

# CHEMISTRY

## International

The News Magazine of IUPAC

January-March 2017

Volume 39 No. 1

### Chemistry Organizations in a Changing World



INTERNATIONAL UNION OF  
PURE AND APPLIED CHEMISTRY

Woodward's Words ►

The Periodic Table (Continued?) ►



# Chemistry International

## CHEMISTRY International

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

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**Front Cover:** In a rapidly changing world, what is the fundamental purpose of chemistry organizations, what should be their roles and how do they need to refresh themselves to best serve the field and also society at large? Stephen A. Matlin, Alain Krief, Henning Hopf, and Goverdhan Mehta examine these questions. See feature page 15. Cover image ©VAlekStudio

**Back Cover Tear-off Page:** IUPAC periodic table of the elements, version 28 November 2016

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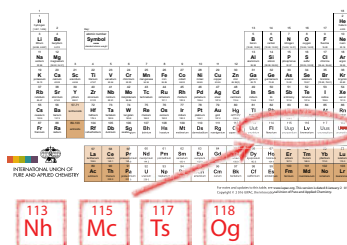
This database is the only product that provides for the quick and easy search and retrieval of IUPAC's standards and recommendations which until now have remained unsorted within the huge *Pure and Applied Chemistry* archive.

- **Useful:** IUPAC's standards and recommendations easily discoverable
- **Comprehensive:** standard values and procedures; nomenclature, terminology and symbols in chemistry and materials properties of elements, etc.
- **Smart:** topical structure, advanced search, cross linked entries



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## On the Path to Rewarding Times

by *Natalia Tarasova*

**I** am grateful for this opportunity to wish members of IUPAC bodies and adhering organizations, fellows, affiliate members, and company associates a successful, fruitful, and healthy year in 2017. Many of us will meet in São Paulo, Brazil, in July, at the IUPAC General Assembly and the 46th World Chemistry Congress, for the first time to be held in South America, to discuss the directions of the Union's activities as IUPAC is moving to its' centenary in 2019.

The year 2016 was rich in events. Let me share with you some examples. On 28 November 2016, IUPAC approved the name and symbols for four new elements: nihonium (Nh), moscovium (Mc), tennessine (Ts), and oganesson (Og), respectively for element 113, 115, 117, and 118. Keeping with tradition, the newly discovered elements have been named after a place or geographical region, or a scientist. From my point of view, the names of the new elements reflect the realities of our present time: universality of science, honoring places from three continents, where the elements have been discovered—Japan, Russia, the United States—and the pivotal role of human capital in the development of science, honoring an outstanding scientist—Professor Yuri Oganessian, the scientific leader of the G. Flerov Laboratory of Nuclear Synthesis at the Joint Institute of Nuclear Research in Dubna, Russia. It should be mentioned that during a 5-month period of public review that preceded the announcement of new names, the Inorganic Chemistry Division, led by its President, Professor Jan Reedijk, has responded to hundreds of questions on the new names, on how to convert or translate them to different languages, and on how to derive (nomenclature) roots from these names.

The exploration of new elements continues, and scientists are searching for elements beyond the seventh row of the periodic table. Some twenty-five years have now elapsed since the criteria that are currently used to verify claims for the discovery of a new element were set down. The recent completion of the naming of the 118 elements in the first seven

periods of the Periodic Table provides a natural opportunity for a necessary expert review of these criteria in the light of the experimental and theoretical advances in the field. IUPAC and the International Union of Pure and Applied Physics (IUPAP) have recently agreed to establish a new joint working group which task will be to examine the criteria used to verify claims for the discovery of new elements.

Another event I would like to mention is the establishment of the Interdivisional Committee on Green Chemistry for Sustainable Development. Green Chemistry which started 25 years ago as the invention, design, and application of chemical products and processes to reduce or eliminate the use and the production of harmful substances, is seen nowadays as a basic instrument for sustainable development that touches many aspects of the environment and human welfare, and is relevant to 17 Sustainable Development Goals set by the United Nations.

The Interdivisional Committee on Green Chemistry for Sustainable Development (ICGCSD) will initiate, promote, and coordinate the work of the Union in the area of green and sustainable chemistry. It superseded the subcommittee on Green Chemistry of the Organic and Biomolecular Chemistry Division successfully led by Professor Pietro Tundo (who is appointed the chair of the ICGCSD). Among the supporters of this new Interdivisional Committee it is worth mentioning professors Paul Anastas, John Corish, Buxing Han, Roger Shelton who are renowned scientists working in the field of Green Chemistry for decades.

The ICGCSD will continue to organise the series of IUPAC International Conferences on Green Chemistry, to manage IUPAC participation in the PhosAgro/UNESCO/IUPAC Green Chemistry for Life programs, the CHEMRAWN Prize in Atmospheric and Green Chemistry, and any other related awards that may be established.

The ICGCSD is expected to actively work with the Committee on Chemistry and Industry (COCI) and the Committee on Chemistry Education (CCE) to stimulate and increase interest in green and sustainable chemistry, in the theory and practice of industrial chemistry and chemistry education, through their external industrial and institutional relationships. Matters relating to harmonisation, regulation, and standardisation in green and sustainable chemistry will also be in the scope of interests of the new Committee, as well as the interaction with other relevant organisations with a common interest. Among them,



the Organisation for the Prohibition of Chemical Weapons (OPCW) should be especially mentioned. OPCW has been a strategic partner of IUPAC for the last decade, sharing the common goal to help chemists all over the world in the adoption of peaceful and sustainable uses of chemicals.

OPCW is the implementing body of the Chemical Weapons Convention, which entered into force in 1997. There are currently 192 Member States, covering 98% of the global population, working together to achieve a world free of chemical weapons, and who share the collective goal of eliminating existing stockpiles of chemical weapons and preventing chemistry from ever again being used for warfare. It should be mentioned that, since 1997, 93% of the world's declared stockpile of 72 304 metric tonnes of chemical agent have been destroyed. In 2013, the OPCW was awarded the Nobel Peace Prize "for its extensive efforts to eliminate chemical weapons."

In 2016, OPCW established an Advisory Board on Education and Outreach on which IUPAC has a permanent observer status. Our collaboration is intended to focus on efforts such as public understanding and education of students about the Chemical Weapons Convention, producing educational materials related to the science of the CWC, education on multiple uses of chemicals, and similar initiatives.

OPCW and IUPAC are actively cooperating to promote knowledge sharing, dissemination of best practices, and capacity building for the peaceful, green and sustainable uses of chemistry. Among the recent examples is the workshop "The best practices to develop the Responsible Care® programs" for the chemical industry representatives of chemical enterprises in the countries of the Russian-speaking regions (CEE and Central Asia) that was held in Moscow, Russia, in March 2016 under the auspice of OPCW and IUPAC. Another example is the active involvement of OPCW in the IUPAC International Conferences in Green Chemistry. The last one was held in Venice in September 2016. The Hague Ethical Guidelines were presented during the OPCW workshop and vividly discussed by the representatives of chemistry community. IUPAC and OPCW will further cooperate on the promulgation of The Hague Ethical Guidelines and initiatives arising from them.

On 1 December 2016, the Memorandum of Understanding between IUPAC and OPCW was signed. Its aim is to outline a framework for co-operation between IUPAC and OPCW with a view towards achieving their common objectives and providing benefits

to their respective programmes and areas of work. The two organizations intend, within the scope of their mandates, to cooperate more closely to achieve their common goals in promoting chemistry for peaceful purposes, and facilitating the exchange of scientific and technical information in support of their work.

My final example deals with the outcome of one IUPAC project, that has been realized as a book recently published by Springer: "Chemistry Beyond Chlorine" (see [www.iupac.org/project/2013-057-3-300](http://www.iupac.org/project/2013-057-3-300)). The international team of authors led by professor Pietro Tundo, states that "Chemistry beyond chlorine... is not committed in any way against chlorine chemistry; this would be out of common sense. Conversely, it should be considered as a useful tool to seek alternative pathways beyond chlorine chemistry when possible".

As chemists, we all know that chemistry attracts a lot of public attention, because of its intrinsic diversity. Elaboration of novel chemical compounds and materials with desirable properties helps to solve such problems as provision of humanity with pure water, food, medicines. On the other hand, it is necessary to pre-empt possible negative consequences, caused by careless exploitation of chemicals. Generations of the Earth's inhabitants have been admiring the austere beauty of the monumental building of fundamental chemistry, while nowadays chemophobia attacks more and more people as the consequence of lack of attention to chemical education and popularization of scientific knowledge. "Chemistry Beyond Chlorine" clearly demonstrates that chemists are ready to meet these challenges.

I am grateful to the IUPAC family for the commitment to the chemical sciences and looking forward to seeing you in São Paulo. 🍷

**Natalia Tarasova** <[tarasnp@muctr.edu.ru](mailto:tarasnp@muctr.edu.ru)> is President of IUPAC since January 2016. She has been a member of the IUPAC Bureau since 2008 and the Executive Committee since 2010. She is a professor at the D. I. Mendeleev University of Chemical Technology of Russia, a Member of the Russian Academy of Sciences, Director of the Institute of Chemistry and Problems of Sustainable Development, a Chairholder of the UNESCO Chair of Green Chemistry for Sustainable Development.

# Woodward's *Pure and Applied* Chemistry Words

*by Jeffrey I. Seeman*

**A**ccording to IUPAC, "*Pure and Applied Chemistry* is the official monthly Journal of IUPAC, with responsibility for publishing works arising from those international scientific events and projects that are sponsored and undertaken by the Union." There is no doubt that PAC has and continues to achieve its goal of being "an authoritative and indispensable holding in academic and institutional libraries."

But I assert, intentionally and rather provocatively (and certainly dramatically), that hardly anyone reads *PAC*. I must explain what I mean. *PAC*, like all journals, is not a literary work. It is meant for browsing, perhaps even just scanning the table of contents, and then, ultimately and for selected papers only, for careful study. *PAC* is also geared as a resource, even as a dictionary, and as an archival record.

That being said, there really are hidden jewels within *PAC*, so much so that I might even go so far as to suggest instances of *belles lettres*. The goal of this article is to share excerpts from the writings of one organic chemist who, within the bookends of *PAC*, was a true *belletrist*! Between 1961 and 1973, he published six papers in *PAC* [1-6]. Clearly, this wasn't just any organic chemist, for how many scientists are invited to give so many IUPAC plenary lectures within their lifetime, let alone within a 13-year period? We speak of Robert Burns Woodward, arguably the greatest organic chemist of the 20th century, perhaps ever. No further introduction is needed.

*Woodward's Words* have been published in a series of articles in the journal *Angewandte Chemie*. These articles—collections of carefully chosen anecdotes and excerpts from the writings of Gilbert Stork, [7] Carl Djerassi, [8] John D. Roberts, [9] and Woodward, [10] all eminent chemists of the 20th Century—have had such an appeal that the Editor of *Chemistry International*, Fabienne Meyers, invited this historian and collector of chemical memoirs to similarly entertain her readership. The *entrée* today is *Woodward's Words* from *Pure and Applied Chemistry*. That this article appears in the first 2017 issue of *Chemistry International* is especially appropriate, as this year marks the centennial anniversary

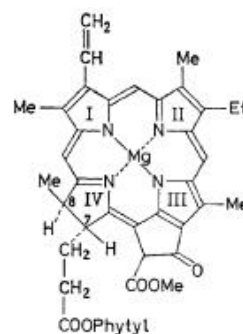
of Woodward's birth, on 10 April 1917.

A follow-up feature will appear in the next issue and hint at emulating Woodward's writing style.

A jewel in this very issue of *Chemistry International* is Dan Rabinovich's Stamps International: Woodward's Birth Centennial, page 15. [11] In this little gem, one of Rabinovich's mini-essays, postage stamps issued by the Republic of Guinea and the Republic of Chad in 2015 honoring R. B. Woodward and his chemistry are reproduced and discussed.

*Note: None of the following excerpts appeared in the previously published Woodward's Words: Elegant and Commanding. [10]*

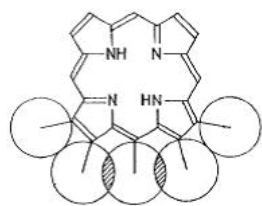
### From *The Total Synthesis of Chlorophyll* (1961)



*Chlorophyll, reproduced  
from [1], p. 384*

"The structural investigations [of chlorophyll] had been carried out almost entirely during the twilight of the classical period of organic chemistry. Only the very simplest basic elements of theory played any role in the whole vast study. Neither was succour or control sought in chemical principle, nor was any attempt made to place the often striking observations in any generalized framework. Would the conclusions from such a study stand scrutiny from the viewpoint of the present day? Was the structure proposed for chlorophyll correct? When we embarked upon the examination of these questions, we entered a chemical fairyland, replete with remarkable transformations which provide unusual opportunities for the testing and further development of principle, and we cannot but urge others to follow us in penetrating what must have seemed to many the monolithic wall of a finished body of chemistry." [1]

“All of these observations baffled us for some time, until they received a very simple rationalization in terms of the principle that two things cannot take up the same space at the same time.” [1]



*Porphyrin, structure IV  
reproduced from [1],  
p. 385*

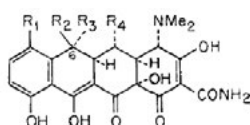
"Now, the porphyrin syntheses of an earlier day, magnificent for their time, were most ill-suited to our purpose. Carried out under bold but brutal conditions, they led in almost all cases to very complicated mixtures of porphyrins, in small, frequently microscopic, yields... By contrast, we required a method which would lead in high yield to a single product of known structure, containing substituent groups of variegated character—for we were well aware that we might have some distance to go after this primary objective had been achieved." [1]

"... which, after oxidation with iodine, small amounts of porphyrin were formed, and more so to succeed, after assiduous variation of experimental conditions, in preparing the porphyrin in the pure condition in a yield approaching 25 per cent. By any previous standard, this result approached the fabulous, but we knew that for our purpose it was still far from satisfactory." [1]

"Such inelegance, not to say impracticality, could not be tolerated. Our plan for expunging it was simple in principle... [but] was by no means mirrored in a comparable ease of its reduction to practice." [1]

"It will be recalled that we considered in our planning the possibility that hydrogen atoms might be induced to wander to the desired positions from another site in a suitably constructed porphyrin. [Since we had] such a suitably constructed porphyrin, it was now time for the wandering to begin—and begin it did—though it stopped short of our desire!" [1]

### **From *The Total Synthesis of a Tetracycline* (1963)**



	R <sub>1</sub>	R <sub>2</sub>	R <sub>3</sub>	R <sub>4</sub>
CHLOROTETRACYCLINE (AUREOMYCIN)	Cl	OH	Me	H
OXYTETRACYCLINE (TERRAMYCIN)	H	OH	Me	OH
TETRACYCLINE	H	OH	Me	H
6-DIMETHYL-6-DEOXYTETRACYCLINE	H	H	H	H

"... the complicated tetracyclic assemblage, adorned with an unusual number of contiguous reactive functional groups of different kinds, and replete with stereochemical imperatives, has presented a synthetic challenge to which many have responded." [2]

"We cannot but direct attention to the fact that it is less remarkable that the discovery of proper conditions for the cyclization was difficult, than that they could be found at all." [2]

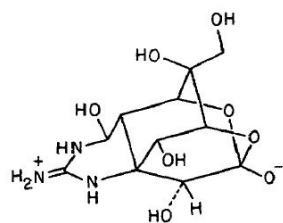
"Among several instances encountered in our work, this final cyclization... must hitherto have been regarded as difficult to the point of improbability." [2]

"... could be isolated in 25 per cent over-all yield. This easy statement should not be allowed to conceal the formidable effort which was required to bring us to a favourable outcome. The detailed mechanism of the oxygenation reaction is obscure—though there is little doubt that metal chelate formation must play a rôle—and the definition of useful reaction conditions required much experimentation; in view of the number of possibly relevant variables, it may strongly be doubted that the optimum has yet been achieved." [2]



*Woodward at the Woodward Research Institute, Basel, Switzerland, 1972, and with a copy of a PAC reprint on his desk, recognizable by the original IUPAC logo. Photograph courtesy of Novartis.*

## From *The Structure of Tetrodotoxin* (1964)



*Tetrodotoxin, Fig. 35 reproduced from [3], p. 73*

“Certain varieties of puffer fish, especially the *tora fugu*, or tiger puffer (*S. rubripes*), and the closely related *ma fugu*, or common puffer (*S. porphyreus*), are highly prized as comestibles in Japan. The indulgence of the taste is fraught with some peril, since the livers and ovaries of the fish contain a powerful poison. The presence of this poison has been known though its effects since antiquity, but its labile nature and its extremely low concentration in its natural milieu made the isolation of the toxic principle extraordinarily difficult . . . Although nearly five hundred persons died from its effects in Japan during 1956-58, the toxic dose for man is not known; if the physiologically absurd equation of men with mice be made, it may be anticipated that half a milligram of tetrodotoxin should be sufficient to deprive an average-sized man of his life.” [3]

“Now, in a wholly imaginary experiment, . . .” [3]

“The simplest manner in which the expression (XVIII) might be disabused of its unwanted carboxyl group was to . . .” [3]

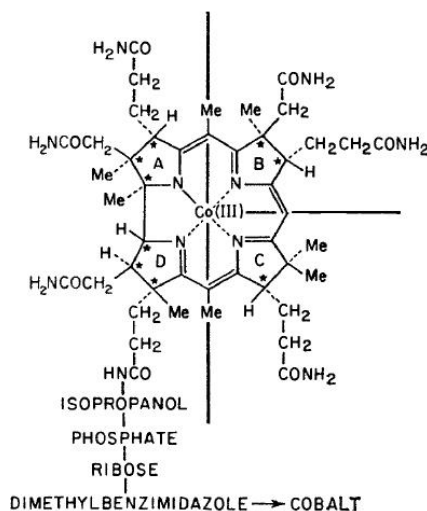
“At this point, however, the argument was simplified through the obtention of the almost ocular evidence provided by a complete three dimensional X-ray crystallographic analysis . . .” [3]

“We see that in the final structure every carbon atom but one bears at least one oxygen or nitrogen atom, while one carbon atom bears two, and two carbon atoms are attached to no less than three hetero atoms. Further, one of the latter arrays—the hemilactal function—is entirely unique, not having been observed before in the structure of any organic molecule, whether of natural or purely synthetic origin.” [3]

“The appearance of the array in the tetrodotoxin molecule presents a clear lesson for the future in its intimation that if normally non-interacting groups are appositely attached to a rigid skeleton, or otherwise

brought into forced proximity, they may be expected to co-operate in the formation of structural groupings which are not observed in simpler systems. It is worthy of note that tetrodotoxin is yet another in the long series of natural products whose study has time and again turned up for the first time new and unique systems, and provided stimulating insights into the fundamental behaviour of organic chemical systems.” [3]

## From *Recent Advances in the Chemistry of Natural Products* (1968)



*Vitamin B<sub>12</sub>, sketch reproduced from [4], p. 520*

“ . . . the crowded concatenation of six contiguous asymmetric centers embedded within the A/D moiety represents a formidable challenge.” [4]

“Perhaps also this is the point at which I should emphasize explicitly the importance of the availability of the ‘unnatural’ enantiomer. Much as had been our progress at this point, we were not unaware that we still had far to go, and that it might be either necessary or desirable—as indeed it turned out to be—to investigate a considerable number of alternatives for further advance. In these explorations we were able to utilize [the enantiomer of the natural series], confident that whatever new route we might establish through its study would be applicable to its counterpart of the natural series; our experience has been such that this is just about the only kind of model study which we regard as wholly reliable! And in fact, although the reactions I shall describe in the sequel will be presented for compounds in the natural series, almost all of them were first discovered using the enantiomeric substances.” [4]



## Woodward's Pure and Applied Chemistry Words



Woodward, with pencil in hand at the Woodward Research Institute (WRI) in Basel, ca. 1965. His offices, either at Harvard or WRI, were often decorated with colorful flowers and cigarette-containing ashtrays. Photograph courtesy Chemical Heritage Foundation.

"Only a single substance was produced . . . we possessed no means of ascertaining which of the two *a priori* possible orientations might be present. Nor in this instance did we have any particularly convincing argument as to which assignment should be made. As we shall see in the sequel the newly placed hydrogen atom appears . . . in the *undesired* orientation. After the fact, we can present a reasonable defense of Nature's action in this respect, but I should hardly feel justified in taking some of the limited time available here today to put forward arguments which we did not regard as convincing before we knew the result. How does it happen that we were so little concerned with the orientation at the centre at issue, by contrast with the very great care we had exercised in the establishment of the desired configuration at each of the other centres? Essentially because we were cognizant of the fact that this centre [would] be susceptible of inversion." [4]

"Quite as important as these changes which do occur is one that does not . . . the survival of the oxime grouping has enabled us to traverse a relatively simple path among a plethora of more complicated possibilities . . ." [4]

"In the light of these considerations we were not surprised to find that our mesylate was indeed quite extraordinarily loath to undergo the desired transformation." [4]

"Many ingenious schemes were devised in attempts to coax the recalcitrant ring to behave properly; their ingenuity was exceeded only by the uniformity with which they turned out to be unsuccessful. The temptation at this stage of our work was to feel that we had been hoist with the petard of a subtle and inherent flaw

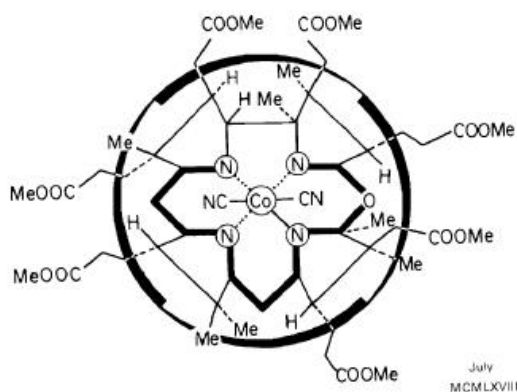
in our plan was strong, but fortunately a most remarkable observation came to our rescue . . ." [4]

"But the danger of such far-flung extrapolations is all too clear, and essentially we regarded the matter as *sub judice*. Now, when our fortunes in our battle . . . were at their lowest ebb, we became mindful of a most remarkable fact . . . seemed so astonishing as perhaps to call in question our [understandings]. However, further reflection not only permitted the rationalization of the remarkable observations in terms of the accepted hypothesis, but provided an insight which was of very great consequence for our further progress, both in understanding and in practice." [4]

"We all know that enforced propinquity often leads on to greater intimacy, and we were able to provide a new illustration of that maxim." [4]

" . . . it need present no occasion for surprise that the real case has exhibited substantial difference in behaviour from the simple analogues." [4]

### From Recent Advances in the Chemistry of Natural Products (1971)



The symbol of the 1968 International Symposium on the Chemistry of Natural Products, London, "which we could not but regard as exhortatory," according to Woodward in 1971, reproduced from [5], p. 283

"This might have seemed a modest objective to those unfamiliar with the magnitude of the challenges which synthetic work with molecules of such complexity and variegated reactivity present, but the event has shown that Professor [Albert] Eschenmoser and I judged our adversary well." [5]

## Taking IUPAC Literally

“Such is the sensitivity of the reactants, and particularly the product, that the successful execution of this operation requires rigorous adherence to the highest standards of experimental precision.” [5]

“The situation at this point may be summarized by depicting the [product] as a substance precariously balanced on a precipice, off of which all of our efforts pushed it into the valley represented by the dormant [compound]. Needless to say, innumerable early efforts to effect [reaction] were made—alas, with anything but encouraging results.” [5]

“This is no place to describe in detail the plethora of mysterious factors which seemed to affect the outcome of the reactions . . . so variable in fact were our experiences that the occasionally successful practitioner was regarded by his frustrated colleagues as quite as much a wizard as a scientist.” [5]

“It remains only to mention that the isolation and purification of [product] presented obstacles only less formidable than those attendant upon the discovery of a satisfactory method for its preparation.” [5]

### From *The Total Synthesis of Vitamin B<sub>12</sub>* (1973)

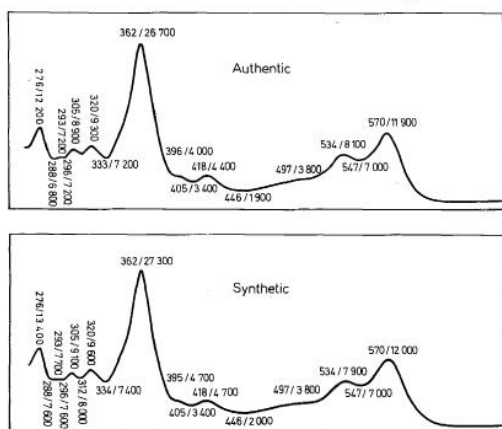


Figure 3 reproduced from [6], p. 147

“In Figure 3 you will see the comparison of the electronic spectra of the synthetic heptamethylbisnorcobyrinate and the authentic heptamethylbisnorcobyrinate. Now I do myself rather object to that term ‘authentic’. I don’t know what’s more authentic about the material derived from natural sources than the synthetic material; so I attribute to Professor Eschenmoser the choice of this somewhat misleading word.” [6]

“Now about the time that we had the thioester in hand, we thought perhaps we should do some of this reading that I am so famous for, and find out about the properties of thioesters. Certainly the idea is current in the minds of most chemists, I think, that thioesters are very much more reactive than the corresponding oxygen analogues. In fact it turns out on examination of the literature that the statement must be severely qualified.” [6]

“You can see what a diabolically clever scheme this is. I didn’t invent it, so I can give it that accolade.” [6]

## Conclusions

For 56 years, *Pure and Applied Chemistry* has served the chemical community well. I applaud the numerous lectures given at over 50 IUPAC conference series which have been permanently archived as publications in PAC. I know this value as a chemist who frequently uses these papers in my own research, as a historian who has cited these papers frequently—this very paper being a prime example!—and as a lecturer myself, for I’ve published one of these conference papers myself. But I now suggest another value of PAC, and that is to read the papers therein for their beauty as well as their scientific and historical value.

What do I mean by “beauty” in this context? It is a characteristic of the publication that combines an aesthetic piece (artistic, beautiful, sensorial compelling) with a chemical piece. Let us consider this proposal using the quote from Woodward’s 1968 PAC article,

“We all know that enforced propinquity often leads on to greater intimacy, and we were able to provide a new illustration of that maxim.” [4]

As lovely and loving as the phrase “enforced propinquity often leads on to greater intimacy” is, for us chemists, knowing that Woodward is referring to the rate enhancing (entropic) effect in, for example, intramolecular reactions, the synergy between the words and the chemistry make the saying ever more entrancing.

Indeed, in the quote immediately below (not from PAC), Woodward lamented that non-chemists cannot possibly be enthralled by some of the pleasures a chemist can, when reading or hearing about an unusual chemical phenomenon. Woodward wrote,

“Not infrequently it is possible to introduce delightful elements of surprise into synthetic work. An apparently rather dull grouping of atoms suddenly, under the impact of especially chosen reactants, undergoes unusual transformations which are of great

## Woodward's Pure and Applied Chemistry Words

utility in progress toward the objective. The impact on an observer may perhaps be compared with that on the traveler down an uninteresting street, who turns through a small hidden doorway into a delightful and charming garden. This kind of satisfaction in chemical synthesis is by its nature suited only for the special delectation of the initiated, and its pleasures are, alas, not transferable to those not fortunate in the possession of detailed chemical knowledge. I am confident that the chemists who read this will share my regret that non-chemists who may venture this far cannot savour with me anew the delights of this short sequence of operations..." [12]

In the same way, non-chemists cannot share the specialness of some of Woodward's writings when they combine linguistic aesthetics and chemical beauty.

### Coda

*Chemistry International's* editor has supported my decision to focus on excerpts from Woodward's PAC articles that were not published in my earlier Woodward's Words. [10] She is rightfully quite proud of IUPAC publications. However, she lamented that perhaps the best of Woodward were already placed elsewhere, and not in this publication. I thus turned the tables around and asked her to choose her favorites from that earlier *Words* paper. Somewhat intrigued by the beauty of Woodward's words, Fabienne Meyers wondered if the younger Woodward wrote already so elegantly or if his style came later with his notoriety. We find *de facto* many excerpts in Woodward's earlier writing that show his tastefulness and the following two excerpts, among Fabienne's favorites, are from when he was not yet 40 years old.

(1956) "In the century that has passed since Berthelot's words were uttered, organic chemistry has literally placed a new Nature beside the old. And not only for the delectation and information of its devotees; the whole face and manner of society has been altered by its products. We are clothed, ornamented, and protected by forms of matter foreign to Nature; we travel and are propelled in, on, and by them. Their conquest of our powerful insect enemies, their capacity to modify the soil and control its microscopic flora, their ability to purify and protect our water, have increased the habitable surface of the earth and multiplied our food supply; and the dramatic advances in synthetic medicinal chemistry comfort and maintain us, and create unparalleled social opportunities (and problems). We do not propose to

examine this vast domain in detail, or to prognosticate the direction of its advance, in response to the need, desire, and fancy of man. We shall leave it that the evidence is overwhelming that the creative function of organic chemistry will continue to augment Nature, with great rewards, for mankind and the chemist in equal measure." [13]

(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." [14]

But I urge those who have enjoyed these excerpts, please find your way to the earlier paper [10] or perhaps just go directly to Woodward's very own publications. Much joy awaits you. 🍷

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# The Periodic Table (continued?)

## Eka-francium *Et Seq.*

by Paul J. Karol

**I**ronically, the IUPAC Gold Book includes no definition of the “Periodic Table”. Nevertheless, Chemistry International’s readership assuredly knows what the Periodic Table is, or at least, what it has been, since that perception might change in the future. If the conversation is to be about prospects beyond the element with atomic number  $Z = 118$ , two essential questions must be answered: Where are we going? How will we get there?

The long-range growth of the Periodic Table, since the dozen or so “ancient elements”, has sat at an effectively constant rate over the last two-and-a-half centuries, with a new element added every two-and-a-half years on average, although not necessarily sequentially. The evolution of the Table is illustrated in Fig. 1.

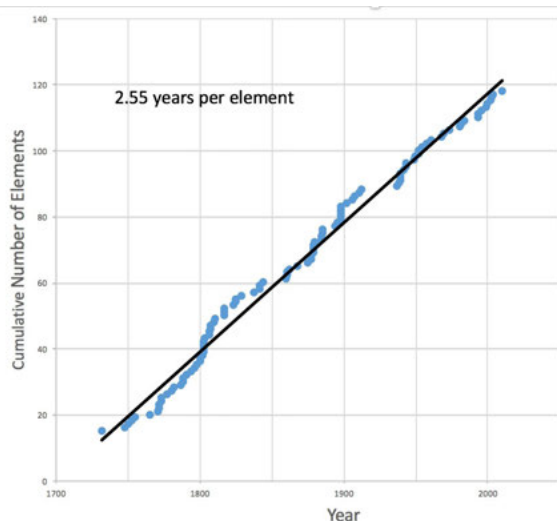


Fig. 1 Total number of known elements as a function of time expressed in calendar years.

Knowing where we are now, let us consider the two questions above. The first question has two aspects: nuclear structure and electronic structure. Without a nucleus, there is no element. A coarse characterization describing nuclear structure is embodied in the liquid drop model, now nearly three-quarters of a century old. The model, which we address only briefly, explains in a semi-quantitative way the broad behavior of nuclei: binding energies, fusion of light nuclei, most stable compositions, decay and reaction energies, fission energies and fissionability, shapes and barriers towards fission, and the location of particle “drip lines” at which

compositions an additional proton or neutron will not “stick”. The total binding energy reaches zero at about the mass number  $A = 3500$ . For heavy nuclei, a greater charge favors alpha decay and binary fission. Even ternary and quaternary fission can occur, as can the emission of clusters larger than alpha particles. Half-lives become shorter for higher  $Z$ . Fission becomes more probable with  $Z^2/A$  and inescapably instantaneous (in the liquid drop model) above  $Z \approx 110$ . But that Periodic Table cutoff was violated years ago. The nuclear shell model, conceptually similar to that for electronic levels in atoms, introduces extra stability at shell closures when merged into the bulk liquid drop behavior. For nuclear systems, both neutrons and protons can have closed shells, in which case nuclear scientists speak of “doubly magic” compositions. The stability associated with shell structure can be sufficient to overcome the high transition rates associated with both alpha-decay and fission and can also affect nuclear shapes and barriers. Seaborg seems to have been the first to reference the “island of stability” beyond the actinides. Exploration of the “island of stability” over the past years, with the anticipated nuclear stability, has focused on predictions of closed shells at  $Z = 114, 120$ , and  $126$ , and also at  $N = 152, 162, 172$ , and  $184$ . Newest to the Periodic Table are the  $p$ -block elements with atomic numbers 113 through 118, [1] whose properties strongly imply an island of stability has been reached (or breached) for those superheavy elements (SHE) where measurements show increasing, but still short lifetimes. SHEs are sometimes referred to as SHNs (superheavy nuclides), considered by chemists to be transactinides ( $Z > 103$ ) and alternatively by physicists to have nuclear mass numbers  $A > 280$ .

Beyond the island (or cluster of islands) now being explored lies a vast ocean of instability that extends to a predicted, though distant, island of stability at  $Z = 164$ , perhaps the last in sight. Arguably,  $Z = 164$  could be deemed the terminal edge of the Periodic Table. However, there are also calculations suggesting that changes in nuclear shape can profoundly affect this expectation. Both nuclear bubble and toroidal shapes suggest there may be “stable” compositions extending to  $Z = 240$  and beyond. Nevertheless,  $Z = 164$  is a huge extrapolation from the recently accessed island, fraught with the usual concerns about placing faith in such leaps. Current indications predict no stable (measurable) nuclides between that remote outlier and the nearer outcropping just being reconnoitered.

If there is a viable nucleus, what about the electrons? Electronic structure emerges from the wave



behavior of electrons electrostatically attracted to a nucleus and repelled by other electrons. Relativistic considerations for atomic structure are exceptionally important: not only spin-orbit splitting, but other more esoteric effects emerge. For hydrogen-like (one electron) systems, we can look at the most tightly bound level, the  $1s$ . The Bohr equation gives a good account of its energy relative to the separated point-nucleus, point-electron arrangement, defining a zero and then including the rest mass energy of the electron itself,  $m_e c^2$ . The problem seems to have been first solved by Walther Gordon (of the Klein-Gordon relativistic Schrödinger wave equation) in 1928 [2]. The total energy, including rest mass energy, can be expressed in terms of the fine structure constant,

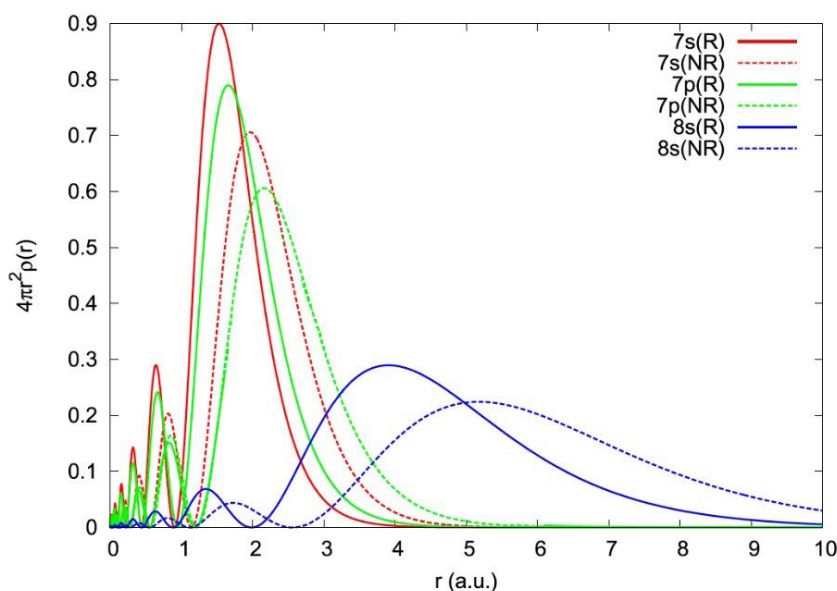
$$\alpha = \frac{1}{4\pi\epsilon_0} \frac{e^2}{\hbar c},$$

as  $E_{1s} = m_e c^2 \sqrt{1 - Z^2 \alpha^2}$ , which gives unphysical results for  $Z > 1/\alpha \approx 137$  and was identified early on as the upper limit for meaningful electron behavior, *i.e.*, a cutoff for the Periodic Table. Nearly four decades later, it was recognized that this obstacle could be circumvented if, rather than a point nucleus, a realistic finite size were considered. In this case, it turned out that the  $1s$  energy would continue to plunge deeper and deeper as  $Z$  grew beyond 137. But at a critical  $Z$  of about 172, the energy was sufficiently negative to allow a positron-electron (particle-antiparticle) pair to be created spontaneously out of the coulomb field in a vacuum, emitting the positron from the system and having the new electron occupy the “ $1s$ ” level, forming a negatively charged vacuum

in the nucleus’ immediate environment [3]. This esoteric description is for the  $1s$  level initially unoccupied. But, of course, what is needed is recognition that the full ensemble of atomic electrons must be considered with whatever effects pertain to their mutual behavior. A many-electron treatment for argon gives essentially the same result for the behavior of the occupied  $1s$  level: a  $Z_{\text{critical}}$  of about 172 [4]. This is basically the cutoff for any theoretical treatment of stable electronic configurations in a neutral superheavy atom, because there is no theoretical salvation beyond this point (yet). Arguably, it is the end of the Periodic Table or, at the least, of discussing the Periodic Table in contemporary language.

However,  $Z_{\text{critical}}$  does not preclude a stable electronic environment at the distant island of stability for  $Z = 164$ . What happens in row eight and beyond, between the two islands? Attempts have been made to derive the appearance of an extended Periodic Table up to about  $Z = 170$ . The influence of relativity is manifest in several different ways. All the  $s$ - and  $p$ -electron radial distributions contract as illustrated in Fig. 2 in the case of calculations for eka-radium [4]. A consequence of the contraction of these orbitals and their influence on higher angular momentum orbitals is that the latter, the  $d$ - and  $f$ -orbitals, expand slightly. A third significant effect imposed by escalating relativistic considerations is the substantial increase in spin-orbit splitting. For example, the threefold degenerate  $p$ -states sever into a  $p_{1/2}$  state and into a twofold degenerate  $p_{3/2}$  state. How these developments are incorporated into projecting the Periodic Table into the 8<sup>th</sup> row and beyond will be briefly sketched out next.

*Fig. 2. For  $Z = 120$ , eka-radium, the radial density distribution functions for the  $7s$ ,  $7p$  and  $8s$  orbitals from the non-relativistic (dashed) and relativistic calculations. Adapted from [4].*



## The Periodic Table (continued?)

Fig. 3. Simplest extension of the Mendeleev-Seaborg construct (see text for details)

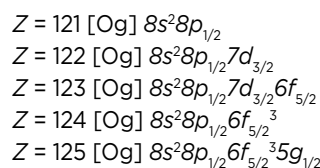
Fig. 4: Frickle et al [6] periodic table extension.

The first, and simplest, of these extensions is the *spdf* (shell partitioned display format) of the Mendeleev-Seaborg construction (Fig. 3), [5] which extends the Madelung (equal  $n+l$ ) aufbau, having the 8th row begin with the  $8s$  level; followed by the  $5g$  block containing 18 “superactinides” or “octadecanoids”; in turn followed by, and sometimes combined with, the  $6f$  block with 14 members; then the  $7d$  with 10 and finally the  $8p$  with 6 elements, completing the 8<sup>th</sup> row at eka-oganesson,  $Z = 168$ .

In the Mendeleev-Seaborg Table, the element with atomic number  $Z = 164$  emerges as a  $p$ -block element, suggestive of its possible chemical behavior. The anticipated first two elements in the 8<sup>th</sup> row, eka-francium and eka-radium, are  $s$ -block elements, and the next few, arguably within reach in the foreseeable future, are  $g$ -block elements. Significantly, for this Table and the alternatives to follow, even though the Table shows the  $5g$  filling after the  $8s$ , the electron configuration for the element with atomic number  $Z = 121$  is predicted to be  $[\text{Og}] 8s^2 8p_{1/2}$ .

Fricke et al. [6] constructed a different extended table, in which the element with atomic number  $Z = 164$  emerges as an  $s$ -block element (in the 9<sup>th</sup> row). See Fig. 4. As with the Mendeleev-Seaborg picture, the first few elements in the 8<sup>th</sup> row show as  $s$ -block and  $g$ -block family members.

Fricke and Soff, in 1977, [7] further refined these predictions: for the first few 8<sup>th</sup> row superheavy elements, they envisage:



Most recently, Pyykkö [8] described a more strongly re-configured Periodic Table, reproduced in Fig. 5. In this view, the element with atomic number  $Z = 164$  projects as a  $d$ -block atom. The first several elements in the 8<sup>th</sup> row would follow the  $s$ -block,  $g$ -block sequence, based on ion configurations that Pyykkö evaluated. For atomic structures through  $Z = 172$  ( $\approx Z_{\text{critical}}$ ), the sequence electron configuration develops as  $8s < 5g \leq 8p_{1/2} < 6f < 7d < 9s < 9p_{1/2} < 8p_{3/2}$ .

Ordering the electron orbital energies is a prodigious task because of the critical imposition of relativistic considerations which themselves are not yet totally resolved *vis-à-vis* quantum mechanics. It is recognized that the various valence orbitals are not anticipated to be pure states but rather confounded by mixed configurations, what nuclear physicists alternatively call “mixed parentage”. As an illustration, Nefedov [9] in 2006 considered the valence configuration of  $Z = 125$ . Eka-nep-tunium? Probably not. The preceding pictures suggest a configuration represented as  $[\text{Og}] 8s^2 5g^5$ . Nefedov instead arrives at a mixed description that contains contributions from  $[\text{Og}] 8s^2 5g 6f^2 8p^2$  and  $[\text{Og}] 8s^2 5g 6f 7d^2 8p$  and  $[\text{Og}] 8s^2 6f^2 7d 8p$ . Where do mixed configurations get placed on a Periodic Table that is founded on simple

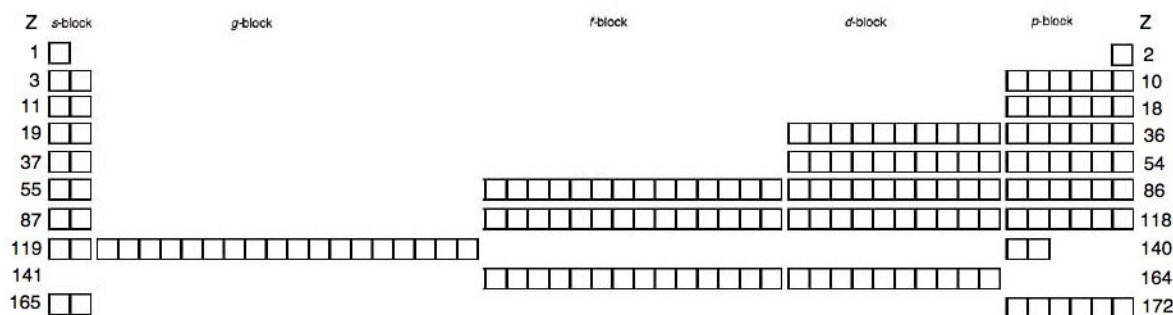


Fig. 5: Pyykkö [8] reconfigured periodic table.

electron configuration pedigree? That modest question is quite profound. But of course, if we don't get much beyond the next few new elements, it becomes moot.

Will new elements be produced? Accelerators used nowadays for superheavy element synthesis are cyclotrons or linear accelerators: the U400 at FLNR (Russia), the 88-Inch at LBNL (United States), the K-130 at JYFL (Finland), the UNILAC at GSI (Germany), the RILAC at RIKEN (Japan) or various cyclotrons at GANIL (France). The most successful methods for the synthesis of superheavy elements have been fusion followed by neutron evaporation reactions using heavy-element targets. Selective physical recoil-separation techniques of reaction products and the identification of nuclei, after implantation into position-sensitive detectors, are supplemented by seeking genetic ties to known daughter decay sequences. Fusion between Periodic Table row 7 elements serving as targets and  $^{48}\text{Ca}$  beams are currently impractical beyond  $^{118}\text{Og}$  because long-lived targets above  $^{98}\text{Cf}$ , such as  $^{99}\text{Es}$  and  $^{100}\text{Fm}$ , are produced only with tremendous cost and effort. Einsteinium is available only in microgram quantities. 100-day  $^{257}\text{Fm}$  availability is about a nanogram. To date, only a half-dozen attempts at row 8 have been made, none reporting convincing success

(see Table 1). Increasing the number of neutrons in superheavy reaction products would increase their stability. But the production of isotopes with more neutrons requires fusion reactions with projectiles heavier than  $^{48}\text{Ca}$ . Increasing the atomic number of the projectile also brings products closer to the stable proton shell(s) at  $Z = 120$  and  $126$ , where longer half-lives are expected. However, this will be a difficult undertaking. Most reaction models predict much lower cross sections for complete-fusion reactions with projectiles heavier than  $^{48}\text{Ca}$ . For cold fusion and hot fusion, decreases by a factor of about 3.6 are evident for every increase in atomic number of the fused systems (see Fig. 6) [10]. However, predictions in the SHE quest have proven challenging, with uncertainties of one or more orders of magnitude in both yields and half-lives being the norm.

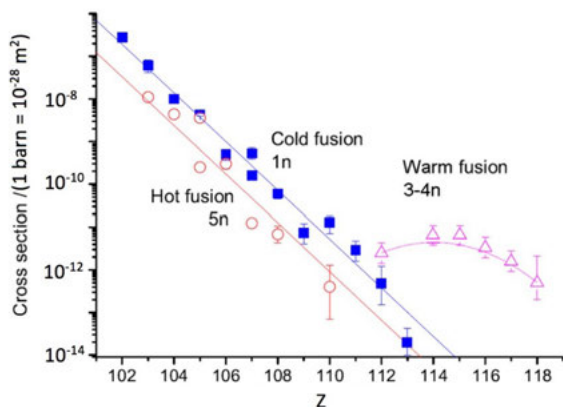
A dedicated facility is under construction: the "SHE Factory" at the Flerov Laboratory in Dubna, which will deliver significantly higher beam intensities than previously available. The French GANIL laboratory will soon open new facilities to study superheavies. The new Facility for Radioactive Ion Beams at Michigan State University will access new neutron-rich species. At GSI in Darmstadt, an accelerator with a beam intensity increased by a factor of 3.8 will serve to study superheavy nuclei. Anticipated improvements in target quantity, beam intensity, and transmission yield all bode well for the next handful of elements.

The possibility of multi-neutron transfer reactions using the heaviest feasible beams and targets has been considered as an alternative to the complete fusion synthesis route. Acceleration of beams of uranium are

Target	Projectile	Products	Year	Facility
$^{254}\text{Es}$	$^{48}\text{Ca}$	$^{119}\text{X}_{183-x} + xn$	1985	Berkeley
$^{244}\text{Pu}$	$^{58}\text{Fe}$	$^{120}\text{Y}_{182-x} + xn$	2007	Dubna
$^{238}\text{U}$	$^{64}\text{Ni}$	$^{120}\text{Y}_{182-x} + xn$	2009	GSI
$^{248}\text{Cm}$	$^{54}\text{Cr}$	$^{120}\text{Y}_{182-x} + xn$	2011	GSI
$^{249}\text{Cf}$	$^{50}\text{Ti}$	$^{120}\text{Y}_{179-x} + xn$	2011	GSI
$^{249}\text{Bk}$	$^{50}\text{Ti}$	$^{119}\text{X}_{180-x} + xn$	2011	GSI

Table 1: Reported attempts at row 8. A number of additional experiments are scheduled for the immediate future. At Dubna, a mixed isotopic target  $^{249}, ^{250}, ^{251}\text{Cf}$  bombarded with  $^{50}\text{Ti}$  is planned. At RIKEN,  $^{248}\text{Cm} + ^{54}\text{Cr}$  will be pursued.

## The Periodic Table (continued?)



**Fig. 6 Measured yields of superheavy elements grouped as evolving from high excitation energy compound nuclei (5 neutrons emitted), low excitation energy (1 neutron emitted) and “warm” excitation.**

included in the designs at several accelerators. The possibility of surprising results from, for example,  $^{238}\text{U} + ^{248}\text{Cm}$  or  $^{136}\text{Xe} + ^{208}\text{Pb}$  are on the horizon, the former seemingly a potential channel to  $Z = 164$ .

On a final note, there is the intriguing possibility of identifying superheavy elements, including new ones, in nature. There are two possible sources. Supernovae explosions, occurring in our galaxy once or twice per century produce rapid, successive neutron captures that can furnish doubly magic, neutron-rich  $^{78}\text{Ni}$ . During the explosive event, fusion with  $^{208}\text{Pb}$  could generate an anticipated 50 teratonnes of (arguably) very long-lived darmstadtium. Also, recently discovered collisions between neutron star pairs and even black hole pairs might be spawning nuclei around  $A = 340$  and stable  $N = 164$ , reactions taking milliseconds and expected to be more efficient than the supernova path, although definitely rarer. Reaction residues dispersed continuously throughout space could have materialized terrestrially at extreme trace levels, if at all.



**Eponymous element hunters in Dubna, Yuri Oganessian on the left, then Georgii Flerov, and fifth is Glenn Seaborg.**

Searches are underway, but appropriate chemistry is needed for their isolation. 🧪

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# Chemistry Organizations in a Changing World

by Stephen A. Matlin, Alain Krief,  
Henning Hopf, and Goverdhan Mehta

**B**uilding bridges between global thinking and local action was the tag line of the 2016 International Year of Global Understanding. [1] This provides an invaluable opportunity for chemistry organizations to rethink their roles and responsibilities in a global context. For IUPAC, its approaching centenary adds a further impetus to the continual quest for sustainability, relevance, and value. Chemistry organizations have a long tradition of helping to develop and promote the interests of the subject and its practitioners. In a rapidly changing world, what is their fundamental purpose, what should be their roles, and how can they refresh themselves to best serve the field and also society at large?

## Spectrum of Chemistry Organizations

Since the earliest chemical societies were formed in the mid-19<sup>th</sup> century, [2] numerous and diverse chemistry organizations have evolved. A web search identified more than 250 that are currently active. [3, 4] At the international level, chemistry organizations have formed as geographical or global federations of national chemical societies and industry associations, as well as of bodies that focus on a specific chemistry subject area, technique, process, or class of substance; or as new entities with a specific goal, such as networking or the promotion of particular objectives. Chemistry organizations have developed a diverse



array of activities (see box below). As a well-known example, the International Union of Pure and Applied Chemistry (IUPAC), formally founded in 1919, includes many national chemical societies among its members and provides global networking opportunities through its diverse activities. It has developed a number of distinctive functions (see box on next page).

## Emerging Changes Necessitate Action

Chemistry organizations are encountering many new challenges and face new realities in the 21<sup>st</sup> century. Externally, the global landscape in which chemistry operates is changing and the field is compelled to refresh both its identity as a science and its relevance to society. Several clusters of issues can be discerned [6-10] in the field of chemistry, especially:

**Position in the ever-expanding space of sciences:** As a mature science where fundamental new discoveries are increasingly rare, chemistry needs to find effective

## Examples of activities of chemistry organizations

- Acting as learned societies—providing opportunities for knowledge exchange and dissemination, outreach between members, and outlets for publications, as well as establishing a framework for recognizing excellence and contributions to industry and society.
- Serving as voices of the profession and liaising with other stakeholders, such as government regulators and the public.
- Protecting the interests of the professionals in diverse ways (e.g. advising on career development, safety standards, and remuneration levels; lobbying with entities that are critical to the profession).
- Protecting the public interest (e.g. by setting standards of professional competence, best practices, and codes of ethical professional conduct).
- Providing professional accreditation and certification to chemists and encouraging or certifying continuing education.
- Communicating about and projecting the value of the subject to diverse target audiences beyond the field, including the public and policy-makers.
- Recognizing the need to address global challenges.

## Some distinctive activities of IUPAC

- Providing a global service in setting criteria for recognizing new elements and definitions, standards, and nomenclature rules in the field of chemistry.
- Hosting meeting-grounds for discussions about aspects of chemistry, including chemistry education and research, through regular cycles of conferences.
- Serving as a publisher of technical reports, recommendations, and books.
- Organizing long-running series of conferences, e.g. Chemical Research Applied to World Needs (CHEMRAWN). [5]

ways to refresh and reinvigorate the understanding of chemistry as a central/enabling science that delivers new knowledge, useful applications and the underpinning of adjacent sciences among practitioners and also those in related fields and those who determine the priorities for funding education and research.

**Ambition as a science that solves large-scale contemporary challenges:** To avoid declining into a science that only progresses through small, incremental, and often predictable changes, chemistry needs to develop the space, ambition, and courage to tackle large-scale and risky undertakings. These include 'grand challenges' (large-scale problems that require collective international effort and funding beyond the normal scope of national programmes), whether relating to fundamental problems that will result in disruptive step-changes to understanding, or to applied problems that will contribute to the benefit of society globally.

**Perception and image of chemistry among scientists, the public, media and policy makers:** Linked closely with the above issues is the need to overcome negative attitudes to chemistry. These include perceptions by some that chemistry is no longer an exciting science and that its practice in both industry and research is sometimes unethical and contributes to pollution and damage to health and the environment.

**The shifting profile of chemistry-related activities across geographies:** With the growth of chemistry research, innovation, production, and publication in countries like China, India, and Brazil, the locus of chemistry has shifted substantially from its traditional locations in Europe and North America and will continue to do so as new regions, including Africa, increase their capacities.

These are deep-seated developments that have been evolving over time and may require new frameworks of thinking, one recent example being the concept of 'one-world chemistry'. [9] Chemistry organizations need to contribute to the substantive adjustments and re-alignments required, including the need to refresh chemistry's sense of its own mission and purpose; reduce internal

fragmentation and barriers to working across disciplinary boundaries; embrace systems thinking within the education, research, and practice of chemistry; ensure the promotion of ethical approaches and research integrity in academia and industry; strengthen the promotion, championing, and steering of the chemical sciences; and strengthen diversity and inclusion. In this endeavour, it is important that all chemistry practitioners—especially educators, researchers, the chemical industry, and chemistry organizations—join forces in contributing to the evolutionary changes required. To be able to do this with objectivity and credibility, some chemistry organizations may need reforms that will amplify their remit and reset their priorities.

Internally, many chemistry organizations, and especially some at the international level, are also experiencing challenges, some of which are:

**Stagnating or declining membership:** Organizations may need to consolidate or expand their membership base, especially among the young, and concomitantly find ways to enhance the organization's relevance and value to all members.

**Stressed finances:** In an era when income from publications and membership are facing headwinds, there is pressure to find a sustainable financial model to support the core purposes of the organization.

**Jaded purpose:** The mission, objectives, strategic plans, and budgets may all require restructuring in order to align them with priorities and expectations in a changing world, rebalancing income generation, service to the membership, and attention to the needs of society. International organizations may additionally need to repurpose themselves to lead in meeting the global challenges by building appropriate networks to implement solutions, harnessing needed strength through partnerships.

**Archaic governance:** To overcome issues related to efficiency, while retaining the confidence of both the membership and society at large, each organization may need to make adjustments to guarantee the adoption of best practices with regard to democratic

# Chemistry Organizations in a Changing World

processes that ensure transparency, inclusion, diversity, rigorous evaluation, and renewal that will induct fresh talent into the decision-making processes. Global and regional federations and unions can be especially vulnerable to being captured by interested parties that wish to control or perpetuate agendas or positions. Special efforts may be needed to overcome this.

## Future Horizons

Responses to the emerging external and internal challenges appear patchy and inadequate. The focus of this article is not to evaluate in detail what the chemistry organizations have been doing, but, notwithstanding their many previous achievements, to suggest directions for reflection.

How can each chemistry organization adapt to help lead and support the repositioning of the field, as well as to ensure its own continued relevance and sustainability? Given the diversity of current organizations, there can be no uniform answer to these questions. What may be useful, however, is a menu of options for consideration that could help to stimulate reflection and focus attention on areas of strength, weakness, and also on opportunities for each organization. Such a menu might cover:



### **Vision, mission, and organizational objectives and strategy:**

Are these clearly stated, publicly visible, and periodically revisited with both internal and external inputs? To what extent do they reflect the changing landscape (in and beyond the field of chemistry) within which the organization works, the changing circumstances in which its membership operates, the changing nature of target groups in and beyond the profession, and the evolving nature of global challenges that require chemistry to contribute to solutions? Is the organization's agenda an inherited one, whose relevance might be eroding but linked with embedded interests that work to perpetuate themselves?



### **Ethics and research integrity:**

Does the organization have formal policies, rules, and procedures for ethical behaviour and integrity regarding its own practices? Does it make systematic efforts to promote these values among its membership and in the wider community? Does it align with the recent initiatives that generated the Hague Ethical Guidelines [11] and the drafting of a global code of ethics for chemists [12] based on these guidelines?



**Building on strengths:** It is important that chemistry organizations working at the national level give attention to factors that relate to the respective country's history, resources, challenges, and opportunities and that recognize its strengths and weaknesses. Strengths may include, for example, a history of success in education, academic research, and the chemical industry or the use of traditional knowledge, such as the use of plant products in medicine. At the global level, strengths may include the convening power of international organizations to bring together diverse views, transcend borders, and orchestrate solutions.



### **International perspective:**

Does the organization have a coherent plan for international engagement, supported by appropriate resources? Global organizations must necessarily take a worldwide view of the field they serve and operate accordingly. But in the 21<sup>st</sup> century national societies, constituted in the first place to serve the field of chemistry and its practitioners in their own country, need to ensure that they also acquire an international perspective to their work. Chemistry organizations can foster engagements in diverse forms, from formal partnerships and collaborative efforts to participation in networks, projects, campaigns, and events. [13]



**Chemistry education:** Whether or not the organization lists education among its primary objectives, does it acknowledge that all those engaged in the chemistry enterprise have an obligation to promote their field, including through education? This may be concerned, at a systemic level, with the formal teaching of chemistry in schools, colleges, or universities; the upgrade of professional knowledge (e.g. through continuing education); or, at a more general level, investment in communication and interaction initiatives that help to promote and develop improved societal scientific literacy and understanding of contemporary challenges. Chemistry organizations should use their capacities to champion and strengthen chemistry education, and ensure it remains contemporary in its content, focus, and methodologies.



**Open access:** The unrestricted flow of scientific knowledge requires open access journals. Does the policy and practice of the organization permit open access to its publications? How free is this access to authors and to

# Chemistry Organizations in a Changing World

readers globally? Many chemistry bodies are changing their approaches, seeking new models. A striking example of innovative change in an adjacent field has been the launch of a free open access, rapid publication journal, *eLife*, which has attracted peer esteem and substantial support from some of the world's biggest private biomedical funders. Why not *eChemistry*?



**Industry interface:** Traditionally there were very strong relationships between the chemical industry and academia (e.g. Liebig's model). These have served as a pivot for the growth, contribution, and common welfare of the discipline for the last century and a half, but have been eroding. Are chemistry organizations developing models and strategies to restore and re-energise this interface?



**Funding for the field:** Funding for chemistry research is woefully inadequate in many places and facing a crisis situation in some parts of the world. Chemistry organizations should do more to draw the attention of policy makers to this problem, help garner public support for remedying the situation, and encourage industry to invest more in the creation of new knowledge on which it depends.




**Periodic evaluation:** Many bodies in diverse fields throughout the world undertake independent external evaluations (IEEs), which serve as a mechanism for accountability to the stakeholders in the organization and as a means to conduct formative policy and strategy reviews that can help move an organization beyond the constraints of its legacy practices and the vested interests of its current staff or sub-groups of influential stakeholders. Does the chemistry organization subject itself to periodic IEEs of its purpose, functions, and performance, set against both internally defined criteria and external criteria that look at the organization's comparative advantage in a competitive world, its long-term viability, and its value to the community it serves and the world at large? As an example, in the 1990s the International Council for Science (ICSU) commissioned an independent review [14, 15] to rejuvenate itself, which resulted in major changes in the organization's approach to strategic planning and methods of work. [16] It is notable that few, if any, chemistry organizations ever undertake such independent external valuations. Some, like IUPAC, [17] maintain an internal evaluation function that focuses on

areas such as project evaluation and delivery. This does not obviate the need to scrutinise the broader strategic vision and performance of an organization and its value to its membership, the field of chemistry, or the world at large.



**Communications and image:** Negative public perceptions of chemistry and its attractiveness to the young are issues of continuing concern, particularly because the discipline is sometimes subject to poorly informed comment. This requires redress through active communication and image refurbishing efforts. There is also a need to create a public forum for articulating views on contemporary issues concerning chemistry and its future. Does the organization have a communications strategy that is linked to the overall organizational strategic plan? Does it include dialogue and communication about and projecting the value of the subject to diverse target audiences beyond the membership and beyond the field, including the media, the public, and policy-makers?

## Conclusion

The field of chemistry faces a number of severe challenges in the 21<sup>st</sup> century as it strives to refresh its purpose, sustain support from society, and continue to provide solutions to contemporary global problems, amounting to no less than planetary sustainability. Chemistry organizations have a central role to play in helping chemistry respond to these pressures, but at the same time they must overcome some major internal challenges that require deep-seated reforms to enable them to give better service to their own chemistry communities and to the field of chemistry. This will require breaking long-standing traditions of many of these associations: champions at both leadership and grassroots levels must step forward and press the case for reform. Each organization needs to do its own critical analysis (with assistance from independent external evaluations as appropriate) to ensure it is fit for its purposes. Implications for national chemistry organizations have been discussed in a separate article. [18] International organizations must also play their part. 

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## IUPAC and the Organisation for the Prohibition of Chemical Weapons Take Partnership to New Level

On 1 December 2016, the Director-General of the Organisation for the Prohibition of Chemical Weapons (OPCW), Ambassador Ahmet Üzümcü and IUPAC President, Professor Natalia Tarasova, signed a Memorandum of Understanding (MOU) pledging to enhance cooperation to keep abreast of developments in chemistry, responsibility and ethics in science, and education and outreach.



OPCW Director-General Ahmet Üzümcü (right) and IUPAC President Natalia Tarasova signed an MOU pledging to enhance cooperation.

Ambassador Üzümcü remarked, “Promoting responsible science is a crucial endeavour to advance the goals of the Chemical Weapons Convention. Without scientists, there is no disarmament. IUPAC’s unwavering commitment to a world permanently free of chemical weapons demonstrates the strength of this norm and the conviction of chemistry researchers and practitioners globally to protect it”.

Professor Tarasova expressed, “Through the co-operation between our organisations, we look to help humanity achieve Sustainable Development Goals in a world free of chemical weapons and in a world in which achievements in chemical science and technology are used only for the benefit of humankind and the environment”.

The MOU opens a new chapter and underscores the long-standing and productive relationship between OPCW and IUPAC.

Read more about IUPAC cooperation with OPCW in the President’s Column page 2 or see [iupac.org](http://iupac.org) News section.

[www.iupac.org/iupac-opcw-take-partnership-new-level/](http://www.iupac.org/iupac-opcw-take-partnership-new-level/)

## IUPAC Announces the Names of the Elements 113, 115, 117, and 118

On 28 November 2016, the International Union of Pure and Applied Chemistry (IUPAC) approved the name and symbols for four elements: nihonium (Nh), moscovium (Mc), tennessine (Ts), and oganesson (Og), for element 113, 115, 117, and 118, respectively.

Following a 5-month period of public review, the names, proposed earlier by the discoverers, have been approved by the IUPAC Bureau.

Keeping with tradition, the newly discovered elements have been named after a place or geographical region, or a scientist. The ending of the names also reflects and maintains historical and chemical consistency: “-ium” for elements 113 and 115, as for all new elements of groups 1 to 16, “-ine” for element 117, belonging to group 17, and “-on” for element 118 as an element belonging to group 18. The recommendations were published in the December 2016 issue of *Pure and Applied Chemistry* ([doi.org/10.1515/pac-2016-0501](https://doi.org/10.1515/pac-2016-0501)). (The earlier provisional recommendations with the explanation of the names were published in CI Sep 2016, p. 30; no changes to the proposed names and symbols were introduced following the public review period).

Comments from the general public during the 5 month public review period were many. Apart from many full agreements, comments were received suggesting other names, in some cases accompanied by petitions from large groups of people. However, these suggestions could not be accepted, given the fact that under the current guidelines only the discoverers have the right to propose names and symbols. Questions were also received about the pronunciation of the names and the translations into other languages. Members of the chemistry community also raised the concern that Ts is one of the two commonly used abbreviations for the t-syl group. Recognizing, however, that many two-letter abbreviations have multiple meanings—even in chem-

INTERNATIONAL UNION OF PURE AND APPLIED CHEMISTRY

For names and symbols to the table, see [www.iupac.org](http://www.iupac.org). The names are dated January 23, 2016. Copyright © 2016 IUPAC, the International Union of Pure and Applied Chemistry.

istry, and for example Ac and Pr— the conclusion was made that the context in which the symbols are used makes the meaning unambiguous.

“Overall, it was a real pleasure to realize that so many people are interested in the naming of the new elements, including high-school students making essays about possible names and telling how proud they were to have been able to participate in the discussions,” said Professor Jan Reedijk, President of the Inorganic Chemistry Division. He added “It is a long process from initial discovery to the final naming, and IUPAC is thankful for the cooperation of everyone involved. For now, we can all cherish our periodic table completed down to the seventh row.”

“The names of the new elements reflect the realities of our present time” said IUPAC President Prof Natalia Tarasova, “universality of science, honoring places from three continents, where the elements have been discovered—Japan, Russia, the United States—and the pivotal role of human capital in the development of science, honoring an outstanding scientist—Professor Yuri Oganessian”.

The exploration of new elements continues, and scientists are searching for elements beyond the seventh row of the periodic table. IUPAC and the International Union of Pure and Applied Physics (IUPAP) have recently established a new joint working group, whose task will be to examine the criteria used to verify claims for the discovery of new elements.

See full release in the News section of [iupac.org](http://iupac.org)  
[www.iupac.org/iupac-announces-the-names-of-the-elements-113-115-117-and-118/](http://www.iupac.org/iupac-announces-the-names-of-the-elements-113-115-117-and-118/)

## IUPAC Periodic Table of the Elements—Updated Release

**A**n updated version of the Periodic Table has been released on 28 November 2016 which includes the recently added elements 113, 115, 117, and 118 and all standard and conventional atomic weights.

The standard atomic weights (abridged to five significant digits) and the conventional atomic weights are extracted from the most recent 2013 review published in *PAC* Vol. 88, No.3, pp. 265-291 (<http://dx.doi.org/10.1515/pac-2015-0305>). For ytterbium, the standard atomic weight is based on the 2015 review. An interval in square brackets provides the lower and upper bounds of the standard atomic weight for that element. For users needing an atomic-weight value for an unspecified sam-

ple without regard to the uncertainty, the conventional values are provided. No values are listed for elements which lack isotopes with a characteristic isotopic abundance in natural terrestrial samples. See *PAC* for more details or visit Commission II.1 at [www.ciaaw.org](http://www.ciaaw.org). Visit [www.isotopesmatter.com](http://www.isotopesmatter.com) for an interactive version of the Periodic Table of the Elements and Isotopes.

A reprint of that table is included as this issue's back cover tear-off page. To download the printable (PDF) version, see the following webpage: [www.iupac.org/what-we-do/periodic-table-of-elements](http://www.iupac.org/what-we-do/periodic-table-of-elements)

## Gender-based Harassment in the Practice of Science

**O**n the occasion of the International Day for the Elimination of Violence against Women—25 November 2016, [www.un.org/en/events/endviolenceday](http://www.un.org/en/events/endviolenceday)—the International Council for Science (ICSU) called for more effective strategies to promote gender equality and equitable access to all resources in the practice of science, notably in the area of field research, and to remove barriers to the full participation in science by women.

This call emerged from a workshop organized by the ICSU Committee on Freedom and Responsibility in the Conduct of Science (CFRS), the Mexican Academy of Sciences, and the ICSU Regional Office of Latin America and the Caribbean on “Gender Issues in Field Research: Mobility and Internationalization of Science,” held in Mexico City on 27 April 2016. (see *CI* Sep 2016, p. 37; doi: [10.1515/ci-2016-0527](https://doi.org/10.1515/ci-2016-0527))

Gender-based harassment can limit the mobility of women researchers and contribute to the under-representation of women in senior careers, as scholars and as leaders in science and industry. Such barriers have the potential to harm the integrity of the research community, relationships amongst its practitioners, and victims' commitment to scientific research and scholarship. The advisory note “**Mobility and Field Research in the Sciences: Gender Equality and Prevention of Harassment**” is available online.

This advisory note, based on the ICSU's Statute 5 on the *Principle of Universality of Science*, commits the council and its members to supporting scientists' freedom of movement, association, expression, and communication, and to promoting equitable and non-discriminatory access to science.

[www.icsu.org/freedom-responsibility/advisory-documentation](http://www.icsu.org/freedom-responsibility/advisory-documentation)

### ICSU to Merge with ISSC

**A**t an extraordinary General Assembly of the International Council for Science (ICSU) and General Assembly of the International Social Science Council (ISSC), held in Oslo on 24 October 2016, members voted overwhelmingly that the two organizations should merge. This in-principle decision followed a recommendation by the two organizations' executives, setting the two councils on a trajectory to become one by October 2018.

For the plans to go ahead, the majority of both councils' voting members needed to vote in favour. 76% of ICSU members and 87% of ISSC members voted in favour of a merger of the two organizations, thereby setting the merger process in motion.

Gordon McBean, President of ICSU, said: "ICSU has long been a champion for excellence in both disciplinary and transdisciplinary science, and seeks to bring that excellence together to address global challenges. Today's vote confirms support for this approach and I want to thank our Unions and National Members for their support. As a unified body, we will be in a stronger position to confront the challenges of the twenty-first century. With a broadened membership base the new organization will be the inclusive global voice of science that we want it to be."

The vote is an *in-principle* agreement to merge the two councils, and to establish a Transition Task Force to develop detailed transition plans, including legal requirements, new statutes, and governance structures for the merged organization. The Task Force proposal will be put to a vote during a joint meeting of ICSU and ISSC Members in October 2017 at the 32nd ICSU General Assembly in Taipei. If the two organizations' members endorse these plans in 2017, the transition will be implemented and overseen by the ISSC and ICSU executives, with a founding General Assembly of the new organization tentatively planned for October 2018.

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

### Remembering Peter Greaves Taylor Fogg (1929-2016)

**A**s a young man, Peter Fogg won an open scholarship to Trinity College, Oxford, where he read chemistry. After gaining a first class degree, he went on to do a doctorate under the supervision of J.D. Lambert. His thesis was on Ultrasonic Dispersion in Gases.



*Peter and Heather at a 1996 IUPAC conference in Hungary*

From 1954-1955 Peter worked as a Scientific Officer at The Atomic Energy Research Establishment in Harwell, Oxfordshire, where he worked on the chemistry of plutonium. He was an assistant lecturer at Queen's University, Belfast from 1956 to 1958 and worked as a research chemist for Monsanto Chemicals, Ltd. between 1958 and 1962. In 1962 he became a lecturer at Flintshire Technical College in North Wales.

Peter taught at the University (formerly Polytechnic) of North London from 1965 until 1986. His undergraduate teaching was primarily concerned with Physical Chemistry and was much appreciated by his students, who found him especially helpful in both practical sessions and tutorials. At the University, Peter supervised the PhD/postgraduate work of several students and gained their gratitude and respect. When joining the University, Peter was active in the research of fast reaction kinetics and then, in collaboration with colleague John Charalambous, on the development of metal complexes for scintillation counting applications, leading to publication in *Polyhedron*.

He was a very active member of the IUPAC Solubility Data Commission V.8 of the Analytical Chemistry Division from its early years, and contributed to the shaping of its successor, the Subcommittee on Solubility and Equilibrium Data. The Solubility Data Project benefited greatly from his expertise in, and passion for, the field of gas solubilities in liquids and solutions. Between 1983 and 2013, Peter was compiler, evaluator, and editor for seven volumes (numbers: 21, 32, 42, 50, 70, 76 and 97) of the IUPAC Solubility Data Series.

Peter was also Chair of Subcommittee V.8.1 (Gases in Liquids) from 1992 to 2000 and was a Titular Member of Commission V.8 in 1987-1989 and again in 1995-1997.

He also actively participated in the International Symposia on Solubility Phenomena (ISSP). He was Co-Chair of the 3rd ISSP (1988, Guildford, University of Surrey) and was Guest Editor for the plenary and invited lectures of the 7th (Leoben, Austria, 1996), 8th (Niigata, Japan, 1998) and 9th (Hammamet, Tunisia, 2000) ISSPs, published in *Pure and Applied Chemistry*.

Peter Fogg and William (Bill) Gerrard collaborated



on the publication of *Solubility of Gases in Liquids: A Critical Evaluation of Gas/Liquid Systems in Theory and Practice* (John Wiley and Sons, 1991), which was a significant contribution to that field, providing extensive information on, and data for, selected systems. Peter was also Editor-in-Chief of the Wiley Series in Solution Chemistry, which comprised authoritative, comprehensive, and up-to-date accounts of many aspects of solution chemistry. Seven volumes were published in this series between 1996 and 2003, including the seminal works: *Octanol-Water Partition Coefficients: Fundamentals and Physical Chemistry* (J. Sangster, 1997), *The Experimental Deter-*

*mination of Solubilities* (G. T. Hefter and R. P. T. Tomkins, eds., 2003) and *Chemicals in the Atmosphere: Solubility, Sources and Reactivity* (P. G. T. Fogg and J. Sangster, 2003).

Peter thoroughly enjoyed his involvement with IUPAC and the opportunities that it gave him and his wife Heather to travel and make friends all over the world. Peter's involvement was characterized by friendship and conviviality, together with passionate professional activity and challenging scientific discussions. Peter was both a gentle man and a gentleman, and both he and Heather enriched the life of all of us.



## Stamps International

### Woodward's Birth Centennial

Much has been written about Robert Burns Woodward (1917-1979), one of the world's leading organic chemists of the twentieth century, from his precocious interest in chemistry to his fearless talent and uncanny intuition as a researcher. His adroit synthesis of complex natural products is legendary: quinine, cholesterol, lysergic acid, strychnine, cortisone, several antibiotics, chlorophyll, vitamin B<sub>12</sub>, and many other intricate molecules. He received numerous honorary degrees, learned society memberships, and awards, including the 1965 Nobel Prize in Chemistry "for his outstanding achievements in the art of organic synthesis". In addition to synthetic organic chemistry, he proposed, in 1952 (with Geoffrey Wilkinson), the "sandwich" structure of ferrocene, a milestone in modern organometallic chemistry, and developed a set of rules to predict and explain the outcome and stereochemistry of pericyclic organic reactions (*i.e.*, the "Woodward-Hoffmann rules"). He authored some 200 publications and trained more than 200 Ph.D. students and postdoctoral research associates, many of who went on to have distinguished careers.



Despite the magnitude of his scientific legacy, Woodward was not philatelically recognized until the year 2015, when postage stamps paying tribute to the eminent chemist were issued in two African nations. The stamp from the Republic

of Guinea illustrated in this note is particularly puzzling, since it portrays Woodward next to a gorilla. It is part of a set of four stamp highlighting early pioneers of the fight against malaria, so it is fair to include Woodward for his well-known total synthesis of quinine (1944). A possible solution to the gorillian conundrum may be surmised from a 2010 study reported in *Nature*, in which an international team of researchers describe how gorillas may have been the original source of *Plasmodium falciparum*, the parasite responsible for the most prevalent and harmful form of malaria infecting humans. Hence, I must conclude that Woodward's companion on the Guinean stamp is a rather obscure but reasonable choice.



In turn, the stamp from the Republic of Chad, with a more conventional design, features the structure of reserpine, an alkaloid with antipsychotic and antihypertensive properties, whose total synthesis was completed by Woodward in 1956. Interestingly, the stamp includes, underneath the structural diagram of reserpine, the actual reference to the full paper published in *Tetrahedron* two years later describing in detail (57 pages!) this synthetic breakthrough.

The only two countries that have honored RBW with postage stamps may seem a bit unusual but I must praise the corresponding postal authorities for doing so in an ingenious and meaningful way!

Written by Daniel Rabinovich <[drabinov@uncc.edu](mailto:drabinov@uncc.edu)>.

## Environmental Fate and Risks of Nano-enabled Pesticides

Nanotechnology is emerging as a highly attractive tool for the formulation and delivery of pesticide active ingredients, as well as enhancing and offering more effective and environmentally friendlier crop protection products. A number of formulation types have been suggested, including emulsions (e.g. nanoemulsions), nanocapsules (e.g. with polymers), and products containing pristine engineered nanoparticles (such as metals, metal oxides and nanoclays). Some nano-enabled pesticides are in the pipeline and are expected to be presented for registration to the regulatory agencies. For example, US EPA recently registered a nano-enabled pesticide, AZteroid, which is based on Vive Crop Protection's Allosperse (a polymer-based delivery system).

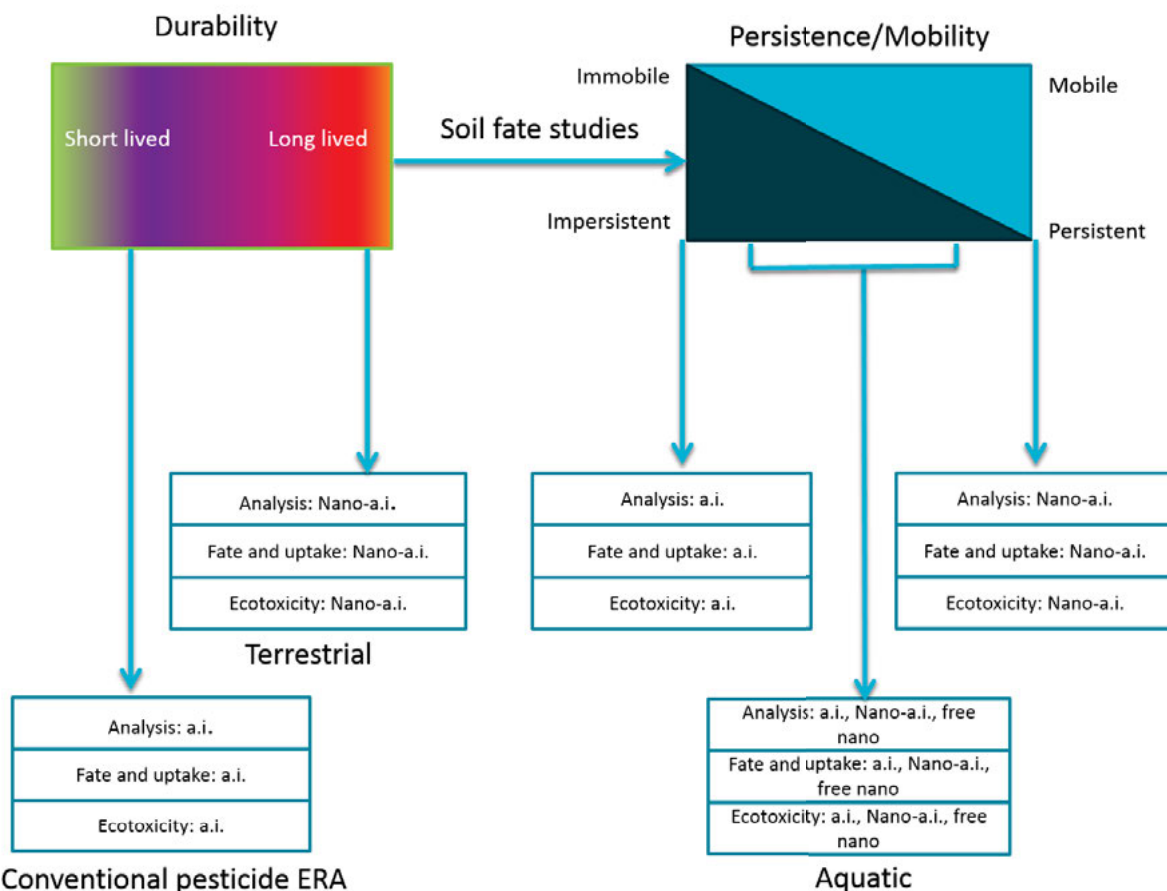
The increasing interest in the nano-enabled pesticides raises questions as to how to assess the environmental risk of these products for regulatory purposes. Therefore, there is a need to develop a set of guiding principles to facilitate a harmonized approach for the

environmental risk assessment (ERA) of nano-pesticides.

In response to the above, we have just concluded an IUPAC project on "Guiding principles to facilitate a harmonized ecological risk assessment framework for nano-pesticides in the environment" ([www.iupac.org/project/2012-020-3-600](http://www.iupac.org/project/2012-020-3-600)). The project has laid down some guiding principles and suggested an approach for consideration by regulatory agencies and industry (Kookana *et al.* 2014).

The project found that the existing tiered risk assessment approach, such as that used in the European Union, remains a useful framework for the risk assessment of nano-pesticides. In many situations, existing approaches can be used with some modifications and adaptations to cover nano-pesticides. In this regard, a crucial decision making step relates to the durability of a nano-enabled pesticide product and the fate of the product in soil (Figure 1). This criteria allows an assessment of whether a new nano-enabled product could be treated as a conventional pesticide, or if it needs to be treated differently, as a product that demonstrates

**Figure 1. Conceptual framework for assessing the environmental risk assessment (ERA) of nanopesticides**  
(taken from Kookana *et al.* 2014, with permission from ACS)





*Project participants in a workshop in York (UK) in May 2013, with Rai Kookana (far right).*

an altered efficacy or fate or toxicity profile. For example, a nano-formulation that is short-lived, *i.e.*, it releases the active ingredient (a.i.) relatively rapidly, the product can be treated as a conventional product. For relatively durable formulations, potential alterations in fate and behavior resulting from the nanoformulation can be accounted for, with some adaptations to existing approaches (Kookana *et al.*, 2014).

The industry feedback received so far indicates that the above appears to be a workable approach. The framework proposed by Kookana *et al.* 2014 is now being considered by regulatory agencies internationally (e.g. USEPA, Environment Canada, APVMA Australia).

Stakeholder consultations undertaken during the above project, especially with industry representatives and regulators, highlighted the need for some specific guidance on data requirements and the associated methodology, based on specific product-types and driven by the problem-formulation stage of risk assessment. Practical information is needed to answer the following key questions:

1. When a new product is presented to the regulators, what are the key questions that they would like to ask? This essentially defines the **problem formulation step** in the ERA framework.
2. What are the key characterizations and analytical requirements for the specific product that may be necessary to answer the question posed at 1 for a specific product type?
3. What are the specific methods or approaches for environmental fate and effects that are readily

available and appropriate to answer the questions for the specific product under consideration?

4. What are the current knowledge gaps and uncertainties that the regulators and industry need to consider for a pragmatic approach to decision making?

It was recognized that there is a need to enhance understanding among industry and regulators on:

- The environmental fate and effects data that regulators will require to determine the risk profile of nano-pesticides.
- What methods/approaches are appropriate and acceptable to give industry confidence in obtaining and submitting the data required to satisfy the regulatory requirements?

Therefore a sequel project has been initiated to develop a practicable approach for generating sound data required for satisfying ecological risk requirements for the purposes of registration of nano-enabled pesticides.

## Reference

Kookana *et al.* 2014, *Journal of Agriculture and Food Chemistry*, **62**:4227-4240; <http://dx.doi.org/10.1021/jf500232f>

For more information about this project contact the Task Group Chair Rai Kookana <Rai.Kookana@csiro.au>  
[www.iupac.org/project/2016-016-2-600](http://www.iupac.org/project/2016-016-2-600)



### Ecological Risk Assessment Workshop for Central America

Substantial amounts of pesticides are used in agriculture in Latin America, in both crops for local consumption and export crops such as bananas, plantains, and pineapples. It is important that the pesticides used do not pose a risk to human health and the environment.

Regarding the environment, it is proposed that an Ecological Risk Assessment Workshop for Central America be held in Costa Rica, in order to:

1. promote and transfer current scientific knowledge on ecological risk assessment
2. highlight the advantages and disadvantages of risk assessment procedures
3. provide a guidance document on the development of ecological risk assessment

This guidance document will give participants more detailed information on risk assessment. However, it is not intended to be a comprehensive handbook, but rather to enable participants to ask the right questions when risk assessments are required.

It is intended that the workshop in Costa Rica will form an integral part of the 6th Latin American Pesticide Residue Workshop (LAPRW 2017, 14-17 May, <https://laprw2017.fundacionucr.ac.cr>), a biennial forum for discussion in which different concepts and future developments are presented on pesticide residues in food and the environment. Key partners will be CropLife International and the Red Analítica de Latinoamérica y el Caribe (RALACA).

For more information about this project contact the Task Group Chairs Elizabeth Carazo Rojas or John Unsworth <[unsworthjo@aol.com](mailto:unsworthjo@aol.com)>



<https://laprw2017.fundacionucr.ac.cr>

[www.iupac.org/project/2016-025-1-600](http://www.iupac.org/project/2016-025-1-600)

### A Critical Review of Reporting and Storage of NMR Data for Spin-Half Nuclei in Small Molecules

The last IUPAC recommendations on nomenclature, nuclear spin properties and chemical shift conventions were published in 2001 [1], and followed by some additional recommendations in 2008 [2]. Recently, a publication by Pauli *et al.* [3] presented some arguments for the need for enhanced precision in  $^1\text{H}$  NMR measurement and concluded by recommending the use of four decimal  $\delta$  values in ppm and one to two decimal  $J$  values in Hz for interpretation and reporting; members of the organic chemistry ("small molecule") community routinely placing NMR data in the literature for characterization purposes would generally resist such a detailed approach.

RSC, ACS, Elsevier, and Wiley journals all use different conventions for reporting NMR data; some journals also use tabular formats, again with inconsistent presentation modes. Practicing organic chemists would prefer a single uniform approach for the routine characterization of small organic molecules, so as to avoid inconsistencies and/or the tedious process of editing data according to individual journal formats. However, conventions for reporting NMR data need to be agreed on together with the specialist spectroscopy and metabolomics communities. In principle, given the availability of NMR processing software, tabular presentation of NMR data could be supplemented and possibly even replaced by the provision of raw FID data.

In view of modern access to (very) high field NMR spectrometers, combined with the data storage capability provided by the internet, the task group aims to revisit the previous IUPAC recommendations (2001, 2008), to reconsider them in the light of access to very high field NMR spectrometers, and to provide a single agreed-upon format for the reporting and storage of (spin-half) NMR data for solution spectra of small molecules in the mainstream chemical literature.

File format specifications need to be assessed (e.g. JCAMP-DX) and explored (e.g., NMRml) with all stakeholders, so as to inform practices for archiving and publication, and ultimately for chemists collecting and managing their raw NMR data. Ideally, consensus on specifications would be achievable as an outcome of TG deliberations, but the specific requirements of individual software manufacturers need to be respected. As the interpretation of the data is crucially important, metadata becomes more and more important for any data format. Thus, this topic is not just a topic for the



hard- and software part of the community, but really for everybody.

### References

1. R.K. Harris, *et al.*, NMR nomenclature. Nuclear spin properties and conventions for chemical shifts (IUPAC Recommendations 2001) *Pure Appl. Chem.* 2001, 73, 1795-1818; <http://dx.doi.org/10.1351/pac200173111795>
2. R.K. Harris, *et al.*, Further conventions for NMR shielding and chemical shifts (IUPAC Recommendations 2008), *Pure Appl. Chem.* 2008, 80, 59-84; <http://dx.doi.org/10.1351/pac200880010059>
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4. A.N. Davies and P. Lampen, JCAMP-DX for NMR, *Appl. Spectrosc.* 1993, 47, 1093-1099.

More information about this project contact the Task Group Chair Mary Garson <m.garson@uq.edu.au>  
[www.iupac.org/project/2016-023-2-300](http://www.iupac.org/project/2016-023-2-300)

## Guides in Metrology

*by Juris Meija and Stephen Ellison*

The Joint Committee for Guides in Metrology (JCGM) is tasked with maintaining and promoting the use of the "Guide to the Expression of Uncertainty in Measurement" (known as the GUM) and the "International Vocabulary of Metrology" (known as the VIM). The JCGM operates through two working groups: JCGM-WG1, with responsibility for the GUM, and JCGM-WG2, with responsibility for the VIM. JCGM has eight member organizations, which include IUPAC. IUPAC is currently represented in the JCGM-WG1 by Stephen Ellison (LGC, UK) and Juris Meija (NRC, Canada).

The June 2016 meeting of WG1 focused primarily on two items of business: actions following member and National Metrology Institute (NMI) comments on the 2015 Committee Draft of a revision of the GUM [1], and steps towards a further JCGM Supplement covering the construction of a 'measurement model' suitable for the evaluation of measurement uncertainty.

The draft revision of the GUM (sometimes referred to as "GUM2") followed from a desire to improve the internal consistency of the GUM and its consistency with later Supplements, and to improve its applicability

across measurement sectors; a summary of the rationale was given by Bich. [2] An on-line survey in 2012 gave further support to some of these objectives, particularly the need to address a wider range of measurement problems. To improve consistency, the JCGM decided to adopt a consistent Bayesian approach. This offers a more general framework, naturally incorporating non-normal distributions and non-linearity. It also provides for more consistent treatment of Type A and Type B evaluations of uncertainty and in many simple cases it avoids the need for a calculation of effective degrees of freedom. In December 2014, a Committee Draft [1] was produced and circulated among the eight Member Organizations, including IUPAC, as well as National Metrology Institutes of the States that have ratified the Metre Convention.

By June 2015, JCGM-WG1 had received a considerable body of feedback on the proposed Committee Draft. IUPAC provided an opinion similar to those given by other member organizations, such as ISO, and by leading National Metrology Institutes, such as NIST (USA), PTB (Germany), NRC (Canada), and LNE (France). Though there was some recognition that the new approach helped in some areas, the great majority of comments strongly opposed replacement of the existing document with the proposed revision. Many did not see sufficient justification for replacement, and it was clear that many felt that the costs associated with changes in procedure in calibration and testing laboratories would be disproportionate where the existing Guide had been found sufficient. [3] Some responses also identified technical issues that would hamper the new version's application in particular fields; for example, the proposed treatment could become problematic if some uncertainties are unavoidably associated with very small degrees of freedom.

JCGM-WG1 has now given careful consideration to all of the comments received. A detailed response to the comments has been prepared and will be made available to member bodies in due course. In general, however, the working group acknowledges that the proposed GUM2 has failed to adequately communicate the rationale for revision of the GUM. The working group has also taken note of concerns relating to the cost of change in laboratories that find the present Guide sufficient. As a result, JCGM-WG1 is considering a wider range of options for moving forward in the light of the feedback received. Replacement of the existing Guide is not envisaged in the short term. One option under active consideration is a "new paradigm" whereby the GUM becomes a multi-part guide, in which different parts differ in scope, complexity, and field of application.

Meanwhile, the working group is moving forward on other guidance. The majority of the JCGM-WG1 June

2016 meeting time, together with a subsequent drafting group meeting in July, was spent on JCGM 103: *Supplement 3 to the Guide to the Expression of Uncertainty in Measurement*. This new guidance document deals with the development and use of measurement models. In addition to setting out the general structure of possible measurement models, the supplement covers a variety of mathematical aspects that are useful in metrology. Example topics include model choice for numerical stability, model parametrization, dealing with implicit measurement models (in which the result cannot be simply written as a function of input variables), and the use of transformations to simplify models or improve the accuracy of computation. A draft of this new Guide is in the late stage of completion and anticipated in early 2017.

## References

1. JCGM 100:201X Committee Draft—Evaluation of measurement data—Guide to uncertainty in measurement, Issued to member bodies December 2014
2. W. Bich, Revision of the 'Guide to the Expression of Uncertainty in Measurement'. Why and how. *Metrologia* **51**:S155–S158 (2014)
3. W. Bich *et al.* Towards a new GUM—an update. *Metrologia* **53**:S149–S159 (2016)

For more information, please contact Juris Meija <Juris.Meija@nrc-cnrc.gc.ca>. Dr. Meija is a Titular Member of the IUPAC Interdivisional Committee for Terminology, Nomenclature and Symbols, Chair of the IUPAC Commission on Isotopic Abundances and Atomic Weights, and IUPAC representative on JCGM-WG1.

## Bookworm

Books and publications hot off the press.  
See also [www.iupac.org/what-we-do](http://www.iupac.org/what-we-do)

### Successful Drug Discovery

János Fischer and Wayne E. Childers (Eds)  
Wiley-VCH, 2016, ISBN: 978-3-527-34115-3

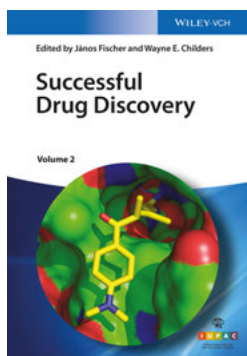
The goal of this book series is to help experts in drug research and development, both in academia and industry, with case histories described by their key inventors or by recognized experts whose contributions can also serve as teaching examples.

Published in December 2016, Volume 2 retains the successful approach found in the previous volume: inventors and primary developers of drugs that made it to market tell the story of the drug's discovery and development and relate the often twisted route from the first candidate molecule to the final marketed drug. Eleven selected case studies describe recently introduced drugs that have not been previously covered in textbooks or general references. These range across six different therapeutic fields and provide a representative cross-section of current drug development efforts. Sections include:

- I. HDAC Inhibitor Anticancer Drug Discovery
- II. Steroidal CYP17 Inhibitor Anticancer Drug Discovery
- III. Anti-infective Drug Discoveries
- IV. Central nervous system (CNS) Drug Discovery

V. Antiulcer Drug Discovery

VI. Cross Therapeutic Drug Discovery (Respiratory Diseases/Anticancer)



2016 marked the 10th anniversary of the approval of vorinostat, the first marketed histone deacetylase (HDCA) inhibitor. This event inaugurated a stream of HDAC inhibitor approvals and confirmed the validity of this drug target and of epigenetic modulation as a viable therapeutic mechanism. To celebrate this important milestone, *Successful Drug Discovery* presents a number of HDAC inhibitor drug discovery stories.

Backed by copious data and chemical information, the insight and experience of the contributors makes this volume one of the most useful training manuals that a junior medicinal chemist can hope to find. The book is the outcome of an IUPAC project.

See detailed Table of Contents on [wiley.com](http://wiley.com).

[www.wiley.com/WileyCDA/WileyTitle/productCd-3527341153.html](http://www.wiley.com/WileyCDA/WileyTitle/productCd-3527341153.html)  
[www.iupac.org/project/2015-026-1-700](http://www.iupac.org/project/2015-026-1-700)

## Source-based Nomenclature for Single-strand Homopolymers and Copolymers (IUPAC Recommendations 2016)

Richard G. Jones, *et al.*

*Pure and Applied Chemistry*, 2016

Volume 88, Issue 10-11, pp. 1073-1100

IUPAC recommendations on source-based nomenclature for single-strand polymers have so far addressed its application mainly to copolymers, non-linear polymers and polymer assemblies, and within generic source-based nomenclature of polymers. In this document, rules are formulated for devising a satisfactory source-based name for a polymer, whether homopolymer or copolymer, which are as clear and rigorous as possible. Thus, the source-based system for naming polymers is presented in a totality that serves as a user-friendly alternative to the structure-based system of polymer nomenclature. In addition, because of their widespread and established use, recommendations for the use of traditional names of polymers are also elaborated.

<http://dx.doi.org/10.1515/pac-2015-0702>

## Comprehensive Definition of Oxidation State (IUPAC Recommendations 2016)

Pavel Karen, Patrick McArdle, and Josef Takats

*Pure and Applied Chemistry*, 2016

Volume 88, Issue 8, pp. 831-839

Oxidation state (OS) gives the degree of oxidation of an atom in terms of counting electrons. [1] It scales trends in redox and acid-base properties, as well as in physical properties such as magnetism, and is a key component when tracking the course of chemical reactions. Thus, the concept of OS is important, and so is an agreed upon definition of what OS is and the algorithmic manner in which it is to be calculated. In the absence of an actual definition, algorithms have thus far been used to define OS.

This recommendation proposes a definition of OS based on ionic approximation of chemical bonds, illustrated on a molecular-orbital scheme and deduced from electronegativity considerations (Allen's scale). Two algorithms are formulated for the determination of OS in molecules, ions, and extended solids, and are illustrated with examples. Limits, beyond which OS ceases to be well-defined or becomes ambiguous, are

*The full scholarly paper providing the 2014 self-consistent set of values of the constants and conversion factors of physics and chemistry recommended by the Committee on Data for Science and Technology (CODATA) was published in September 2016 in Review of Modern Physics 88, 035009 (2016); <https://doi.org/10.1103/RevModPhys.88.035009>. The full text article, a wall chart, and a wallet card (reprint below) are available from the NIST website at <http://physics.nist.gov/cuu/Constants>*

## 2014 CODATA RECOMMENDED VALUES OF THE FUNDAMENTAL CONSTANTS OF PHYSICS AND CHEMISTRY NIST SP 959 (Aug 2015)

See: P. J. Mohr, D. B. Newell, and B. N. Taylor, [arxiv.org/pdf/1507.07956v1.pdf](http://arxiv.org/pdf/1507.07956v1.pdf) (2015).

A more extensive listing of constants is available in the reference given above and on the NIST Physical Measurement Laboratory Web site: [physics.nist.gov/constants](http://physics.nist.gov/constants).

Quantity	Symbol	Numerical value	Unit
speed of light in vacuum	$c, c_0$	299 792 458 (exact)	$\text{m s}^{-1}$
magnetic constant	$\mu_0$	$4\pi \times 10^{-7}$ (exact)	$\text{N A}^{-2}$
electric constant $1/\mu_0 c^2$	$\epsilon_0$	$8.854 187 817 \dots \times 10^{-12}$	$\text{F m}^{-1}$
Newtonian constant of gravitation	$G$	$6.674 08(31) \times 10^{-11}$	$\text{m}^3 \text{kg}^{-1} \text{s}^{-2}$
Planck constant	$h$	$6.626 070 040(81) \times 10^{-34}$	$\text{J s}$
$h/2\pi$	$\hbar$	$1.054 571 800(13) \times 10^{-34}$	$\text{J s}$
elementary charge	$e$	$1.602 176 6208(98) \times 10^{-19}$	$\text{C}$
fine-structure constant $e^2/4\pi\epsilon_0\hbar c$	$\alpha$	$7.297 352 5664(17) \times 10^{-3}$	
inverse fine-structure constant	$\alpha^{-1}$	137.035 999 139(31)	
Rydberg constant $\alpha^2 m_e c/2h$	$R_\infty$	10 973 731.568 508(65)	$\text{m}^{-1}$
Bohr radius $\alpha/4\pi R_\infty$	$a_0$	$0.529 177 210 67(12) \times 10^{-10}$	$\text{m}$
Bohr magneton $e\hbar/2m_e$	$\mu_B$	$927.400 9994(57) \times 10^{-26}$	$\text{J T}^{-1}$

exemplified; moving outside these requires additional measurements, round offs, estimates, or plain postulates. Specific uses that justify a nominal OS are also explained.

<http://dx.doi.org/10.1515/pac-2015-1204>

## Glossary of Terms Used in Developmental and Reproductive Toxicology (IUPAC Recommendations 2016)

John H. Duffus, Michael Schwenk, and Douglas M. Templeton

*Pure and Applied Chemistry*, 2016  
Volume 88, Issue 8, pp. 713-830

The primary objective of this glossary is to give clear definitions for those who contribute to studies relevant to developmental and reproductive toxicology, or who must interpret them, but are not themselves reproductive physiologists or physicians. This applies especially to chemists who need to understand the literature of reproductive and teratogenic effects of substances without recourse to a multiplicity of other glossaries or dictionaries. The glossary includes terms related to basic and clinical reproductive biology and teratogenesis, insofar as they are necessary for a self-contained document, particularly terms related to

diagnosing, measuring, and understanding the effects of substances on the embryo, on the fetus, and on the male and female reproductive systems. The glossary consists of about 1200 primary alphabetical entries and includes Annexes of common abbreviations and examples of chemicals with known effects on human reproduction and development. The authors hope that, in addition to chemists, toxicologists, pharmacologists, medical practitioners, risk assessors, and regulatory authorities are among the groups who will find this glossary helpful. In particular, the glossary should facilitate the worldwide use of chemical terminology in relation to occupational and environmental risk assessment.

<http://dx.doi.org/10.1515/pac-2015-1202>

Quantity	Symbol	Numerical value	Unit
electron mass	$m_e$	$9.109\,383\,56(11) \times 10^{-31}$	kg
proton mass	$m_p$	$1.672\,621\,898(21) \times 10^{-27}$	kg
proton-electron mass ratio	$m_p/m_e$	1836.152 673 89(17)	
Avogadro constant	$N_A, L$	$6.022\,140\,857(74) \times 10^{23}$	mol <sup>-1</sup>
Faraday constant $N_A e$	$F$	96 485.332 89(59)	C mol <sup>-1</sup>
molar gas constant	$R$	8.314 4598(48)	J mol <sup>-1</sup> K <sup>-1</sup>
Boltzmann constant $R/N_A$	$k$	$1.380\,648\,52(79) \times 10^{-23}$	J K <sup>-1</sup>
Stefan-Boltzmann const. $\pi^2 k^4/60\hbar^3 c^2$	$\sigma$	$5.670\,367(13) \times 10^{-8}$	W m <sup>-2</sup> K <sup>-4</sup>
magnetic flux quantum $h/2e$	$\Phi_0$	$2.067\,833\,831(13) \times 10^{-15}$	Wb
Josephson constant $2e/h$	$K_J$	$483\,597.8525(30) \times 10^9$	Hz V <sup>-1</sup>
von Klitzing constant $h/e^2$	$R_K$	25 812.807 4555(59)	$\Omega$
electron volt ( $e/C$ ) J	eV	$1.602\,176\,6208(98) \times 10^{-19}$	J
(unified) atomic mass unit $\frac{1}{12}m(^{12}\text{C})$	u	$1.660\,539\,040(20) \times 10^{-27}$	kg

The number in parentheses is the one-sigma (1  $\sigma$ ) uncertainty in the last two digits of the given value.



# 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 of 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**

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[www.iupac.org/project/2011-047-1-500](http://www.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 complex compounds on the basis of structure-based nomenclature for regular and irregular organic polymers, including adjustments required for specifying dendritic and hyperbranched macromolecular structures. These recommendations and the examples 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](mailto:alain.fradet@upmc.fr)>  
[www.iupay.org/project/2001-081-1-800](http://www.iupac.org/project/2001-081-1-800)

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# Conference Call

## WMFmeetsIUPAC

by *Hans van Egmond and Rudolf Krska*



“WMFmeetsIUPAC” is a unique event, combining the 9th Conference of the World Mycotoxin Forum and the XIVth IUPAC International Symposium on Mycotoxins. It was held in Winnipeg,

Canada, 6-9 June 2016. The conference built on the success of the previous edition, which was held in Rotterdam, the Netherlands (2012). The IUPAC symposia on Mycotoxins has existed since 1972. Traditionally, these symposia had a strong focus on (applied) chemistry and attracted in particular attendees from academia, research institutes, and government agencies. The World Mycotoxin Forum (WMF) is a younger series of conferences, organized since 2001 by Bastiaanse Communication. WMF conferences put more emphasis on issues such as prevention and control, and practical solutions for the food and feed industry receive a more prominent place in the conference programs compared to the IUPAC symposia.

Mycotoxins, produced by fungi, are an important class of natural toxins. They are of significant concern to the health of humans and animals. The conference WMFmeetsIUPAC aims to increase the awareness of human and animal health risks due to mycotoxins in food and feed, and of potential risk management options, technologies, and integrated strategies for minimized contamination. The Winnipeg conference attracted more than 400 attendees, representing 34 countries. With the support of renowned members of the International Advisory Committee, a program was built which included more than 100 invited lectures and oral contributions in two plenary meetings and 13 parallel sessions; speed presentations; over 130 posters; spotlight presentations, and an instrument/manufacturers exhibition.

After various welcoming words, Laura McConnell, Past President of the IUPAC Division on Chemistry and the Environment (Division VI), gave an inspiring introductory talk showing how IUPAC has evolved over a century, from an institution particularly focusing on nomenclature, standards, and norms into what it is today: an organization with a clear eye on present-day concerns such as globalization, energy crisis, and climate change. Following the introductory presentations, four respected keynote speakers set the stage by sharing their views on various contemporary mycotoxin issues in the perspective of a changing world.

The following days were characterized by a variety of parallel and poster sessions, which allowed conference participants to select the most appealing subject areas for attending and interacting with presenters. As a special end to the third day of WMFmeetsIUPAC, an exclusive dinner was organized for conference attendees in the new Canadian Museum for Human Rights, with its breathtaking architecture and its interactive exhibitions, a must-see in Winnipeg! The fourth and last conference day included the traditional ceremony of the IUPAC Best Poster Award. The winning poster “Optimal sampling and extraction procedures for ergot measurements” was prepared and presented by Taylor Grusie, Veterinary Biomedical Sciences, University of Saskatchewan, Canada.

At the close of the conference, a few upcoming international conferences of relevance to the audience were announced, including the next WMFmeetsIUPAC conference, which will be held in Austria, October 2019, the year of the IUPAC Centenary.

A post-conference activity was the visit to a nearby grain elevator. This excursion was facilitated by the Canadian Grain Commission, Canada's scientific research organization on grain quality. Participants gained an understanding of the operation of a commercial grain elevator and had the chance to learn about equipment and methods used in the Canadian grain industry for sampling whole grain, visually inspecting grain for grading factors related to fungal infection, as well as how industry manages and mitigates risks due to the presence of mycotoxins in grains.

From the various conference sessions and the subsequent discussions, five generalized “lessons” could be distilled, each broken down with information, observations and conclusions summarized and provided by the session chairs.



*Canadian Museum for Human Rights in Winnipeg, where the conference dinner was held*

**Lesson 1: We are living in a changing world with new developments, changed attitudes, challenges, and chances.**

- A changing world means: changes in technology, mycotoxin patterns, and dietary behavior.
- Climate change, including more extreme weather conditions, may mean that old problems may become new ones (e.g. ergot in western Canada).
- Large collaborative projects have been launched in various regions of the world to combat mycotoxins, with more involvement of Africa and Asia.
- Food authorities and international organizations work more towards proactive approaches than reactive approaches.
- Economic and human health costs associated with mycotoxins can be equated, but the methods for assessment are arbitrary.

**Lesson 2: We need to consider that co-exposure to multiple mycotoxins and other contaminants is a reality.**

- Recent mycotoxin surveys prove that co-occurrence of multiple mycotoxins, including modified forms, is the rule rather than the exception.
- Food authorities now recognize mycotoxin co-occurrence as a priority in exposure assessment.
- In vitro models for risk assessment still prevail, moving to in vivo models seems challenging.
- Different modes of action are a major challenge for toxicological evaluation.
- New technologies (such as High Content Analysis) may assist in assessing combined effects of various food contaminants.

**Lesson 3: New advanced tools for sampling and analysis of mycotoxins offer opportunities to increase knowledge and understanding in various respects: “the numbers tell the tale”.**

- An on-line FAO sampling tool is now available to visualize effects of sampling plan parameters on the risk of mischaracterizing commodity lots.
- State-of-the-art MS methods lead to a clearer picture on the range of occurring (masked) fungal secondary metabolites.
- Innovative approaches for biomarker analysis (including blood spot analysis) provide new insights into the exposure of mycotoxins, their metabolism and the efficacy of detoxifiers.
- Omics technologies are becoming an important data source for improved risk assessment and better understanding of plant-fungi interactions.

**Lesson 4: Success stories and promising techniques are stimulating elements in our further efforts to tackle mycotoxin problems.**

- Expanding the application of biocontrol with atoxigenic *Aspergillus* technology in Africa has dramatically reduced aflatoxin contamination of maize.
- Using novel compounds, including natural products, may inhibit toxin production in the plant and may mitigate the physiological impact on intestinal tissue.
- Use of hyperspectral imaging or NIRT as non-invasive analytical techniques offer promise in sorting.
- A clear trend towards ICT-based tools, including novel handheld devices, allow on-line data provision via apps and instantaneous management decisions.

**Lesson 5: Integrated approaches are the way forward to the effective and efficient reduction of mycotoxins in the food and feed chains.**

- New approaches go beyond “field-to-fork” and consider the entire cycle, including waste management and alternative energy sources.
- Understanding the fungi’s life cycle and its interaction with host and environment is of key importance in sustainable prevention strategies.
- Innovative post-harvest techniques, including novel milling, thermal processing, and detoxification techniques become increasingly attractive to minimize mycotoxin content.
- In order to be effective to avoid adverse health effects, mycotoxin regulations have to impact the whole food and feed chains.

Hans van Egmond <[hans.vanegmond@worldmycotoxinjournal.org](mailto:hans.vanegmond@worldmycotoxinjournal.org)> is senior scientist, retired from the RIKILT Institute of Food Safety, Wageningen University and Research Centre, the Netherlands; Rudolf Krska is full professor at the University of Natural Resources and Life Sciences, Vienna (BOKU) in Austria, where he serves as Head of the Center for Analytical Chemistry at the BOKU-Department IFA Tulln.

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

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## Chemistry Education

*by Datuk Dr. Soon Ting-Kueh*

The 24th IUPAC International Conference on Chemistry Education (ICCE) 2016 was successfully organised by the Institut Kimia Malaysia (IKM), under IUPAC auspices, at the Borneo Convention Centre Kuching,

## Conference Call

Kuching, Sarawak, Malaysia, 15–20 August 2016. At the same time and while celebrating its 30th anniversary, the Institut Kimia Malaysia (IKM) Sarawak Branch held the International Symposium on Pure and Applied Chemistry (ISPAC), in conjunction with ICCE 2016 and with the support of the Foundation of Interaction of Science and Technology (FIST), Japan.

The ICCE is a major international chemistry education conference held biennially all over the world. It usually attracts a large number of chemistry and science educators, practitioners and researchers, and education decision and policy makers, including heads of education and research institutions from around the globe. ICCE-2016 ranked among one of the largest ICCEs, with 456 registered delegates including 260 foreign delegates representing 38 countries. Of course, the Malaysian delegation was the biggest, at 196, followed by Japan (109), India (15), Taiwan (14), China (13), and Australia (10). 50 teachers from Sarawak schools were provided with complimentary registration under the Tan Sri Law Hieng Foundation and the Lee Foundation. IKM also supported 14 teachers from Peninsular Malaysia with a grant of RM 1,500 each to enable them to participate in ICCE 2016.

The Chief Minister of Sarawak, YAB Datuk Patinggi Tan Sri (Dr.) Haji Adenan Bin Haji Satem, officiated the Opening Ceremony of ICCE and ISPAC 2016 at the Borneo Convention Centre Kuching, Kuching, Sarawak on Tuesday, August 16, 2016

### Highlights

One of the highlights of ICCE & ISPAC 2016 was the presence of the 2010 Nobel Laureate in Chemistry, Ei-ichi Negishi, from Purdue University, USA. Professor Negishi delivered two plenary lectures, one at ICCE 2016 and the other at ISPAC 2016.

Another highlight was the Global Launch of the new Electronic Interactive IUPAC Periodic Table of the Elements and Isotopes by Peter Mahaffy.

The third was the presentation of the IUPAC Committee on Chemistry Education (CCE)'s Award for Distinguished Contribution to Chemistry Education to Kazuko Ogino of Tohoku University, Japan.

ICCE's technical program included a total of 141 presentations, comprising 6 Plenary Lectures, 13 Key-note Lectures, and 96 oral and 26 poster presentations. The 6 Plenary Lectures were as follows:

- Pursuit of My Dreams for Half-a-Century, by **Ei-ichi Negishi** (Nobel Laureate in Chemistry 2010, Purdue University, USA);
- Sustainability Through Attainability, by **Peter**

**Atkins** (CCE inaugural chair, Oxford University, UK);

- Faculty and Student Goals for Undergraduate Laboratory: The Conflicts Between Hands-on Skills, Critical Thinking and Efficacy, by **Marcy Towns** (Purdue University, USA);
- Models of Life Long Learning: Professional Development of Teachers, by **Rachel Mamlok-Naaman** (The Weizmann Institute of Science, Israel);
- Globalization of Chemistry Education: Comparison of K-12 Chemistry Standards across the World, by **Mei-Hung Chiu** (National Taiwan Normal University, Taiwan); and
- Motivation and the Undergraduate Chemistry Student, by **Robert (Bob) Bucat** (The University of Western Australia, Australia)

ICCE 2016 also included activities for teachers and students from Kuching and the surrounding areas. These were a IUPAC Young Ambassador for Chemistry (YAC) event for 40 teachers and 60 students; Microscale Laboratory Training for schools involving 20 teachers and 30 students; and Microscale Laboratory Training for 20 undergraduates and 20 lecturers at Universiti Malaysia Sarawak (UNIMAS).

### Social & Cultural Events

Close to 200 delegates attended the ICCE 2016 Welcome Reception at Hilton Kuching on Monday, 15 August 2016. The delegates were treated to sumptuous local cuisines and pastries with a free flow of cordials and beer. There were lots of renewed acquaintances and networking among the delegates. This was truly a happy and joyous social occasion.



*Cultural Dance Performance at Banquet*

The ICCE 2016 Conference Banquet on Wednesday, 17 August 2016 was a grand occasion. 400 delegates, invited guests, and VIPs attended. The Chief



## Conference Call



**Prof. Dr. Sim Kui Hian officiating the Opening Ceremony**  
From left, Peter Atkins, Marck Cesa, Ong Eng Long, Sim Kui Hian, Ei-ichi Negishi, Soon Ting Kueh, and Alvin Chai.

Minister of Sarawak was represented by YB Prof. Datuk Dr. Sim Kui Hian, the Minister of Local Government Sarawak. YB Prof. Datuk Dr. Sim gave a Welcome Address to invite all delegates to sample the delicious Malaysian food and local dishes. He also welcomed them to visit and tour various interesting places and tourist attractions in Sarawak.

At the Banquet, IKM Sarawak Branch also presented the 30th Anniversary Distinguished Service Award to Chan Woon Peng, the Founding Chair of the Branch, who has contributed tremendously to the development of the Branch and to chemistry in Sarawak.

Besides the wonderful foods, the delegates were entertained by a performance of Sarawak cultural dances by a group of dancers from Kumpulan Kesenian JKKN Sarawak. Kyoko Mori from Japan entertained with a performance on the flute, and then Ei-ichi Negishi serenaded the attendees with three songs accompanied by Miss Mori on the flute. The Chair of ICCE 2016 also entertained the guests with two songs, followed by two songs from the Taiwanese delegation, led by Mei-Hung Chiu. The Japanese delegation, led by Tamotsu Takahashi, followed with the song "Sukiyaki". Other performers included Puan Sri Law Hieng Ding nee Ngui Soon Leng, Lau Seng from UNIMAS, and the German delegation. Zuriati Zakaria from IKM also rendered a hot Tina Turner number, "What's Love Got To Do With It". It was a fun-filled evening of merry-making that the delegates truly enjoyed.

About 240 delegates participated in the ICCE 2016 Discovery and Cultural Tour on Friday, 19 August 2016. A first group visited the Semenggoh Wildlife Centre in the morning and the Sarawak Cultural Village in the afternoon. A second group visited the same sites in the reverse order.

It was really exciting that both groups witnessed



**Mustafa Sozibilir presenting souvenir to CCE Past Chair, Prof. Mei-Hung Chiu at Closing of ICCE 2016**

the feeding of the orang-utan. In the morning, the delegates managed to come face-to-face with six orang-utans, while the afternoon group saw three and had a close encounter with a male named Anuar. Then came the rain and many of us saw how Anuar used the large leaves to cover himself from the rain. They are almost human.

The tour of the Sarawak Cultural Village was equally entertaining. They saw the dwellings of seven local tribes of Sarawak and witnessed their ways of life and their cultures. There was a performance of cultural dances from the various tribes.

### Appreciation

On behalf of the Organisers, IKM would like to extend our sincere appreciation to the Chief Minister of Sarawak, YAB Datuk Patinggi Tan Sri (Dr.) Haji Adenan Bin Haji Satem, for officiating the Opening Ceremony of ICCE 2016 and for the strong support of the Sarawak Government. We would also like to thank the Sarawak Convention Bureau and the Malaysia Convention and Exhibition Bureau for their support in the bidding and management of ICCE 2016. To the other major sponsors, including Tan Sri Law Hieng Ding Foundation, Lee Foundation, Chemsain Konsultant Sdn Bhd, KISM Sdn Bhd, and Foundation for the Interaction of Science and Technology Japan, we would like to convey our utmost sincere gratitude and appreciation for their strong support.

As Chair of the National Organising Committee (NOC) of ICCE & ISPAC 2016, I am personally indebted to the members of NOC who have worked so hard to put everything together to make a successful ICCE & ISPAC 2016. To members of the International Advisory Committee and the National Advisory Board, we are really grateful for advice and technical input.

The success of ICCE & ISPAC 2016 is largely due to the delegates, including the Session Chairpersons,

## Conference Call

the Plenary Speakers, oral and poster presenters, and the other participants. Last but not least, I am very much indebted to ICCE & ISPAC 2016 Secretariat staff, headed by Ms. Ong Bee Kwan, Dr. Alvin Chai Lian Kuet and members of the IKM Sarawak Branch Committee, and Associate Prof Dr. Sim Siong Fong and her UNIMAS team.

The 25th ICCE will be organized in Australia in 2018 by The University of Sydney and chaired by Dr. Sigi Schmith. See you there!

<http://www.icce2016.org.my>

## Green Chemistry

*by Pietro Tundo*

After Dresden, Moscow, Ottawa, Foz do Iguaçu, and Durban, the **International IUPAC Conference on Green Chemistry** (ICGC) moved to Italy. ICGC-6 took place 4-8 September 2016 in Venezia, one of the most beautiful cities in the world, filled with history and culture, which welcomes more than 20 million visitors from all over the world each year. The Centro Culturale Candiani and the Teatro Toniolo of Venezia Mestre hosted the five-day scientific event. The conference belongs to a series developed by the IUPAC Subcommittee on Green Chemistry (a subcommittee of the Organic and Biomolecular Chemistry). Pietro Tundo, chair of the subcommittee, managed the event organization, together with the Organizing Committee, composed of Fabio Aricó, Lucio Ronchin, and Andrea Vavasori from Ca' Foscari University of Venice, and the Secretary of the Conference, Emilia G. Pasta.

The Conference was organized in collaboration with the Consiglio Nazionale dei Chimici and obtained the endorsement of UNESCO, Italian National Commission for UNESCO, Italian National Committee for IUPAC, ICSU, CNR, Società Chimica Italiana, AIRI, IUAV, Royal Society of Chemistry, Ordine dei Chimici di Venezia, Città Metropolitana di Venezia, Città di Venezia, and 7 Italian Ministries: Ministero dell'Ambiente e della Tutela del Territorio e del Mare, Ministero dello Sviluppo Economico, Ministero della Giustizia, Ministero dei Beni e delle Attività Culturali e del Turismo, Ministero dell'Istruzione, dell'Università e della Ricerca, Ministero della Salute, and Ministero degli Affari Esteri e della Cooperazione Internazionale. It was supported by Ca' Foscari University of Venice and Regione del Veneto and was sponsored by: PhosAgro, the Organisation for the Prohibition of Chemical Weapons (OPCW); Milestone as platinum sponsor;

Mapei, Cefic, L'Oréal and Ecopneus as gold sponsors; Nemo Glass and Perkin Elmer as silver sponsors; and Biogest and Pirelli as bronze sponsors.

The conference was divided into five topics: Green Materials, Green Industrial Processes and Molecular Innovation, Green Bioprocesses, Green Energy, and Green Policy and Education.

ICGC-6 kicked off on Monday, 4 September, at the Teatro Toniolo of Venezia Mestre with Tundo's welcome message. Then, the following personalities took the floor: Michele Bugliesi, Rector of the University of Venice; Paolo Pellegrini, City of Venice; Romain Murenzi, UNESCO Director for Science Policy and Capacity Building; Andrei Guriev, CEO of PhosAgro; David Black, Secretary General of International Council for Science (ICSU); Xiaohui Wu, Head of the OPCW International Cooperation Branch; Nausicaa Orlandi, President of the Consiglio Nazionale dei Chimici; Mauro Marchetti, Consiglio Nazionale delle Ricerche; and Carlos Tollinche, CHEMRAWN Chair, IUPAC.



**Presentation of the IUPAC-CHEMRAWN VII Award: from left, IUPAC President Natalia Tarasova, Award recipient Ali Makeji, CHEMRAWN Chair Carlos Tollinche, and ICGC-6 Chair Pietro Tundo.**

After these contributions, two awards were presented: CHEMRAWN Award for Green and Atmospheric Chemistry and the PhosAgro/UNESCO/IUPAC awards. The 2016 IUPAC-CHEMRAWN VII award for Green Chemistry was presented to Ali Maleki from the Iran University of Science and Technology. Next, J. Corish (University of Dublin, Ireland) presented the six awards of the 3<sup>rd</sup> edition of the PhosAgro/UNESCO/IUPAC "Green Chemistry for Life" to: A. Akhmetshina (Russia), I. Carrera (Uruguay), M. Ismail (Pakistan), E. Ravera (Italy), A. S. Elsayed Sayed (Egypt) and W.C. Wanyonyi (Kenya).

ICGC-6 success is in the numbers: 580 registrations from 76 countries, 400 active participants from more than 60 different countries, 4 daily parallel ses-

## Conference Call



sions, 6 plenary lectures, 20 keynote speeches, 2 symposia, 3 round tables, and about 250 original scientific reports. The detailed program listing plenary and keynote is available online. Selected lectures will be published in a special issue of the IUPAC journal *Pure and Applied Chemistry*.

Two symposia of international relevance took place: one organized by UNESCO, PhosAgro, and IUPAC, and the other sponsored by the Organisation for the Prohibition of Chemical Weapons (OPCW). With UNESCO support, new ideas arose from the application of Green Chemistry to restoration and cultural values conservation, while the pharmaceutical industry brought experiences and data on chemical reaction performed by using water in place of chemical solvents. With OPCW, Green Chemistry as a principle and a means to oppose military usage of chemical compounds was explored.

Three open roundtables gave the opportunity to the attendees to deepen some of the issues addressed by the participants. The first was dedicated to the industries. Indeed, the massive participation of industries and companies, both Italian and international, was one of the great success of the Conference. Industries and companies from different



production sectors agreed on future industrial strategies proposed by IUPAC, considered a scientifically valid, independent, and trustworthy institution. As examples, Eni thoroughly explained Marghera hydrogenation plant technical aspects, Mapei showcased the usage of recycled materials in building industry, and Pirelli talked about innovative production coming from renewable materials.

As the Conference Secretariat received many scientific proposals concerning the analysis, utilization, and exploitation of plants in Africa and India, the Conference Organizing Committee decided to organize a second roundtable to open a dialogue among people from these regions. In fact, considering the vastness of the African continent and of a country like India, it is often difficult for people in these geographical areas to meet.

The theme of the third roundtable was education. It took place after the education-dedicated session and was an interesting opportunity for comparison and for dialogue, as many young researchers, students, and representative of international organisations gave their opinion on the best way to teach, to learn, and to share knowledge.

The closing ceremony saw the contribution of Ali Maleki, who illustrated the project that allowed him to win the CHEMRAWN prize. The title of his oral presentation was "Green Reaction Media Protocols: From Solvent-Free to Catalysis State-of-the-Art".

The awarding ceremony of the poster prizes also took place during the closing ceremony. The participants presented their poster contributions on Monday and on Tuesday. The poster sessions could be considered one of the greatest success of ICGC-6, for the originality and the high scientific value of the contributions, for the significant number of young people who shared their interesting researches with the other attendees, and for the interest demonstrated by the participants in the session.



*Hands-up for the success of ICGC-6 from the cheerful group of local organizers.*



## Conference Call

The winners of the certificates were:

- Daichi Nakayama, Muroran Institute of Technology (Japan);
- Yuki Takada, Graduate School of Science, Nagoya University (Japan);
- Klara Čebular, Department of Physical and Organic Chemistry, Jožef Stefan Institute (Slovenia).

The winners of the publications were:

- Stefan B. Lawrenson, Green Chemistry Centre of Excellent, Department of Chemistry, University of York (UK);
- Stefania Trita, TU Kaiserslautern (Germany);
- Roxanne Brion-Roby, Université du Québec à Rimouski (Canada).

ICGC-6 was not only a great scientific event, it was also a place and time dedicated to social gathering and networking. A boat trip around the Venice lagoon was organized. On board a big motor ship, attendees saw the city of Venice from the Giudecca Canal, visiting Burano and Torcello, and were rewarded with a panoramic view of the Venetian Arsenal. The Organizing Committee also chose an exclusive location for the conference Gala Dinner, which was hosted by Ca' Vendramin Calergi and held at the Venice Casino, an historical building on the Grand Canal, a great example of renaissance style, and Wagner's last dwelling place. The dinner was accompanied by live classical music.

The Organizing Committee's expectations were met. During several sessions, issues of national relevance were discussed. New challenges in different sectors were also undertaken: restoration and cultural values conservation, chemical weapons prohibition, innovative pharmaceutical production processes, and environmental protection. The chemical industry, moving from the image of a "Twentieth Century Monster," responsible for development, but also environmental and health issues for mankind, is becoming the leader of sustainable development through decades of day-by-day research in thousands of universities and laboratories, looked at as a new hope for populations around the world. The next editions of the International Conference on Green Chemistry will be held in Moscow, Russia, 2-5 October 2017 (<http://greeniupac2017.muctr.ru>) and in Bangkok, Thailand, in September 2018.

For more pictures from Venice and the full conference program, see [www.greeniupac2016.eu](http://www.greeniupac2016.eu)

## Solid State Chemistry

by *Adriana Lančok*



The **12<sup>th</sup> Solid State Chemistry conference (SSC 2016)**, endorsed by IUPAC, was

held 18-23 September 2016 in Prague, Czech Republic. The conference was organized in honour of Professor Miloslav Frumar (University of Pardubice, Czech Republic) on the occasion of his 80th birthday, to celebrate his life-long scientific contribution, particularly to the fields of solid state chemistry and inorganic chemistry.

SSC 2016 is a part of the series of conferences on solid state and materials chemistry, with the scope and themes of special significance and challenges currently interlinking research, development, and technology. The conferences are held biannually, alternatively in Slovakia and the Czech Republic. SSC 2016 was a forum for the presentation of new research results in the area of solid state chemistry to bridge the gap between scientific understanding and technical requirements and applications, so that the enormous future potential of solid state chemistry, materials, and technologies can be realized effectively. SSC 2016 encompassed different facets of solid state chemistry, physics, and related fields, and therefore attracted an extremely wide audience. In total, 101 scientists from 24 countries around the world participated. Specific topics included: preparation and synthesis; phase and properties characterization; nanomaterials, nanocomposites and catalysis; magnetic, metal, and alloy materials; optical and photovoltaic materials; and theoretical approaches to solid-state chemistry.



*IUPAC representative, Milan DRÁBIK, made a short presentation about IUPAC, its mission and role.*



## Conference Call



The scientific program consisted of five plenary lectures, 16 invited lectures, 28 lectures, and 41 posters. The IUPAC representative, Milan Drabik, gave a presentation on the scope and activities of the Union. Young authors of 7 oral presentations and 15 posters entered the sponsored Student Awards competition. The jury of Student Awards competition has proposed to award:

(1) Best Oral Presentation Certificates to three young scientists”:

- Daniela Nýblová—Comenius University Bratislava, Faculty of Natural Sciences, Department of Inorganic Chemistry - *Synthesis of layered alpha alumina by heat-treatment of aluminium carbide*
- Filip Varga - University of Pardubice, Department of General and Inorganic Chemistry - *Synthesis, crystal structures and spectral, redox and magnetic properties of cobalt(II)/(III) complexes with chelating *s*-, *p*-donor ligands*
- Bo Zhang - University of Pardubice, Department of General and Inorganic Chemistry - *Investigation of the resistive switching in  $\text{Ag}_x\text{AsS}_2$  layer by conductive AFM*

(2) Best Poster Certificates to three young scientists:

- Eunji Lee - Gyeongsang National University, Jinju, South Korea - *Anion-controlled assemblies of silver(I) coordination polymers and their anion-exchange exhibiting dimensional changes in the solid state*
- Vasyi Karabyn - University of Pardubice, Department of General and Inorganic Chemistry - *Physico-chemical properties of the  $\text{Ge}_8\text{Sb}_{2-x}\text{Bi}_x\text{Te}_{11}$  bulks and thin film*
- Max Fraenkl - University of Pardubice, Department

of General and Inorganic Chemistry - *Study of ionic properties of Ag-Ge-Sb-S glasses by electrochemical impedance spectroscopy and radioactive tracer diffusion*

The SSC 2016 conference has enabled the mutual exchange of knowledge and ideas directly during the oral and poster sessions, as well as at various informal discussions in the course of the six days of the conference. Selected contributions, mostly plenary and invited lectures representing the content of the conference, will be published in the special issue of IUPAC scientific journal *Pure and Applied Chemistry* (PAC), with Dr. Mariana Klementová as the Conference Editor. We are convinced that the quality of plenary and invited lecturers guarantee that the special issue of PAC will be a representative profile not only of SSC 2016, but also of the challenging fields of Solid State and Materials Chemistry.

**Dr. Adriana Lancok, SSC2016 chair, works at the Laboratory of Moessbauer Spectroscopy at the Institute of Inorganic Chemistry, in Prague, Czech Republic**

# RACI2017 Centenary Congress

23-28 July 2017  
Melbourne



**Theme: Chemistry addressing sustainable development and other challenges of the 2020s**

**SAVE THE DATE 23-28 July 2017 | Melbourne, Australia**

The RACI 2017 Centenary Congress will be the biggest chemical congress ever held in Australia and Melbourne's thriving chemistry community makes it the ideal city to advance the science and practice of chemistry.

That's right, the RACI will soon be 100 years old! The Congress is being held in collaboration with nine prestigious chemistry conferences that will attract 3,500 delegates over five days from across the breadth of the chemical sciences and technologies.

The novel congress concept involves all of the partner conferences running concurrently during the week allowing delegates to access sessions across a wide variety of chemistry disciplines. Each day will commence with a common Congress plenary speaker for all delegates followed by the various conferences running their individual programs.

A single Congress fee will allow delegates to attend any conference or session they wish. No one will be limited to a single conference stream.



Set on the shores of picturesque Port Phillip Bay, Melbourne, the capital of the state of Victoria, is rich in aesthetics. The city's charm is characterised by its enchanting laneways, stunning waterfront precincts and trendy neighbourhoods, and provides an endless range of shopping hot spots and attractions in weird and wonderful locations.

We look forward to seeing you at the RACI Centenary Congress in Melbourne in July 2017.

*Mark Buntine (Centenary Congress Chair)*



**Celebrate the  
festival of  
Chemistry**

## Confirmed Plenary Speakers

**Professor Frances Arnold**

University of California, Berkeley

**Professor Oliver Einsle**

Spemann Graduate School of Biology and Medicine  
Freiburg | Germany

**Professor Robert Grubbs**

Californian Institute of Technology | USA

**Professor Andrew B. Holmes**

Australian Academy of Science | Australia

**Dr Laura Kiessling**

University of Wisconsin, Madison | USA

**Dr Andrew Makarov**

hermo Fisher Scientific Bremen | Germany

**Professor Molly Stevens**

Imperial College of London | United Kingdom

**Professor Ning Yan**

Tsinghua University | China

**Professor Ada E. Yonath**

Director of the Helen and Milton A. Kimmelman Center  
for Biomolecular Structure and Assembly of the  
Weizmann Institute of Science | Israel

## KEY DATES

Abstract submission opens **Now open**

Registration opens **Now open**

Abstract submission closes  
**23 March 2017**

Early bird deadline  
**23 April 2017**

Congress dates  
**23-28 July 2017**

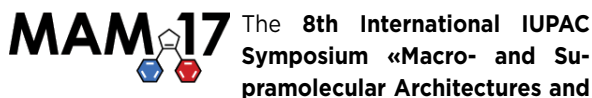
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## Where 2B & Y

### Macro- and Supramolecular Architectures and Materials

6-10 June 2017, Sochi, Russia



**The 8th International IUPAC Symposium «Macro- and Supramolecular Architectures and Materials: Multifunctional Materials and Structures» (MAM-17)** will be held from 6-10 June 2017 in Sochi, Russia and organized by the Lomonosov Moscow State University.

An important field in the recent development of science, technology, and society is associated with novel materials. This Symposium provides an international forum for presentation and discussion about the most recent progress and future trends in the rapidly expanding interdisciplinary field of macromolecular and supramolecular architectures and materials, as well as multifunctional realms of their application.

This symposium continues a series of conferences that have been organized biennially at different places around the world. The previous MAM conferences were held in South Korea, USA, Japan, Germany, Jamaica, India, and South Africa. Russia will host the 8<sup>th</sup> symposium in 2017. MAM-17 will bring together top scientists and experts from all over the world to share and discuss theoretical and practical knowledge about novel materials and to chart out future scientific and technological research directions.

The main topics of the symposium are:

- Catalysis and applications
- Membrane technologies
- Energy conversion and storage
- Materials for next generation manufacturing processes
- Biomedicine and bio-engineering
- Macromolecular design
- Engineered materials with high performance
- Nanomaterials and multifunctions
- Chemo- & biosensors
- Environmental applications
- General topics

Plenary and breakout sessions, poster sessions, and a contest for young scientists are scheduled within the framework of the event. An exhibition, where leading domestic and foreign companies will present their products and developments, will be arranged.

The host city, Sochi, promises not only its well-preserved historical and tourism background with modern facilities, but also the scenery of the lovely Black sea and delicious Russian cuisine, as well. The participants will be able to enjoy optional post-symposium tours to the Black Sea and different other tourist destinations in Russia.

For further information, please contact: [mam-17-program@yandex.ru](mailto:mam-17-program@yandex.ru)  
[www.mam-17.org](http://www.mam-17.org)

### POLYCHAR World Forum on Advanced Materials

2-6 October 2017, Kuala Lumpur, Malaysia



**POLYCHAR 25** follows the large number of POLYCHAR conferences that have come before, establishing a measure of excellence and a special culture of friendship and collaboration between participants. POLYCHAR 1 to 11 were held in the USA, while POLYCHAR 12 was held in Portugal, 13 in Singapore, 14 in Japan, 15 in Brazil, 16 in India, 17 in France, 18 in Germany, 19 in Nepal, 20 in Croatia, 21 in South Korea, 22 in South Africa, 23 in the USA and POLYCHAR 24 in Poland. Now, in 2017, POLYCHAR 25 is coming to Malaysia for the first time—giving an opportunity to students and young scientists from Asia, in particular from neighboring ASEAN countries, but of course also to their peers from other parts of the world.

POLYCHAR conferences offer an eminent setting for the presentation and discussion of materials, especially on materials characterization, properties, syn-

thesis, processing, and manufacturing. POLYCHAR 25 hopes to provide participants with an exciting range of presentations in these areas, and to provide the opportunity for professors, students, and people from industry to meet and discuss them with experts in their fields. In addition, POLYCHAR is the event where the prestigious Paul J. Flory Polymer Research Prize and International Materials Research Prize are presented to distinguished researchers. The Forum also has a strong tradition of promoting students and young investigators through other prizes and awards.

The traditional “Short Course on Polymer Characterization” will be held on the first day of POLYCHAR. The Short Course serves as a tutorial for newcomers in the field of Polymer Science, as well as an update on recent developments in the analysis and characterization of polymer systems, provided by specialists in the field.

[www.25POLYCHAR.org.my](http://www.25POLYCHAR.org.my)



### Coordination and Bioinorganic Chemistry

4-9 June 2017, Smolenice, Slovakia

The XXVI International Conference on Coordination and Bioinorganic Chemistry (ICCBIC) will be held in Smolenice Castle 4-9 June 2017, organized by the Slovak Chemical Society in cooperation with the Slovak University of Technology and the Slovak Academy of Sciences in Bratislava.

The conferences on coordination chemistry, held regularly in Slovakia, have a long tradition. The First Conference was organized in 1964. Many coordination chemists, including Nobel prize winners from all over the world, have attended past Conferences and Smolenice Castle has become the place where many new scientific and personal contacts are established.

The XXVI Conference will deal with current prob-



lems of coordination, bioinorganic, and inorganic chemistry and the progress achieved in these fields. The scientific program will be concentrated on the following themes:

- Electronic, molecular and crystal structures
- Solution and solid state reactivity
- Applied inorganic and coordination chemistry
- Complexes in human medicine and the environment

[www.iccbic.stuba.sk](http://www.iccbic.stuba.sk)

### Chemists and IUPAC: Taking Responsibility and Taking Action

29 August - 2 September 2017, Trondheim, Norway

Since its foundation in 1919, many famous chemists have contributed to the International Union for Pure and Applied Chemistry (IUPAC), fueling the drive to improve standardisation of methods, nomenclature, units and standards, among other things. Without a doubt, progress has been made, despite power struggles, uncompleted projects, and unproductive commissions.

A special session titled, **“Chemists and IUPAC: Taking Responsibility and Taking Action,”** to be held during the 11th International Conference on the History of Chemistry, will aim at shedding light on the activity of chemists invested with responsibilities in IUPAC, whose actions are often overlooked in nation-

al biographical dictionaries. This session falls into the broader project on the centennial of the IUPAC in 2019. Each paper will focus on the responsibilities and actions of individual chemists, alone or combined in a small national or disciplinary group, inside IUPAC. The case study can, however, expand to roles in other international organisations (e.g. IRC, ICSU, SDN or UNESCO). A first survey is provided by the books of R. Fennell (1994) and S. S. Brown (2001). By focusing on individual actions, the aim is to get a better sense of the articulation between the local and the international, and how this articulation was constructed through the work and actions of chemists dispersed across the world.

For more information, please contact Danielle Fauque ([danielle.fauque@u-psud.fr](mailto:danielle.fauque@u-psud.fr)) or Brigitte Van Tiggelen ([vantiggelen@memosciences.be](mailto:vantiggelen@memosciences.be))

### Small Satellites for Space Research

18-22 September 2017, Jeju Island, South Korea

Hosted by the Korean Astronomy and Space Science Inst. (KASI) / Korean Space Science Society, the 3rd Symposium of the Committee on Space Research (COSPAR) 2017 continues on the success of the previous symposia, with topics including:

- New ideas for upper atmosphere research with micro- and nano-satellites
- Interaction of solar wind and Earth's bow shock: recent progress in observations and modelling
- Dynamics of the magnetospheric process through coordinated experiment and modelling
- Advances in astrophysical research with small

satellites

- Planetary exploration of the solar system
- Enabling technologies

Selected papers will be published in *Advances in Space Research* and *Life Sciences in Space Research*, fully refereed journals with no deadlines and open to all submissions in relevant fields. The deadline for abstracts is 31 March 2017.

For more information, contact [cospar@cosparhq.cnes.fr](mailto:cospar@cosparhq.cnes.fr)  
<http://cospar.kasi.re.kr/cospar-symposium-2017/>

## 2017

### 23 Jan 2017 • Validation of Test Methods • Tel Aviv, Israel

*International Workshop on Validation of Test Methods, Human Errors and Measurement Uncertainty of Results, in conjunction with the Isranalytica Conference and Exhibition (24-25 Jan 2017)*

Dr. Ilya Kuselman, Chairman of the International Workshop Advisory Committee, [ilya.kuselman@bezeqint.net](mailto:ilya.kuselman@bezeqint.net); c/o Isranalytica, Reut Lazar, Bioforum Applied Knowledge Center, E-mail: [reutl@bioforum.co.il](mailto:reutl@bioforum.co.il) <http://bioforumconf.com/satellite-event2017> and [www.isranalytica.org.il](http://www.isranalytica.org.il)

### 3-5 April 2017 • Solutions for Drug-Resistant Infections (SDRI 2017) • Brisbane, Australia

SDRI 2017 is the first multi-disciplinary scientific conference for the Asia Pacific region focused on Solutions for Drug Resistant Infections. Chair of Local Organizing Committee: Mathilde Desselle, E-mail: [m.desselle@imb.uq.edu.au](mailto:m.desselle@imb.uq.edu.au), c/o ASN Events Pty Ltd, 9/397 Smith Street, Fitzroy VIC 3065, Australia, Tel. +61 (0) 3 8658 9530; [info@sdri2017.org](mailto:info@sdri2017.org), [www.sdri2017.org](http://www.sdri2017.org)

### 10-13 April 2017 • Macromolecules & Materials • Stellenbosch, South Africa

*14th Annual UNESCO/IUPAC Workshop and Conference on Macromolecules & Materials*

Prof B Klumperman (Conference Chair), University of Stellenbosch, Department of Chemistry & Polymer Science, Private Bag X1, Matieland 7602 South Africa, E-mail: [bklump@sun.ac.za](mailto:bklump@sun.ac.za); Conference Secretariat: [aef2@sun.ac.za](mailto:aef2@sun.ac.za), <http://academic.sun.ac.za/unesco>

### 19-22 April 2017 • Croatian Chemical Congress • Poreč, Croatia

*25th Meeting of Croatian Chemists and Chemical Engineers (25HSKIKI)*

Dr.sc. Ana Šantić, PhD, Co-chair, Department of Materials Chemistry, Ruđer Bošković Institute, Bijenička c. 54, HR-10000 Zagreb, Croatia; E-mail: [asantic@irb.hr](mailto:asantic@irb.hr), [www.25hskiki.org](http://www.25hskiki.org)

### 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](mailto:unsworjo@aol.com)

### 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](mailto:filip.duprez.ugent.be), [www.apme2017.org](http://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](mailto:kar@petrol.chem.msu.ru), [www.mam-17.org](http://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@moleculardiagnosics.gr](mailto:haliassos@moleculardiagnosics.gr); Organising Secretariat, MZ Congressi: Patrizia Sirtori, E-mail: [patrizia.sirtori@mzcongressi.com](mailto:patrizia.sirtori@mzcongressi.com), [www.athens2017.org](http://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](mailto:dulivo@pi.iccom.cnr.it); [www.csi-conference.org](http://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](mailto:tatfil@imc.macro.ru), [www.onlinereg.ru/mmops2017](http://www.onlinereg.ru/mmops2017)



## Mark Your Calendar (cont.)

### 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](http://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](mailto: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](mailto:IMEBORON16@cuhk.edu.hk); [www.imeboron16.org](http://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](http://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](http://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](mailto: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](mailto:Roger.stapleford@raci.org.au); [www.racicongress.com](http://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](mailto:Elias.Arner@ki.se), [www.se2017.se](http://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](mailto:steve@inchi-trust.org), [www.inchi-trust.org](http://www.inchi-trust.org)

## Visas

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

## How to Apply for IUPAC Endorsement

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

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

## Mark Your Calendar (cont.)

### 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-mm17

### 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: reviakine@uw.edu and Robert Latour (Clemson University), E-mail: latour@clmson.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

### 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

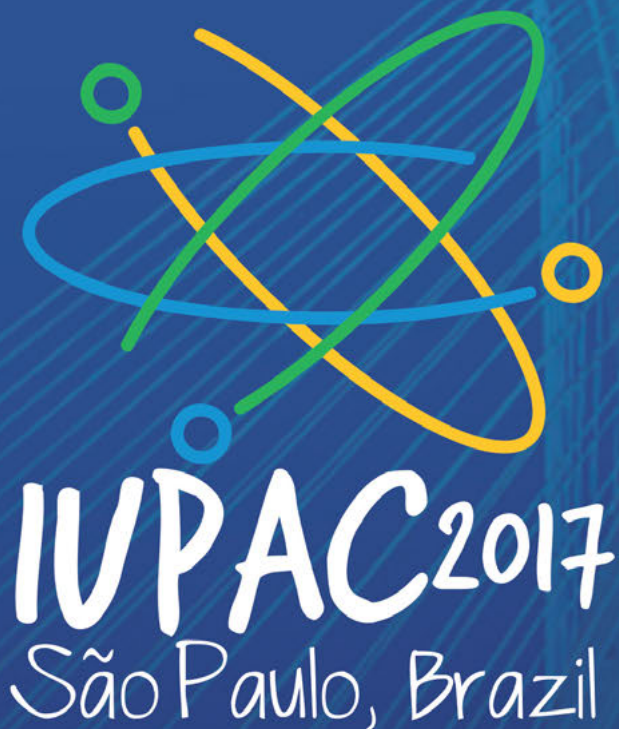
### 5-9 November 2017 • HPLC 2017 • Jeju Island, Korea

*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

## CI Goes Seasonal and Digital First

As indicated in the previous issue, beginning with this issue, *Chemistry International* will be published in print format only four times a year. However, and throughout the year, IUPAC members and *CI* subscribers will have access to new and updated content via *Chemistry International: Digital First*—a new electronic version that is currently in the early stages of development. The Digital First edition will provide a preview of what is new since the last print and what is being worked on for the next issue, including news, project updates, books and publications, conference updates, and feature articles - all of the *CI* sections with you are familiar with. Ultimately the print edition will be compiled every three months and thus will remain a sort of time capsule for reference. See iupac.org for updates.



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**We are ready to make it happen!**

**São Paulo – Brazil  
July 9-14, 2017  
Venue: WTC Sheraton**

[www.iupac2017.org](http://www.iupac2017.org)

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ADVANCING THE WORLDWIDE ROLE OF CHEMISTRY FOR THE BENEFIT OF MANKIND

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Version 2/2016, last updated 4 Jan 2016



# IUPAC Periodic Table of the Elements

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