboratory Accreditation Authority (ISRAC), was held 23 January 2017, in Kfar Maccabiah, Israel. The event was sponsored by Sigma-Aldrich Corporation (now a part of Merck) and arranged by Bioforum Ltd. Reports on the previous two workshops are available in *Chemistry International*. [1, 2]

The present workshop, titled, "Validation of Test Methods, Human Errors and Measurement Uncertainty of Results," was planned as a milestone of IUPAC project 2016-007-1-500. Validation of test (chemical analytical) methods is one of basic requirements for the competence of testing and calibration laboratories (ISO/IEC 17025) [3] and reference measurement laboratories in laboratory medicine (ISO 15195). [4] The same is required by national regulators, such as the U.S. Food and Drug Administration, the UK Medicines and Healthcare products Regulatory Agency, and others. There are also a number of guidelines in different industries and chemical analytical societies adapting these requirements for specific purposes and laboratories. The main aim of the workshop was to facilitate the discussion of the experience of chemists-analysts, metrologists, and quality specialists in method validation in pharmaceutical industry, food analysis, environmental analysis, and other fields. This discussion included the following topics:

- use of results of human error study at validation of an analytical method;
- evaluation of measurement uncertainty of the test (analytical) results as a part of the method validation task;
- evaluation of probabilities of false decisions at conformity assessment of test results obtained by the method under validation.

Opening remarks were given by Dr. Ilya Kuselman, Independent Consultant on Metrology, Israel, Chair of the Workshop International Advisory Committee. Dr. Bertil Magnusson, SP Technical Research Institute of Sweden, then delivered the keynote lecture "The fitness for purpose of analytical methods: a laboratory method validation and related topics", explaining the Eurachem guide. [5] Mr. Ilan Landsman, ISRAC, Israel, informed the workshop participants in his lecture about changes in requirements to method validation and verification at accreditation of measurement and testing laboratories in the new upcoming issue of ISO/IEC 17025, under voting now. The next lecture was on setting and using target uncertainty in chemical measurement by Prof. Ricardo J.N.B. da Silva, University of Lisbon, Portugal. It was dedicated to understanding the key concept of method validation "fit for purpose" or 'fit for intended use" in terms of measurement uncertainty and its target value, as in the Eurachem/CITAC guide. [6] Evaluation of probabilities of false decisions (risks) in conformity assessment of test results caused by measurement uncertainty was the subject of the lecture of Dr. Francesca Pennecchi, Istituto Nazionale di Ricerca Metrologica (INRIM), Italy. This lecture, based on the guidelines of JCGM 106, [7] Eurachem/CITAC, [8] and IUPAC/CITAC, [9] helped the participants to understand the metrological and mathematical background necessary for an evaluation of the risks. Dr. Pennecchi also announced the IUPAC task team's lecture on evaluating total risk of false decisions on conformity of a multicomponent material at

A group of the lecturers in the Baha'i Gardens, Haifa. From left to right: Dr. Mikhail Zayats, Dr. Ilya Kuselman, Dr. Bertil Magnusson, Dr. Francesca Pennecchi. Mr. Ron Sinai (our local tour guide), Dr. Michela Sega, Prof. Ricardo J.N.B. da Silva, Dr. Markus Obkircher and Prof. Emil Bashkansky.

the Isranalytica conference. [10]

In the lecture "Human error study as a part of method validation task", Dr. Kuselman proposed to use a method validation mapping possible human error scenarios according to the IUPAC/CITAC guide. [11] Results of such a study can be helpful in the correct formulation of the measurement uncertainty budget and the improvement of the standard operating procedure, as well as for training (how to avoid the errors) and for supervision. The map of the error scenarios, included in the validation report, may also be useful as a check list for prior assessment of an analyst before assigning the task, etc. Ms. Karen Ginsbury, PCI Pharmaceutical Consulting, Israel, talked in her lecture about the practical applications of risk management to analytical testing, paying attention mostly to human errors. She said that error prevention in analytical methods is possible by 1) investing in education and improving the technical writing skills of analytical personnel responsible for writing methods; 2) performing robust method validation after formal risk assessment; 3) monitoring the risk of method performance using control charts and continued methods (process) verification; 4) implementing corrective and preventive actions (CAPA), auditing, oversight, and feedback as risk communication; and 5) engaging management review for risk review and risk assessment updates.

After these lectures, Dr. Michela Sega, INRIM, Italy, moderated the round-table discussion, "Are there relationships between method validation, human errors and estimation of measurement uncertainty?" Dr. Kuselman presented a question on the treatment of bias for measurement uncertainty evaluation in legal metrology. In the recommendations of the International Organization for Legal Metrology (*e.g.*, OIML R111-1 [12] and OIML R126 [13]), bias is limited by comparison with 'maximum permissible error'. However, in addition, it is taken into account as a part of measurement uncertainty at conformity assessment of a measurement/test result, compared with the nominal value, *e.g.*, the weight or the alcohol content in a driver's breath relative to the national law. Dr. Magnusson supposed that in this way the level of confidence of the measurement/test results for legal metrology purposes is larger than the usual 95 %. Dr. Markus Obkircher, Merck, Switzerland, discussed the role of certified reference materials (CRMs) for bias evaluation at method validation, and described briefly the Sigma-Aldrich (Merck) activity in the field of CRMs.

The second half of the workshop day started with a lecture by Prof. Emil Bashkansky, ORT Braude College, Israel. This lecture was dedicated to the validation of qualitative methods: evaluation of repeatability and reproducibility. The applications of statistical methods, such as "Categorical Analysis of Variance" (CATANOVA) and "Ordinal Analysis of Variance" (ORDANOVA), to the analysis of test results of nominal and ordinal properties were discussed. A study of freshwater cultured pearls colour test results was demonstrated as an example.

Dr. Anneli Kruve, University of Tartu, Estonia, talked about handling different matrices in the validation of analytical methods based on LC/MS. Dr. Shulamit Levin, Waters (TC), Israel, reported on the use of peak purity and spectral matching during the validation of LC methods. The topic of the lecture by Dr. Bianca Avramovitch, Teva Pharmaceutical Industries Ltd., Israel, was "Analytical quality by design (AQbD) in practice: risk assessment based on failure mode and effects analysis (FMEA) methodology, applied for complex sample preparations and chromatographic impurities separation". As at the previous workshop, Dr. Orna Dreazen, Nextar Chempharma Solutions Ltd, Israel, summarized the day, asking the workshop participants in her lecture, "Can the theory (of method validation) work in reality?" Dr. Dreazen said that her experience in pharmaceutical industry indicates a number of problems. Validation design is affected by practical considerations, such as the availability of samples and their cost, the duration of the study, etc. Validation study may often detect imprecision, inaccuracy, requiring a return to the method development stage. Thus, it is important to understand that method validation is not a routine task.

The round-table discussion, "How can validation be planned to provide a method user with maximum information?" was moderated by Dr. Raphael Bar, BR Consulting, Israel. Dr. Kuselman informed the participants about method performance criteria in recently published AOAC International Guidelines. [14] Dr. Hellmuth Broda, PerkinElmer, Switzerland, reported on novel services of his company for analytical method validation and other method lifecycle activities. Dr. Mikhail Zayats, Institute of Plant Protection, Belarus, discussed challenges in the validation of a GC method.

More details about the workshop and presentations in pdf format are available at http://bioforumconf.com/satellite-event2017.

On the two days following the conference, 24-25 January, workshop participants took part in the Isranalytica 2017 Conference and Exhibition. A summary of these events is available at www.isranalytica.org.il.

www.iupac.org/project/2016-007-1-500

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Dr. Ilya Kuselman <ilya.kuselman@gmail.com> is a member of the IUPAC Interdivisional Working Party on Harmonization of Quality Assurance.

Chemistry in a Multidisciplinary, Interdisciplinary World

World Chemistry Leadership Meeting 2017
49th IUPAC General Assembly
7-14 July 2017, São Paulo, Brazil

Chemistry is an essential element of modern society, providing vital solutions in a sustainable fashion to such basic societal needs as food, energy, and water. Chemistry enables solutions in healthcare that detect and cure disease and will do so increasingly. Even the most sophisticated forms of computation and communication depend on chemistry to provide its materials and devices. At the same time, although chemistry has never been more important to so many societal needs, there is an air of uncertainty regarding future steps the discipline must take. Palermo, in her report on the future of chemistry for RSC, emphasizes the need for an even greater role by chemists in solving challenges of significant societal need. [1] As noted in their commentary in *Nature Chemistry*, Matlin and colleagues report that chemistry in general has not identified grand challenges the way other disciplines have. [2] For example, the Human Genome Project depends on advances in chemistry, but is driven by the fields of biology, genetics, and medicine. They suggest that "chemistry must go beyond 'being a science' and embrace the concept of 'being a science for the benefit of society'". Chemistry should be multidisciplinary, interdisciplinary and even transdisciplinary, "recognizing that valuable knowledge can be found in the spaces between defined disciplines, addressing the complexity of problems and the diversity of perceptions of them".

The areas in chemistry between disciplines are forefront research topics and often the career focus of the younger scientist community. Chemistry does not work alone in addressing these challenges. Whitesides, in his perspective in *Angew. Chem. Int. Ed.*, states that chemistry is limited by its traditional organization into specialties and needs to break down those barriers. [3] The problems that chemistry must address are increasingly multidisciplinary and interdisciplinary, as they also depend closely on chemistry in its broadest sense and other scientific (*e.g.* physics, biology) and engineering disciplines to tackle. New tools in computation and data mining promise to revolutionize our approach to chemistry and discovery. It is the objective of WCLM2017 that these multidisciplinary and interdisciplinary themes will now be developed in depth. This work will be facilitated through the inter-divisional committee on Green Chemistry for Sustainable Development (ICGCSD) and the inter-divisional sub-committee on materials chemistry (ISMC) using them as a launch pad for developing shared languages and activities.

This WCLM follows in the tradition established in the 2011 meeting to prepare groundwork for a debate on the future of chemistry, its role in sustainable development, and IUPAC's part in advancing this future. Attendance is for IUPAC members at large, including members of Divisions and Standing Committees, NAOs and Associate NAOs and their delegates, and the representatives of Company Associates and Associated Organizations. WCLM2017 aims to facilitate the specific involvement of Young Observers (YOs) by targeting interdisciplinary topics and cross divisional/committee collaboration.

The YOs and invited leaders will have the opportunity to discuss and identify gaps in existing knowledge and practice of chemical science and how to address them. The YOs will assess the future of chemistry in breakout sessions and then present their findings to a panel of experienced leaders of the global chemical community. The outcome should help generate new projects in line with IUPAC's strategic vision. We ask the NAOs in particular to invite YOs to participate in the WCLM programme.

The programme will begin with a session in which the different IUPAC divisions and committees will intro-

Young Observer workshop during the WCLM 2015 in Busan, Korea.

duce themselves to participants using a "speed dating" concept. In a following workshop, YOs will assemble and work on projects in line with the themes of the WCLM. Finally, a symposium featuring outstanding speakers will be capped with a panel discussion and a report by the YOs on possible IUPAC projects. The progamme will be as follows:

Monday Evening, July 10: Reception for YOs hosted by IUPAC Divisions and Committees to introduce WCLM activities. This will be done in a speed-networking format in which we will have a round table discussion at each station with representatives from each Division/ Committee and up to 10 YOs in each discussion. This networking opportunity will continue and extend during the reception held with the International Young Chemists Network and around their poster session (To learn more about IYCN, see feature page 4) .

Tuesday Morning, July 11: Following a workshop with ISMC and ICGCSD representatives, the YO teams will work with IUPAC volunteers to develop their ideas into a presentation for the WCLM.

Wednesday Morning, July 12: Plenary presentations will be made by noted leaders from academia and industry. Presentations from YO teams will be given to the assembled audience. Group discussions and identification of highest priority tasks will take place.

Post-GA Activities: Outcomes from the WCLM will be as a means to develop interdisciplinary projects. YOs will be encouraged to participate in working groups and newly formed project teams.

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https://iupac.org/project/2016-032-2-020

Trace Elements Analysis of Environmental Samples with X-rays

Zurich, Switzerland, 16-20 July 2017

The use of X-ray methods for the analysis of trace elements in environmental samples has become a modern tool for scientists around the world. With dedicated instrumentation, X-ray analyses of trace elements in environmental matrices can be successfully performed both at synchrotron facilities and in the lab.

This Symposium aims to inform the audience about the most recent developments in trace elements analysis in environmental samples with X-rays, available both at synchrotron beamlines and as laboratory instrumentation. In particular, the latest developments in X-ray technology (sources, optics, detectors) and sample preparation will be presented, as well as new X-ray based analytical methods for the analysis of trace elements in the environment.

New developments in the fields of X-ray diffraction, X-ray fluorescence, and X-ray absorption will be discussed, in both 2D and 3D applications, with a special emphasis on spatially resolved microscopic and submicroscopic analyses of minor and trace elements in environmental matrices.

The Symposium will be organized in oral and poster sessions, with invited keynote lectures. Three poster prizes, including an award certificate and prize money, will be awarded by IUPAC Division VI to young participants.

The Symposium, co-sponsored by IUPAC Division VI, Chemistry and the Environment, and by Bruker Nano Gmbh, is part of the International Conference on the Biogeochemistry of Trace Elements (ICOBTE 2017)– www.icobte2017.ch

This Symposium is part of a project task group which includes Roberto Terzano (IT, chair), Koen Janssens (BE), Ryan Tappero (US), Melissa Anne Denecke (UK), Gerald Falkenberg (DE), David Paterson (AU), Bradley Miller (US), Armin Gross (DE), and Fang-Jie Zhao (CN)

https://iupac.org/project/2016-019-2-600

Ionic Polymerization

17-22 September 2017, Durham, UK

The 12th **International Symposium on Ionic Polymerization** (IP 2017) will be held at Durham University in the UK from 17 to 22 September 2017, organised and hosted by the Durham Centre for Soft Matter and endorsed by IUPAC. IP 2017 will be the latest in a series of successful meetings, the most recent of which were held in Bordeaux (France, 2015), Awaji (Japan, 2013), Akron (USA, 2011), and Krakow (Poland, 2009).

IP 2017 has its roots in the series of international symposia on Cationic, Anionic, and Ring-opening Polymerizations which were merged into the inaugural International Symposium on Ionic Polymerization held in Istanbul (Turkey, 1995).

The focus of IP 2017 will be on academic and industrial research in the areas of anionic, cationic, and ring-opening polymerization mechanisms. Contributions related to other methods of living/controlled polymerization (catalytic, controlled free-radical, and step-growth polymerizations) are welcome.

We invite all participants to submit an abstract for contributed oral presentations (20 minutes), short talks for younger researchers (15 minutes) or posters.

Contact l.r.hutchings@durham.ac.uk for more info.

www.dur.ac.uk/soft.matter/ip2017

Global Challenges and Data-Driven Science

8-13 October 2017, Saint Petersburg, Russia

The International CODATA 2017 Conference, "Global Challenges and Data-Driven Science", will explore the fundamental issues relating to the availability, (re-)use, and scientific analysis of data that relate to the most significant contemporary global challenges.

Global science is increasingly data-driven. Major international scientific programmes contribute to a collective endeavour to understand contemporary global processes and phenomena that are of deep relevance to contemporary societies. The unprecedented volume of data generated by the digital revolution of recent decades has led to the emergence of distinctive and powerful means of characterising and understanding the complex systems that are at the heart of many global challenges. These developments raise major questions around data collection, stewardship, and analysis and there are timely lessons to be shared between the academic and commercial sectors.

This major scientific conference aims to explore the intersection between data-driven technological and scientific approaches and specific global challenges. It will explore the nexus between:

1. approaches that permit vast quantities of data to be created, stored, recombined, and analysed, with the capacity to integrate data from disparate domains to reveal unanticipated relationships, and, with the use of powerful learning algorithms, to establish deep relationships in complex systems; and
2. their application to major global challenges, including disaster risk, smart cities, and urban development and global environmental change.

Scope of the Conference

Topics to be covered by the conference include:

- concrete achievements in data-driven science across all research areas;
- data collection, analysis, and integration for Earth observations and the study of the Earth's system;
- data collection and analysis for disaster risk research;
- data-driven cities and sustainable urban development;
- shared data challenges, Big Data Management, and analysis in the scientific and commercial sectors;
- the fundamental and practical issues of data analysis, event recognition, and application;
- coordination and development of national and international data services;
- the development of research data services in universities and other research organisations;
- coordination of data standards and interoperability;
- issues around "Intelligently Open" and FAIR data.

The conference will be of interest to researchers in many domains, particularly those relating to the global research programmes sponsored by the International Council of Science (Future Earth, Integrated Research on Disaster Risk, Urban Health and Wellbeing), as well as research around the Sustainable Development Goals, ecological and environmental challenges and assessments, and the Sendai Framework on disaster risk reduction. The conference will foster constructive and continued dialogue between transdisciplinary researchers and data experts.

http://codata2017.gcras.ru

Mark Your Calendar

Upcoming IUPAC-endorsed events
See also www.iupac.org/events for links to specific event websites

2017 (after 1 May)

13-14 May 2017 • Ecological Risk Assessment of Pesticide • San Jose, Costa Rica
IUPAC workshop, an integral part of the 6th Latin American Pesticide Residue Workshop (LAPRW 2017: https://laprw2017.fundacionucr.ac.cr)
Dr. John Unsworth, chair of IUPAC project 2016-025-1-600 ; E-mail: unsworjo@aol.com

17-18 May 2017 • Stat Test in Clinical Laboratory • Barcelona, Spain
9th European Symposium on Clinical Laboratory and In Vitro Diagnostic Industry
Ariadna Arbiol-Roca, Laboratori Clinic Hospital Universitari de Bellvitge, 08907 L'Hospitalet de Llobregat, Catalonia, Spain; E-mail: ariadna.arbiol@bellvitgehospital.cat
www.acclc.cat

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

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

11-15 June 2017 • EuroMedLab • Athens, Greece
22nd IFCC-EFLM European Congress of Clinical Chemistry and Laboratory Medicine
Alexander Haliassos, Congress President, E-mail: haliassos@moleculardiagnostics.gr; Organising Secretariat, MZ Congressi: Patrizia Sirtori, E-mail: patrizia.sirtori@mzcongressi.com, www.athens2017.org

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

19-23 June 2017 • Molecular Mobility and Order in Polymer Systems • St Petersburg, Russian Federation
9th International Symposium on Molecular Mobility and Order in Polymer Systems,
Symposium coordinator: Dr.T.V. Filippova, Institute of Macromolecular Compounds of RAS; Bolshoi pr.31, St.-Petersburg, 199004, Russia, Tel. +7 (812) 323 29 07, E-mail: tatfil@imc.macro.ru, www.onlinereg.ru/mmops2017

25-29 June 2017 • Organometallic Chemistry • Jeju Island, South Korea
International Symposia on Organometallic Chemistry Directed Towards Organic Synthesis (OMCOS 19)
Prof. Sukbok Chang (chair), Department of Chemistry, Korea Advanced Institute of Science and Technology (KAIST), Daejeon, Korea, E-mail: sbchang@kaist.ac.kr, www.omcos19.org

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

9-13 July 2017 • Boron Chemistry • Hong Kong, China
16th International Meeting on Boron Chemistry (IMEBORON XVI)
Zuowei Xie, Chair, Department of Chemistry, The Chinese University of Hong Kong, Shatin, N.T., Hong Kong SAR, China, E-mail: IMEBORON16@cuhk.edu.hk; www.imeboron16.org

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

16-20 July 2017 • Trace Elements Analysis • Zurich, Switzerland

Special IUPAC symposium on "Trace elements analysis of environmental samples with X-rays", part of International Conference on the Biogeochemistry of Trace Elements (ICOBTE 2017, www.icobte2017.ch), Dr. Roberto Terzano, Department of Soil, Plant and Food Sciences, University of Bari, Bari, Italy; chair of IUPAC project 2016-019-2-600; E-mail: roberto.terzano@uniba.it

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

Chemistry addressing sustainable development and other challenges of the 2020s
Dr. Roger Stapleford, CEO RACI, 21A Vale Street, North Melbourne, Australia, E-mail: Roger.stapleford@raci.org.au; www.racicongress.com

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

The 11th International Symposium on Selenium in Biology and Medicine and The 5th International Conference on Selenium in the Environment and Human Health (Se2017)
Prof. Elias Arnér, Department of Medical Biochemistry and Biophysics, Karolinska Institutet, SE-171 77 Stockholm, Sweden, E-mail: Elias.Arner@ki.se, www.se2017.se

16-18 August 2017 • Chemical Identifier • Bethesda, MD, USA

The IUPAC International Chemical Identifier, InChI, 10th anniversary workshop
Steve Heller, workshop coordinator, Division VIII InChI Subcommittee Chair and the InChI Trust project director, E-mail: steve@inchi-trust.org, www.inchi-trust.org

28-31 August 2017 • MacroMolecular Complexes • Tokyo, Japan

17th IUPAC International Symposium on MacroMolecular Complexes (MMC-17)
Hiroyuki Nishide, Chair of Program Committee, Department of Applied Chemistry, Waseda University, Tokyo 169-8555, Japan, E-mail: nishide@waseda.jp; Kenichi Oyaizu, Chair of Local Organizing Committee, Waseda University, E-mail: oyaizu@waseda.jp, www.waseda.jp/assoc-mmc17

10-14 September 2017 • Organic Materials for Electronics and Photonics • Prague, Czech Republic

81st Prague Meeting on Macromolecules (PMM): Polymers and Organic Materials for Electronics and Photonics: Science for Applications
Prof. Jiří Pfleger, Pogram chair, E-mail: pfleger@imc.cas.cz ; and Daniela Illnerová, Institute of Macromolecular Chemistry, Czech Academy of Sciences, Tel.: +420-296 809 331, E-mail: sympo@imc.cas.cz www.imc.cas.cz/sympo/81pmm

17-20 September 2017 • BloodSurf • Clemson, SC, USA

Blood-biomaterial interface: where medicine and biology meet physical sciences and engineering
Ilya Reviakine (U Washington/Seattle, WA), E-mail: reviakin@uw.edu and Robert Latour (Clemson University), E-mail: latourr@clemson.edu, co-organizers; www.ireviakine.net/Bloodsurf

17-22 September 2017 • Ionic Polymerization • Durham, United Kingdom

International Symposium on Ionic Polymerization – IP 2017
Professor Lian Hutchings, Chair of Local Organizing Committee, E-mail: l.r.hutchings@durham.ac.uk; Dr Mike Shaver, Chair of Program Committee, E-mail: michael.shaver@ed.ac.uk; www.dur.ac.uk/soft.matter/ip2017/

27-29 September 2017 • Bioorganic Chemistry • Konstanz, Germany

11th International Symposium on Bioorganic Chemistry (ISBOC-11)
Program Committee Chair: Andreas Marx, University of Konstanz, Dept. of Chemistry, Universitaetsstr. 10, Postf. 726, D-78457 Konstanz, Germany, T:+49 7531 88-5290, andreas.marx@uni.kn, www.uni-konstanz.de/isboc-11/

2-5 October 2017 • Green Chemistry • Moscow, Russian Federation

7th IUPAC International Conference on Green Chemistry
Prof. Natalia P. Tarasova, Conference Chair, D. Mendeleev University of Chemical Technology, Moscow. Dr. Anna S. Makarova, Chair of Local Organizing Committee, E-mail: annmakarova@mail.ru; http://greeniupac2017.muctr.ru

Mark Your Calendar (cont.)

8-11 October 2017 • Chemistry Education • Sétif, Algeria

ACRICE 2017, 3rd African Conference on Research in Chemistry Education

Prof Djafer Benachour, Department of Process Engineering, Ferhat Abbas University SETIF 1, Sétif 19 000, Alegria; E-mail: bendjafer@univ-setif.dz

www.univ-setif.dz/OCS/FT/ACRICE

9-13 October 2017 • Advanced Materials • Kuala Lumpur, Malaysia

25th Annual World Forum on Advanced Materials (POLYCHAR 25)

Ong Eng Long, Organizing Chair, E-mail: ongelong@gmail.com; ikmhq@ikm.org.my. 25th POLYCHAR 2017 Secretariat, Institut Kimia Malaysia, 127B, Jalan Aminuddin Baki, Taman Tun Dr Ismail, 60000 Kuala Lumpur, Malaysia, Tel.: +603 77283272, E-mail: secretariat@25polychar.org.my, www.25polychar.org.my

11-13 October 2017 • Smart Materials • Jeju Island, Korea

IUPAC-FAPS 2017 Polymer Congress on Smart Materials for Emerging Technology

Jungahn Kim, Chair of the Organizing Committee, Department of Chemistry, Kyung Hee University, Seoul, Korea, E-mail: jakim05@khu.ac.kr; www.faps2017.org

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

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

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

2018

21-23 February 2018 • Chemistry Conference for Young Scientists • Blankenberge, Belgium

Chemistry Conference for Young Scientists (ChemCYS 2018)

Koninklijke Vlaamse Chemische Vereniging vzw; E-mail: support@chemcys.be

www.chemcys.be

4-7 June 2018 • Polymers and Organic Chemistry • Montpellier, France

Polymers and Organic Chemistry 2018 (POC 2018)

Dr Ghislain David (Chair), Institute Charles Gerhardt, School of Chemistry of Montpellier, 8 rue de l'Ecole Normale, F-34296 Montpellier Cedex 5, France, E-mail: ghislain.david@enscm.fr

4-7 June 2018 • Isotopes and Isotopically Labelled Compound • Prague, Czech Republic

13th International Symposium on the Synthesis and Applications of Isotopes and Isotopically Labelled Compounds

Prof. Tomáš Elbert (Chair of the Local Organising Committee), E-mail: elbert@uochb.cas.cz

www.iis-prague2018.cz

1-5 July 2018 • MACRO2018 • Cairns

World Polymer Congress

Prof. Sébastien Perrier and Prof. Martina Stenzel (conference co-chairs); Conference Coordinator: Taylor Mills, Leishman Associates, E-mail: taylor@leishman-associates.com.au

www.macro18.org

8-13 July 2018 – Photochemistry • Dublin, Ireland

27th IUPAC International Symposium on Photochemistry

Dr. Miguel A. Garcia-Garibay (Conference co-chair), Department of Chemistry and Biochemistry, University of California, Los Angeles, E-mail: mgg@chem.ucla.edu, and Dr. Susan Quinn, School of Chemistry, University College Dublin, Belfield, Dublin 4, Ireland, E-mail: susan.quinn@ucd.ie

16-21 September 2018 • Organic Synthesis • Florence, Italy

22nd International Conference on Organic Synthesis (22-ICOS)

Professor Alberto Brandi (Conference Chair) and Professor Maurizio Taddei (Vice-Chair), E-mail: secretariat@22-icos-florence.it

www.22-icos-florence.it

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Asociación Química Argentina *(Argentina)*
Australian Academy of Science *(Australia)*
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Bangladesh Chemical Society *(Bangladesh)*
The Royal Academies for the Sciences and Arts of Belgium *(Belgium)*
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Chinese Chemical Society *(China)*
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Russian Academy of Sciences *(Russia)*
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Serbian Chemical Society *(Serbia)*
Slovak Chemical Society *(Slovakia)*
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