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The Garden Party at Wiltzangk

The Table of Standard Atomic Weights ▶

The Search for Biodegradable Drugs ▶

INTERNATIONAL UNION OF
PURE AND APPLIED CHEMISTRY

Chemistry International

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

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Cover: In July 1928 in The Hague, The Netherlands, there was sufficient attention at the IUPAC conference for cheerfulness and entertainment. On Saturday, 21 July, all chemists "and their wives" were invited for a cup of tea at the Wiltzangk estate. This made for a memorable garden party. See the story behind the picture, page 6.

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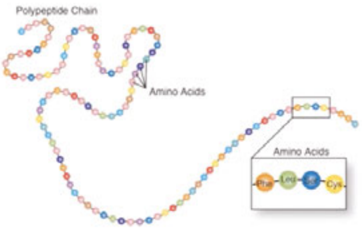

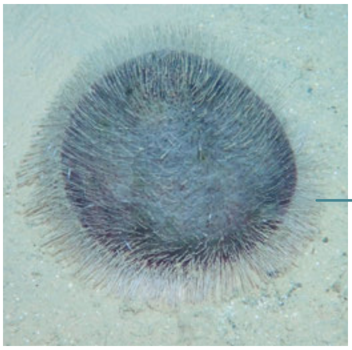

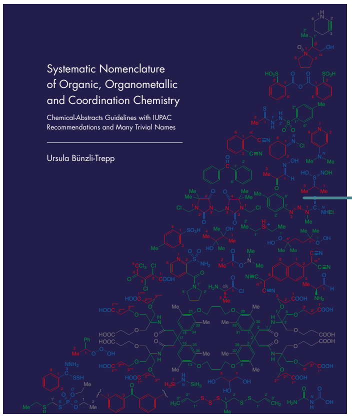

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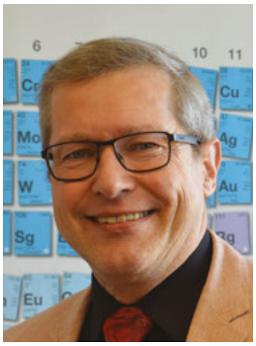

Wir schaffen das!

by Wolfram Koch

This is my first Editorial for *Chemistry International* as newly elected Treasurer of the Union. I feel very honored and proud that you have given me this mandate to serve the International Union of Pure and Applied Chemistry and am grateful for your trust. When I was first asked to write this column, back in early February of this year, I planned to elaborate primarily on IUPAC's financial situation, the effects of the pandemic and the way to a new normal. But then the unthinkable happened when Russia attacked Ukraine on 24 February. Since then we have experienced a terrible and inhumane war in the middle of Europe and thousands innocent people have lost their lives, are fleeing their country, and suffering terribly.

On 1 March IUPAC, as did many other scientific organizations around the globe, published a statement in which the Union strictly condemned the use of violence as a means to resolve a conflict and appeals to the Russian government to stop violating international conventions. Unfortunately to no avail. While writing this article the situation has deteriorated further. A new Russian offensive has been started at the end of April in the Eastern part of Ukraine and there is even the fear that internationally banned weapons of mass destruction, including chemical weapons (sic!), might be used by the aggressors. As an international science organization IUPAC plays a decisive role in facilitating cross border cooperation and keeping the doors open between researchers of all nations. Particularly in terrible times like this, science can be a catalyst to rebuilding bridges, and I hope and pray that we will see an end to this human catastrophe very soon.

While the war in Ukraine dominates the news and has shifted the Covid-19 pandemic somewhat out of focus, the pandemic is everything but over and still has significant influence on our lives and on the functioning of organizations such as IUPAC.

On the one hand, due to the pandemic and the lack of personal meetings, many projects of the Divisions and Standing Committees are negatively affected. At the most recent Bureau meeting on 9 April, many Division Presidents and Committee Chairs reported that while some progress could be achieved, a number of projects lie behind schedule and enthusiasm was lost because no travel and no meetings were possible. On the other hand, the Covid-19 induced restrictions which made face-to-face meetings impossible had also a positive effect on the Union's critical financial situation.

The past biennium was budgeted with an unhealthy deficit of more than 250,000 USD with expenses for travel and meetings of impressive (or better frightening) 907,000 USD. However, we actually spent only 27,500 USD for travel and meetings in 2020 and 2021, which is just 3 percent of the originally budgeted sum. The biennium closed with a surplus of almost 340,000 USD, an improvement of almost 600,000 USD against plan. An important contributor to this gain was however the good performance of our investment portfolio, which, as we all know, cannot be taken for granted in the future.

Therefore, as Colin Humphries, my longtime predecessor as Treasurer correctly pointed out, the last biennium has been something of a financial "timeout" helping IUPAC to consolidate its financial situation, which in the previous years became more and more problematic and unsustainable. Thanks to the reduced expenses we were also able to pay back completely our line of credit which adds to the good news. However, we must be aware that these good results are solely due to the very special circumstances of the pandemic and do not change the structural deficit that the Union was experiencing in the past years. This is where we must put our focus; we definitely need to come back to a financially sustainable situation. Hence, even if the pandemic—hopefully soon—will be overcome, a return to the *status quo ante* cannot be an option. Rather, we need to learn our lessons. It will be good to have the opportunity to meet in person again. But we should very carefully consider for which occasions this is really worth the expenses and limit our physical meetings to only those where it is necessary and justified.

We have all learned that virtual meetings are an alternative (even though I totally agree that there are a lot of disadvantages of such meetings, such as no informal but usually extremely valuable conversations or the time zone problem, which we as a global organization face in particular). But to re-iterate: It is my duty as Treasurer to make sure that the financial basis of the Union remains stable and healthy. And I take this duty very serious, even though I am very well aware that some of the necessary consequences will hurt and will not find everyone's support. But this is one of the Treasurer's unpleasant roles: I have to hold the tiller when it comes to finances and sometimes this means that I need to recommend to our governance to change or adapt routines, because it is necessary to ensure the well-being of the organization.

This brings me to my last point: The extreme importance of the organizational review which was adopted by the special Council meeting very recently on 4 June. Aside from the strategic arguments which clearly speak for the replacement of the current Executive Committee and Bureau by an Executive Board and a Science Board, also the financial consequences are extremely important. I was definitely not amused to learn that the last traditional (*i.e.* in person) Bureau meeting in Bratislava in 2018 costed us a fortune! My reaction as Treasurer has to be: Stop! We cannot afford this anymore.

Hence, the new structure with fewer people on the two Boards is a good step in the right direction, strategically and financially, and I am very happy that Council approved it. Let me close by reassuring you that I know what I am saying. As many of you know, the job I am getting paid for is to be the Executive Director of one of the largest global chemical societies, the German Chemical Society (GDCh) with around 30,000 members in Germany and beyond. And we are facing very similar challenges to IUPAC. The digital dimension will be more and more important in all areas we operate and also we will reduce significantly our in person meetings because we have learned that many issues can be dealt with in front of the screen. Not as fun as in the past, but unavoidable.

Lastly, but certainly not least, with reduced travel we also pay in for a lower CO_2 emission, something particularly well suited for a chemistry organization. I end with a quote from the former German Chancellor (and chemical physicist!) Angela Merkel who once said: “*Wir schaffen das!*” (“we can do it!”).

Wolfram Koch <wkoch@iupac.org> is IUPAC Treasurer since January 2022. Koch was appointed Professor of Theoretical Organic Chemistry at TU Berlin 30 years ago. In November 1998 he joined the Gesellschaft Deutscher Chemiker (GDCh, German Chemical Society) in Frankfurt and is GDCh’s Executive Director since November 2002. From 2002 until the end of 2020, he was also Executive Director and General Secretary of the German NAO to IUPAC.

The IUPAC Global Women’s Breakfast was born during the International Year of Chemistry in 2011, and it was reborn in 2019 during the International Year of the Periodic Table. Since 2019, the GWB has grown into an annual event in February of each year in support of the United Nations Day of Women and Girls in Science.

The goal is to build a network of women and men in support of closing the Gender Gap in Science.

In 2022, more than 30,000 people participated in 400 breakfast events in 75 countries.

We invite women and men from all science disciplines to organize breakfast events on 14 February 2023 as part of the IYBSSD.

Go to iupac.org/gwb to register your event today.

Le petit-déjeuner mondial des femmes de l'IUPAC est né lors de l'Année internationale de la chimie en 2011, et réétabli en 2019 lors de l'Année internationale du tableau périodique. Depuis 2019, le Global Women’s Breakfast (GWB) est devenu un événement annuel en février en soutien de la Journée des Nations Unies pour les femmes et les filles de science.

L'objectif est de créer un réseau de femmes et d'hommes de scientifiques pour soutenir la réduction des inégalités entre les femmes et les hommes dans le domaine scientifique.

En 2022, plus de 30 000 personnes ont participé à 400 petits-déjeuners dans 75 pays.

Nous invitons femmes e hommes de toutes les disciplines scientifiques à organiser des petits-déjeuners le 14 février 2023 dans le cadre de l'IYBSSD.

Allez sur iupac.org/gwb pour enregistrer votre événement dès aujourd'hui.

The Garden Party at Wiltzangk

The Garden Party at Wiltzangk

by Jorrit Smit [1]

What is the story behind this photo, of the "Garden party at Wiltzangk"? It first caught my attention over eight years ago when I was researching interwar chemistry during my studies. Since then, I moved to post-war science policy in my PhD, and the photo faded into the margins of my attention. Yet recently the image of this fabulous garden party came back to me—and I finally wondered what was actually going on there [1].

After three years in the lab, for my bachelor degree in chemistry, I decided to explore new areas of research: a master program in history of science at Utrecht University. In the course "Dilemmas of Modernity" I was for the first time—still half chemist— confronted with the empirical richness of the archive. I thoroughly enjoyed the strange feeling of connecting with an earlier time. Whenever you thought you figured it out, an unexpected letter, photo or scribble in the sidelines could turn the story upside down. And I enjoyed the physical contact with my century-old sources: from the thick yellowed paper and the beautifully published booklets, to the clumsy, cozy places in the library or museum where you could suddenly plow through piles of paper. As research space the archive is thus both very different from the lab, and not so different at all—especially when you consider the practical discipline required and the surprises that the empirical world holds for the researcher.

Luckily, all this toil not only ended up in chaos, but also a paper that was allowed to appear in a special issue about the First World War in *Studium* (a magazine that has recently become archival material itself!) [2]. In short, this paper followed the attempts of a few Utrecht chemists to bring the chemists of all countries back into conversation after the Great War—that was especially sensitive for chemists, since chemical expertise had been used for offensive (and defensive) purposes on all sides of the conflict. The newly established International Organization for Pure and Applied Chemistry (IUPAC) temporarily excluded the chemists from Central Powers (Germany, Austria, Hungary) from participating. The Dutchman Ernst Cohen was one of the neutral champions who tried to change this in the 1920s [3].


Ernst Cohen

Looking back at these papers, I am a little bothered by the need I felt to emphasize again and again that this war marked a break with the scientific images of "Comtean" and "positivist" optimists (what we would today probably call scientism). The science-critical scholar I had decided to become had to deal with the chemist I might have been. But, the archival sources that I gathered for these papers still fascinate me: from a cozy group photo in Cohen's garden in Utrecht, in 1921, and the "chemical-historical" menu they were served that evening, to a poem by the Latvian-German chemist Paul Walden who, with healthy poetic exaggeration, compared the work of the Dutch with their struggle against the raging sea.

Subsequently, I wrote my thesis on the same Cohen and his so-called "pure" physical chemistry, and so I collected his remaining documents throughout the Netherlands. That is how I came to visit the Utrecht University Museum, where I not only found a few beautiful letters from an exchange between Cohen and Fritz Haber— the German Nobel Prize winner who became a notorious symbol for poison gas development—but was also surprised by a classy photo album.

Most of the photos were from the IUPAC conference that took place in The Hague in July 1928. I quickly snapped some memories of the prettiest—including the garden party photo that I started this piece with. But I didn't dwell on it very long and didn't figure out what exactly was happening there, and it disappeared in a folder, tucked away deep on my hard drive.

It was a few years later, in 2019, that I opened this digital drawer again. The occasion was the centenary of the IUPAC, in honor of which chemistry historians prepared a special issue of *Chemistry International* [4]. As it turned out, they knew about my *Studium* article (which had a wider international reach than I suspected!) and asked me to tell more about Ernst Cohen's years as IUPAC president [5]. The article that I thought I had left behind for a long time suddenly turned out to be relevant again.

It was the editor of *Chemistry International*, Fabienne Meyers, who inquired about the photos I supplied with the text. Where were these photos taken, and why? The easiest was the photo of the opening of the IUPAC conference—where German chemists were again present as guests for the first time. This clearly took place in the "old" room of the House of Representatives in the Binnenhof [See photograph of the opening of IUPAC Conference in the "old chamber" of the *"Tweede Kamer"* (House of Representatives)" in The Hague in July 1928, reproduced in ref. 5, p. 9]. Although it's not officially in use anymore for the main Dutch political debates, it

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[1] *This feature in English is based on an original blogpost published in Dutch on 19 Oct 2019; see ref. 1*

Can you find Cohen?

still houses events. And, in 2020, it was again used, as it could accomodate distancing measures, to hold political meetings on the appropriate (scientifically validated) response to the covid pandemic.

Even though they have put up some gloomy blue lights in the meantime, the hall remains easily recognizable.

In both 2020 and 1928, this room was a crossroads of science and politics [6]. Cohen opened the meeting in four languages (French, English, Latin and Esperanto) to emphasize the international nature of science. He then gave the floor to the Minister of Labour, Trade and Industry, Dr J.R. Locksmith de Bruine. As a "former professor" of theology, he praised not only "pure" science, but also, as a minister, "applied" chemistry, because "industry" increasingly learned to "reap the fruits" of science. Cohen concluded with some science-historical jokes: History had examples of ministers proficient in chemistry—Joseph Priestley discovered both oxygen and soda water ('laughter')—so the Minister could become "one of them" if only he would hang out long enough with chemists ("cheerfulness").

Indeed, there was sufficient attention at the 1928 IUPAC conference for cheerfulness and entertainment. On Friday, the delegates visited Rotterdam, where they enjoyed lunch at City Hall, took a boat trip on the Maas river to visit the port and passed by the monument of the first Dutch Nobel prize winner J.H. van 't Hoff (which can still be visited today!).

And on Saturday, 21 July, a procession of cars drove from the Peace Palace in The Hague to the woody Wassenaar. All IUPAC chemists "and their wives" were invited for a cup of tea at the Wiltzangk estate. The invitation came from "S. van den Bergh and Mrs. Van den Bergh-Willing." That is to say, Samuel van den Bergh, at that time a member of the board of directors of the Margarine Unie, and thus one of the founders of today's Unilever. The Jewish Van den Berghs had been spending their free time on Wiltzangk since 1922, and would do so until the Wehrmacht requisitioned and looted the house during World War II. Today it is the residence for the Iranian ambassador, at Rust en Vreugdelaan 5.

At the closing dinner, in the Kurhaus in Scheveningen, the Minister for Industry Slotemaker de Bruine again reflected on the relationship between pure and applied science, in chemistry and theology: "If I review what you have done in the last four days . . . I wonder how to classify this. For example, was the 'garden party' on the Wiltzangk and your visit to the ports of Rotterdam to be regarded as pure or applied chemistry?" Both, Cohen could have answered, because the international chemical conference was an opportunity for him to establish himself internationally on the scientific map, as well as an opportunity to strengthen ties with politics and industry within Dutch borders, so as to convince them of the social relevance of his science. That was more or less the conclusion of my master's thesis on Cohen's chemistry, which I now saw expressed in these few images. The garden party photo has continued to follow me over the years—and I'm excited to see it resurface here again in *Chemistry International* and who knows, at the IUPAC conference next year in The Netherlands.

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Title page reprinted with permission from the photo album of Professor Dr. E.J. Cohen, 1928-1933, Utrecht University Museum, inv.nr 0285-25630.

A Global Conversation on the Use of Artificial Intelligence in Chemistry

by Jeremy Frey, Bonnie Lawlor, Leah McEwen, Christopher Ober, and Antony Williams

The 2021 IUPAC World Chemistry Leadership Meeting (WCLM) was more than a year in the making and it was quite a roller coaster ride. Originally planned as a traditional in-person meeting, the pandemic required that the entire IUPAC World Chemistry Congress (WCC) be held virtually. Rather than view this as a negative outcome, the WCLM organizers decided to leverage the situation as an unexpected opportunity to do something unique and innovative that would allow the session to reach a much larger portion of the global scientific community than is the norm at an in-person meeting. The meeting format was designed to stage not one plenary session, but four virtual sessions spread over 24h and covering three different time zones (vide infra). The topic, The Future of Chemistry in the World of Artificial Intelligence, was chosen because artificial intelligence (AI) has been receiving a lot of press—not only in the sciences, but across all industries [1]. In addition, AI was selected in 2020 by a panel of experts as one of IUPAC's top ten emerging technologies in chemistry—one that will have major positive impacts on how research is conducted and the speed with which science is advanced [2].

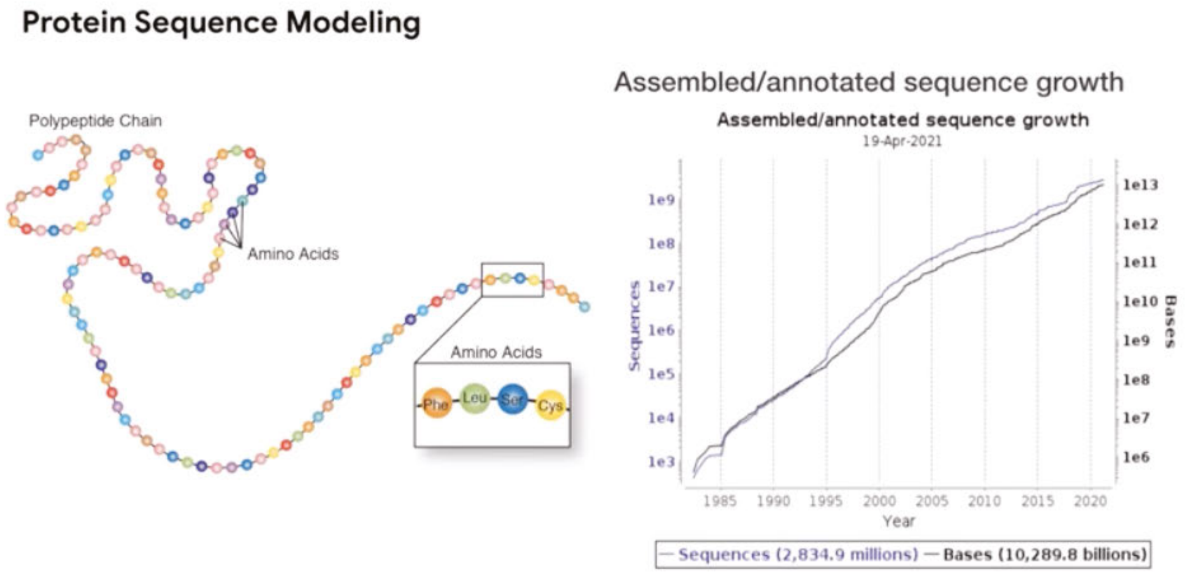
The topic, just one aspect of digital science, exemplifies IUPAC's new direction which began almost a decade ago in 2014 with Jeremy Frey's proposal for "Digital IUPAC." [3] He recommended that IUPAC create a consistent global framework for human AND machine-readable (and "understandable") chemical information. He also recommended that IUPAC not do it alone, but rather in collaboration with other science communities, industries, and governments. IUPAC extended the Committee on Printed and Electronic Publications to the Committee on Publications and Cheminformatics Data Standards (CPCDS) to focus on both data sharing and the storage and management of digital content through the development of standards that would ensure both the human and machine-reading/sharing of chemical information.

By the time of IUPAC's 100th anniversary in 2019 it has become apparent that the IUPAC is emerging as a strong leader in the digital world through partnerships with broad international data initiatives, including CODATA and GO FAIR [4]. The goal is to develop standards and a global infrastructure that promotes the machine-readability of chemical data and other digital resources building on IUPAC's founding principle to provide a common language for human chemists so that they could efficiently and effectively communicate irrespective of their geographic location. The next logical next step is for IUPAC to develop the standards required to ensure that the computers and other equipment used by chemists share a common language for the dissemination, exchange, and FAIR re-use of data. A 2021 article details the implications of this relationship with CODATA that you can read at your leisure [5].

By the time that the 2021 WCLM was being planned in its virtual format the forces of change within IUPAC itself had converged. The journey to a Digital IUPAC had already begun and was exemplified by the WCLM global conversation.

As noted above, the move to a fully online meeting meant that it was possible to engage not only scientists ostensibly in Montréal, but the global science community, independent of location, in a 24-hour event. Working with the Canadian hosts of the 2021 World Chemical Congress a small team consisting of the listed authors of this paper and coordinating with Lynn Soby and Fabienne Meyers from the IUPAC Secretariat, assembled the event. For each of the organizers, the impact of AI is already clear, its future is astonishing, and this event offered an opportunity to share their collective excitement at the impact this field will have on chemistry. They also elected to engage two additional groups, the future hosts of the next two WCC, the Netherlands (2023) and Malaysia (2025), and both groups were willing, on rather short notice, to hold a local event on the theme of AI.

As planning developed, the team realized the need to set the stage for an interested but non-expert audience to consider the many possibilities of artificial intelligence as applied to chemistry. To do this they identified six expert practitioners of this developing field: Andreas Bender (University of Cambridge), Nathan Brown (BenevolentAI), Lucy Colwell (Google Research/University of Cambridge), Thomas Fleming (Arctoris), Wendy Poulsen (Bayer Crop Science) and Christoph Steinbeck (Friedrich-Schiller University) to record short presentations on their work and the



Lucy Colwell (Google Research/University of Cambridge) discussed chemical structure insight through analysis and modeling, and taking advantage of large data sets.

impact that AI is having, and may have, on chemistry. These short video presentations were then made available to people interested in attending the WCLM and form the basis of panel discussions held during the WCLM. They covered topics that ranged from laboratories and instrumentation of the future, products and services using AI, informatics and data sets, chemical modeling and using AI to identify candidate systems.

Bender described computer-driven drug discovery made possible by the growth in data today. With that comes new methods for sifting through data. However, in this period established complex processes are difficult to change. Building new tools can lead to new discoveries by using data-driven starting points and optimization with increased amounts of data. Compared to materials discovery, drug discovery is more challenging. In materials research usually the researcher knows what they want and how to measure properties. In contrast with drug research, scientists may not know precisely what they want and responses are difficult to measure. In drug discovery with AI, the question needs to come first, then appropriate data, and finally the representation and the method.

Brown presented a discussion of using AI to speed drug discovery. The goal of his organization is that no disease goes untreated. Biology is incredibly complex and must also deal with vast amounts of data. The cause of a disease is often misunderstood which complicates interpretation. In a discussion of this topic, Brown described aspects of their process flow for drug discovery which is to first map a knowledge graph, make target identification, develop precision medicine, and finally identify molecular design.

Colwell discussed chemical structure insight through analysis and modeling, and taking advantage of large data sets. Challenges include cleaning data for analysis, how to represent molecules, choosing the right modeling strategy, and training test sequences that mimic real world use cases. She described protein modeling using data collected from real world examples and used AlphaFold to discuss examples of prediction success. She noted that 3D-structure can constrain folding. Accurate predictions can be produced given enough sequence homologs. Finally, she described a progression in strategies for using AI to provide more sophisticated and successful folding models.

Fleming showed efforts for drug discovery. A new drug can take 10 years and $2B to develop, and in pharma drug discovery, costs keep increasing with time. Other industries (*e.g.* microelectronics) have opposite trends. In pharma, labs are expensive to build and to maintain. He described total automation for biochemistry, cell biology, molecular biology and biophysics, and how to take the laboratory beyond high throughput screening.

Poulsen explained that data is used in agriculture to plan plantings and crop selection. Using AI enables an improved pace of innovation, improves sustainability and accessibility, and creates new experiences and value for farmers and consumers. By using digital sensors on tractors and unmanned systems (*e.g.* drones) it is possible to extend the spectrum of parameters and provide new insights for agriculture. Examples of the of use Machine Learning (ML) and computer vision to interpret data means we can better ensure safety of bees and pollinators to improve sustainability or use robotics to make decisions about what weed control products to spray.

AlphaGo vs Fan Hui
London, October 2015

'Our goal is to beat the best human players not just mimic them'
Google Deep Mind

In his presentation, Steinbeck highlighted the importance of Artificial Intelligence winning against a human opponnent in a game of Go.

Steinbeck began by mentioning the impact of AlphaGo winning against a human player in the game of Go. This win showed the potential of AI in areas previously limited to human intelligence, and taught us that unlimited training data (created by AlphGo playing itself) and both hardware and software improvements also enabled this advance. A next development was AlphaFold (already mentioned by Colwell) and was able to best other AI systems in determining protein folding. Steinbeck asks, given the need for data, do we have enough data for deep learning in chemistry? He asserts that useful data must be open and bulk-downloadable and that the life sciences is generating lots of that data while chemistry is not. He talks about how chemistry can get out of its data drought and he says chemistry needs to begin using proper data management and making it openly available.

The WCLM started in Montreal with a plenary talk given by Yoshua Bengio (U Montréal), an A.M. Turing Award winner [6] and pioneer in artificial intelligence, and was introduced by the conference lead, Bruce Lennox, Chair of the WCC. Comments were provided by IUPAC VP Javier Garcia-Martinez on the importance that AI will play in IUPAC's future and that of the chemical community. Bengio's talk on Machine Learning for Chemical Discovery was inspirational and presented an exciting vision to all the WCLM participants on the use of Machine Learning to sift through vast amounts of data to identify new solutions to chemical and biological problems.

That evening (Montréal time) the WCLM baton would be passed to Malaysia where a mini symposium was organized by Datuk Soon King Tueh and his associates. The symposium centered on chemistry in the developing world around themes of economic development, environmental protection, societal harmonization, and sustainable development, and a special session on the role of AI in the future of chemistry and de novo drug design was held. Speakers on AI included Luhua Lai (Peking U), David Winkler (LaTrobe U), and speakers on other topics were Mayume Nishida (Hokkaido U), Mazlin Mokhtar (U Kebangsaan Malaysia), Mei-Hung Chiu (National Taiwan Normal University), and Chulhee Kim (Inha U).

The Netherlands hosted the next event in the early hours of the morning (Montréal time), a panel discussion that considered the short previously recorded presentations by the six experts and AI in general. Timothy Noël (U Amsterdam) was the moderator of a panel discussion. The panelists in this session were: Ola Engkvist (AstraZeneca), Hugo Ceulemans (Janssen R&D), Barbara Zdrazil (UVienna) and Maarten Honing (Maastricht U). The debates on the six videos and points of view expressed reflected the rapidly evolving and increasingly sophisticated methods of AI.

And finally, 24h after the initial session, the event returned to Montréal where participants were welcomed by Christopher Ober and Bonnie Lawlor. Following their remarks, they introduced Antony (Tony) Williams (US-EPA) who moderated a virtual panel convening the six expert speakers who previously shared short videos and to discuss their presentations and the future of AI.

The presenters each gave a short overview, about 5 minutes each, of their recorded presentations before moving on to the panel discussion. The discussion was initiated with prepared questions as well as some submitted during the session. Example questions included: 1) How will AI change the way we teach chemistry (at all levels); 2) How should IUPAC work with other computer & information scientists to set the standards for a digital age?; and 3) What data interoperability challenges are you facing?

The panel was ideal as the presenters were highly engaged and offered their opinions, insights and experiences when answering these and many other questions throughout the panel discussion. The collective wisdom shared was concluded with the consensus opinion that while there have been many achievements to date, and these are indeed exciting times in terms of the expanding applications and benefits of AI, there is still much to do and unforeseen impacts to come. Tony concluded by acknowledging the speakers for the significant work invested in writing and recording the presentations, getting them delivered on schedule, and showing-up to participate in the panel discussion. Finally, the session was closed with a comprehensive summary of what the audience had heard and a personal perspective by Jeremy Frey on the importance of AI.

Jeremy Frey highlighted the fact that the use of Artificial (or as he said in his view this would be better considered as Augmented) Intelligence and the specific area of Machine Learning, that has become very prominent in the last five years, is a major part of the digital revolution in chemistry (and the wider chemical sciences) [7]. AI has already had a dramatic influence in some areas of chemistry (*e.g.* AlfaFold2 for protein structure prediction) and is poised to be a revolution in most of chemistry R&D. It is highly likely that AI will drive even more dramatic changes in the approach taken to teaching chemistry in higher education (and indeed perhaps even in earlier years, ML is available for the Scratch programming environment [8]).

AI/ML technologies are developing rapidly, interdisciplinary work between pure mathematics, statistics, data science, and chemistry are moving the field forward by taking advantage of faster computers, dedicated hardware, improved software, and new algorithms. Huge investments are being made in AI/ML in both drug and materials design, and in digital twins to model and control chemical processes both by traditional players and new start-ups. The confluence of AI and simulation, seen already in digital twins for process chemistry, will further the analysis of the complex formulations that abound in industry and will be a step along the path to integrating chemical, biochemical, and medical pathways to deliver the potential of personalized medicine (at an affordable cost?).

AI/ML will help in predicting properties of molecules and materials, how to make them, and how well they will integrate into devices and serve the circular chemical economy; they will not do this alone. The need for reliable quality data means that the parallel development of automated, high-throughput, synthesis, and new characterization methods that work with increasingly small amounts of material are essential. However, it is also essential that the AI models be explainable. Understanding why a model works is essential to imbue the systems with trust that is a necessary component for AI to enhance chemical discovery. AI together with human insight will help us develop a more sustainable and personalized economy.

Through its mission and proven process for defining a rigorous parlance of chemistry, IUPAC has an imperative to provision digitally enabled standards that meet these needs for both accessible data and expert exchange. We are honored to engage so many experts and members worldwide in this exciting and timely dialogue on behalf of the global scientific community.

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Jeremy Frey, Professor of Physical Chemistry and Principal Investigator for the AI for Scientific Discovery Network, University of Southampton; Bonnie Lawlor, Vice Chair, U.S. National Committee for IUPAC; Leah McEwen, Chair, IUPAC Committee on Publications and Cheminformatics Data Standards and Chemistry Librarian, Cornell University; Christopher Ober <cko3@cornell.edu>, Francis Norwood Bard Professor of Materials Engineering, Cornell University; Antony Williams, Computational Chemist, U.S. Environmental Protection Agency.

See video at https://iupac.org/event/wclm2021/.

The search for biodegradable drugs

by Anthony King

When Israeli scientists tested vegetables for the epilepsy drug carbamazepine, they detected it in cucumbers, carrots, lettuce, and peppers. More surprisingly, people who ate the vegetables had a surge of the epilepsy drug in their urine—albeit in the nanograms.

"So much reclaimed wastewater is being used for irrigation that we wanted to see whether some residues can pass from water to the soil to the crop to people," explains study author Benny Chefetz of the Hebrew University of Jerusalem, Israel. The quantities were minuscule (one thousand-millionth of a gram) and there was no risk of death or instant illness from the drug residues, so the vegetables stayed on the market.

It's an oft-told tale. Most drugs we take, we excrete. The remnants flow on to treatment plants, and some drugs flow out in treated water—more, it turns out, than we previously thought. As chemistry instruments advanced over the past decade, scientists expanded the list of leftovers detected in rivers, streams, and wildlife. The US Geological Survey reported in 2016 that it had detected at least one out of 108 pharmaceuticals it tested for in small streams in the eastern US. The average number detected was six.

Our prescription habit, it seems, has blanketed the Anthropocene with a variable drug cocktail.

One solution is to intensify the cleaning process. Switzerland has spent huge sums upgrading its treatment facilities to remove micro-pollutants. Yet many countries cannot afford this strategy. Eighty percent of active pharmaceutical ingredients are made in China and India, where water treatment standards are generally poor. What's more, some argue, treatment is not just expensive but potentially harmful. Professor Klaus Kümmerer at Leuphana University in Lüneburg, Germany, is of this view. He says high-tech treatments can convert pharmaceuticals into biologically active molecules that we know even less about.

Kümmerer began his academic career looking at pollutants in the environment. What he saw forced him to switch his attention to the other end of the pipeline—the creation of new drugs. He advocates "benign by design," a concept he began promoting more than ten years ago. Under this new creed, drug companies should look at biodegradability as desirable during drug development. Drugs would be designed to break down naturally.

When he first talked about this concept at a pharma conference in London in 2006, his audience sat stunned. Drug developers were horrified: it is already difficult to come up with a new drug, and now you want it to biodegrade. That's crazy talk, they said. Drug developers and regulators seek stability, not instability. But Kümmerer persisted. Tests he carried out indicated that between 15 and 20 percent of drugs on the market were already—accidentally—biodegradable.

It is normal to have a lead drug structure and to alter parts of the molecule to improve it, to optimize its biological effect, or to reduce side effects. "Designing for biodegradable drugs would just add another criterion when selecting from promising candidates," says Kümmerer.

There are chemistry basics that guide whether a compound will biodegrade. Many molecules in nature are linear carbon chains, made up of carbon-to-carbon bonds; natural enzymes in bacteria chew these bonds apart. However, highly branched carbon chains with three carbons stuck together resist natural enzymes and persist. Knowing and tweaking the chemistry of drug molecules could ensure they break down in the environment, not in storage.

Kümmerer hasn't just campaigned. He's walked the walk. As a proof of concept, Kümmerer and his colleagues modified a beta-blocker used to treat high blood pressure (propranolol). He blasted it with UV light and then picked out molecules that blocked the drug target and were biodegradable. He tested candidates for toxic effects until he selected two winners.

His lab also developed a new cipro-floxacin-class antibiotic that is biodegradable. Low-dose antibiotics in the environment encourage drug resistance. This happens when bacteria are continually pressured to defend themselves against antibiotics. Harmless bacteria in the environment can then come up with ways to evade antibiotics and transfer this ability via resistance genes to bacteria that infect patients. In fact, many of the resistance genes found in hospitals today originated in harmless bacteria. Researchers say this phenomenon threatens the usefulness of existing and future antibiotics. Yet there are few strategies to tackle this problem. One solution is for drugs to self-destruct rather than persist and encourage resistance to antibiotics.

> *When he first talked about this concept at a pharma conference, his audience sat stunned. Drug developers were horrified: it is already difficult to come up with a new drug, and now you want it to biodegrade.*

But societal benefits and chemical structures notwithstanding, the biggest hurdle to environmentally benign drugs may be a lack of incentives. "We need a mix of sticks and carrots," says Kümmerer. Incentives could include patent extension if

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Adding Responsibility to the Three R's

Design on different levels for circularity (adapted from Zuin and Kümmerer, Nature Rev Mat. 2022, ref. 8)

1) Responsibility

Take ownership of your own product throughout the whole lifecycle beyond the value chain and required function and application

2) Reduce

Avoid consumption and thereby the amount of waste generated: the first and most effective step toward producing less waste, needing less energy and resources; relates to flows of substances, materials, building blocks and products at all levels including

- size (tonnage)
- chemodiversity (atomic, molecular, complexity of composition, mixing)
- dynamics (size, composition)
- space (size, composition)
- time (rate of change, change of rates)

3) Reuse (and extended use)

Use an item again and again in its original form: this eliminates the need to reprocess materials (whether it is for disposal or for recycling). Reduces dissipative losses, save energy, material resources and waste)

4) Recycle

1. keep form and size (for example, do not cut track tarpaulin into pieces for bags)
2. keep material (remould thermoplastics and alloys, avoid thermosets)
3. keep the composition (do not add or remove constituents or additives when re-melting alloys)
4. keep molecules (constituents, additives)
5. keep building blocks (molecules, monomers)
6. keep atoms (pyrolysis, metallurgy)
7. keep energy (e.g. "thermal recycling", which is in fact combustion)

a drug is made biodegradable, or faster authorization. The stick: to include biodegradability in the drug-approval process. The idea that drugs could be kept from market for polluting is one that the industry finds shocking. They argue that it would be unethical for regulators to stop a drug getting to patients because of pollution. Kümmerer is unrepentant.

He counters that industry will cease drug development for lethal diseases for economic reasons. Moreover, says Kümmerer, there is a need to break the industry's dogma that stability in a drug is desirable, instability undesirable. We tend to think of the drug industry as innovative, but they are highly conservative. They want to stick to the business strategy that has kept them profitable.

Kümmerer believes that new regulations, rather than being a burden, can spark innovation. Big drug companies will be pushed to be chemically creative or surrender market share to nimble newcomers. They could also re-examine drugs previously jettisoned for stability reasons. One market-driven solution, adopted by Sweden, is to make doctors and patients aware of the green credentials of drugs when making choices.

With water shortages a growing issue around the world, water re-use is likely to become more popular. This makes it more likely drug residues will end up in our food and drinking water.

Bryan Brooks, a biologist at Baylor University in Texas, is especially concerned about mega-cities in developing countries; most will not install sophisticated water treatment anytime soon. "There are a number of streams in semi-arid regions that would not flow at times of the year without wastewater discharge," he says.

Brooks became intrigued by urban water cycles and subsequently made landmark discoveries of antidepressants in the brains of fish as well as subtle effects on their behavior. Like many researchers in this area, he notes the difficulty of deciphering the effects of the motley mix of drugs and other chemicals in the environment on different animals.

"Our understanding of potential consequences of pharmaceutical exposure to biodiversity is very limited," Brooks says. The same is true for people. We do not know the damage we are doing. Moreover, the variability in what we are exposed to makes it practically impossible to set up endless experiments in a lab, so we should take a precautionary approach and minimize the risks.

Getting there will require investment, drug research, and a change in attitude. Kümmerer radiates belief that industry will eventually see the light. Attitudes in some companies are shifting. "Some people recognize that this is an opportunity for new molecules and new patents," he says. The issue of drugs in the environment is not fading from public view, and the political pressure is heating up in Europe. "It is still in its infancy, but this can be a business opportunity," Kümmerer concludes. "Old thinking could be dangerous to a drug company's future."

Anthony King is a freelance science journalist based in Dublin, Ireland. His article was first published in *Anthropocene* in July 2018 <https://www.anthropocenemagazine.org/2018/09/benign-by-design/>, and reprint here with permission

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Not just Good Chemistry

Design at All Levels and for All Stages of Life Going Beyond Sheer Circulation is Key for Chemistry and its Products

by Klaus Kümmerer and Vânia G. Zuin-Zeidler

Chemistry as a science and an industrial sector plays a determining and indispensable role in all parts of our lives as it is the only science that can change matter (apart from nuclear physics). What we call a chemical product is often highly complex; elements and chemicals are most often applied as mixtures in products. For example, there are several hundred grades of steel (*i.e.* iron alloys) marketed. Electronics relies on many complex materials. Other examples of products are pesticides, pharmaceuticals, biocides, laundry detergents, personal care products and many others composed of several chemicals each. Estimates indicate that the number of chemicals in use today exceeds 340 000 worldwide. There are many kinds of polymers. The polymers themselves are made-up by manifold building blocks of different size, stereochemical arrangement, functional groups, branched or interlinked segments, *etc.* Today more than 10 500 plastic-related additives are in use. Often

during synthesis, manufacturing, and use, and at the end of their lives, all these materials and products are transformed ("degraded"), resulting in new chemical entities of often unknown properties, impact on the product and toxicity. In other words, at all stages of the chemical products lifespan there is enormous chemodiversity, from the atomic to the molecular, from material to building blocks and products, as well as in sectors of applications and usage. Owing to their high diversity and adaptability, chemicals and synthetic materials are literally used everywhere nowadays.

The downside of this impressive success story is that chemical products are ubiquitous in places also where we do not want to have them, *i.e.* in human beings, organisms and the environment. Another downside is an increasing shortage of resources and an increase in waste and an increase in energy demand. One attempt to address issues of a shortage of resources, waste and pollution simultaneously is the concept of Circular Economy (CE).

To understand chemistry as an important building block of a future CE, we must understand CE prerequisites, opportunities, and limitations from a chemical point of view. Chemical products (and the downstream products containing them) need to be designed from the very beginning for both circulation and later recycling. This includes design for easy use and further reuse, collection, as well as physical and chemical dismantling and separation processes; all this to keep unintended losses as low as possible. Just applying "good chemistry" is not sufficient by far. Chemistry, in the broadest sense, has to fit into a CE. If a broader view is taken, there can only be down-cycling, and no up-cycling. Recycling is governed by thermodynamics, *i.e.,* entropy increases. For example, to gain the desired quality of the products of recycling, fresh or virgin material needs to be added often (*e.g.* alloys, aluminum, fibres for textiles and paper, and polymers and additives in case of plastics). In order to lose as little as possible of materials and to generate as little entropy as possible, we need to avoid unsustainable extraction, mixing and separation, and upgrading processes including the obtention of natural and renewable resources such as (bio)waste. Therefore, we have to design both products and processes for as simple as possible. This relates—among other things—to the chemical structure and its change, as well as the composition of related material flows. Extreme efficiency (either maximal or minimal) may result in rebound effects, when optimization is preferable. The cradle to cradle thinking that everything is abundant and easily available "food" within the technosphere would result in an economy where efficiency is not be taken into consideration. This thinking denies thermodynamic principles which also apply. It is guided by a misunderstanding of natural cycles: in contrast to the matter flows in the technosphere, those in nature consist of a few basic building blocks only and low chemodiversity.


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There are always unavoidable losses of products or their constituents during their lifetime, as by thermal degradation in the case of moulding thermoplastics, unintended disaggregation (*e.g.* plastics and additives) or abrasive losses (*e.g.* tyres, paint, metal corrosion, and facades). These products cannot be collected and therefore neither can they be recycled. In addition, the use of many chemical products is linked to their direct introduction into the environment (*e.g.* surfactants and other constituents of laundry powder, pesticides, biocides, personal care products, and pharmaceuticals). For these, a design for full and fast environmental degradation, *i.e.* mineralisation, is necessary.

This demonstrates that CE in its different forms is neither necessarily a greener nor a more sustainable contribution of chemistry to a more sustainable future. A broader system thinking-based view accounting for needed service and function is integral part of sustainable chemistry ("chemistry for sustainability"). Different behaviours and business models that focus on knowledge instead of tonnage can reduce the number and the amount of chemicals and chemical products. If the desired service and function can only be delivered requiring chemical products, we should aim to making them fit into a CE ("chemistry within a circular economy"). The synthesis and properties of these chemicals and products must be aligned with the principles of green chemistry then, in fact "greener chemicals."

Becoming more sustainable means to design for less diversity, less complexity, and lower tonnage. This may be the biggest challenge for chemistry and chemists, as the character of chemistry is to invent or to introduce new molecules, materials, and products by changing matter.

Further Reading

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The 2030 Agenda for Sustainable Development, adopted by all United Nations Member States in 2015, provides a shared blueprint for peace and prosperity for people and the planet, now and into the future. At its heart are the 17 Sustainable Development Goals (SDGs), which are an urgent call for action by all countries—developed and developing—in a global partnership. Reprinted from [1]. Additional Goal 12 infographic, source: https://unstats.un.org/sdgs/report/2021/


the end is near
everything will be okay

IUPAC Periodic Table of the Elements

Key:

atomic number
Symbol
name
abridged standard atomic weight

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1 **H** hydrogen 1.0080 ± 0.0002																	2 **He** helium 4.0026 ± 0.0001
3 **Li** lithium 6.94 ± 0.06	4 **Be** beryllium 9.0122 ± 0.0001											5 **B** boron 10.81 ± 0.02	6 **C** carbon 12.011 ± 0.002	7 **N** nitrogen 14.007 ± 0.001	8 **O** oxygen 15.999 ± 0.001	9 **F** fluorine 18.998 ± 0.001	10 **Ne** neon 20.180 ± 0.001
11 **Na** sodium 22.990 ± 0.001	12 **Mg** magnesium 24.305 ± 0.002											13 **Al** aluminium 26.982 ± 0.001	14 **Si** silicon 28.085 ± 0.001	15 **P** phosphorus 30.974 ± 0.001	16 **S** sulfur 32.06 ± 0.02	17 **Cl** chlorine 35.45 ± 0.01	18 **Ar** argon 39.95 ± 0.16
19 **K** potassium 39.098 ± 0.001	20 **Ca** calcium 40.078 ± 0.004	21 **Sc** scandium 44.956 ± 0.001	22 **Ti** titanium 47.867 ± 0.001	23 **V** vanadium 50.942 ± 0.001	24 **Cr** chromium 51.996 ± 0.001	25 **Mn** manganese 54.938 ± 0.001	26 **Fe** iron 55.845 ± 0.002	27 **Co** cobalt 58.933 ± 0.001	28 **Ni** nickel 58.693 ± 0.001	29 **Cu** copper 63.546 ± 0.003	30 **Zn** zinc 65.38 ± 0.02	31 **Ga** gallium 69.723 ± 0.001	32 **Ge** germanium 72.630 ± 0.008	33 **As** arsenic 74.922 ± 0.001	34 **Se** selenium 78.971 ± 0.008	35 **Br** bromine 79.904 ± 0.003	36 **Kr** krypton 83.798 ± 0.002
37 **Rb** rubidium 85.468 ± 0.001	38 **Sr** strontium 87.62 ± 0.01	39 **Y** yttrium 88.906 ± 0.001	40 **Zr** zirconium 91.224 ± 0.002	41 **Nb** niobium 92.906 ± 0.001	42 **Mo** molybdenum 95.95 ± 0.01	43 **Tc** technetium [97]	44 **Ru** ruthenium 101.07 ± 0.02	45 **Rh** rhodium 102.91 ± 0.01	46 **Pd** palladium 106.42 ± 0.01	47 **Ag** silver 107.87 ± 0.01	48 **Cd** cadmium 112.41 ± 0.01	49 **In** indium 114.82 ± 0.01	50 **Sn** tin 118.71 ± 0.01	51 **Sb** antimony 121.76 ± 0.01	52 **Te** tellurium 127.60 ± 0.03	53 **I** iodine 126.90 ± 0.01	54 **Xe** xenon 131.29 ± 0.01
55 **Cs** caesium 132.91 ± 0.01	56 **Ba** barium 137.33 ± 0.01	57-71 lanthanoids	72 **Hf** hafnium 178.49 ± 0.01	73 **Ta** tantalum 180.95 ± 0.01	74 **W** tungsten 183.84 ± 0.01	75 **Re** rhenium 186.21 ± 0.01	76 **Os** osmium 190.23 ± 0.03	77 **Ir** iridium 192.22 ± 0.01	78 **Pt** platinum 195.08 ± 0.02	79 **Au** gold 196.97 ± 0.01	80 **Hg** mercury 200.59 ± 0.01	81 **Tl** thallium 204.38 ± 0.01	82 **Pb** lead 207.2 ± 1.1	83 **Bi** bismuth 208.98 ± 0.01	84 **Po** polonium [209]	85 **At** astatine [210]	86 **Rn** radon [222]
87 **Fr** francium [223]	88 **Ra** radium [226]	89-103 actinoids	104 **Rf** rutherfordium [267]	105 **Db** dubnium [268]	106 **Sg** seaborgium [269]	107 **Bh** bohrium [270]	108 **Hs** hassium [269]	109 **Mt** meitnerium [277]	110 **Ds** darmstadtium [281]	111 **Rg** roentgenium [282]	112 **Cn** copernicium [285]	113 **Nh** nihonium [286]	114 **Fl** flerovium [290]	115 **Mc** moscovium [290]	116 **Lv** livermorium [293]	117 **Ts** tennessine [294]	118 **Og** oganesson [294]

57 **La** lanthanum 138.91 ± 0.01	58 **Ce** cerium 140.12 ± 0.01	59 **Pr** praseodymium 140.91 ± 0.01	60 **Nd** neodymium 144.24 ± 0.01	61 **Pm** promethium [145]	62 **Sm** samarium 150.36 ± 0.02	63 **Eu** europium 151.96 ± 0.01	64 **Gd** gadolinium 157.25 ± 0.03	65 **Tb** terbium 158.93 ± 0.01	66 **Dy** dysprosium 162.50 ± 0.01	67 **Ho** holmium 164.93 ± 0.01	68 **Er** erbium 167.26 ± 0.01	69 **Tm** thulium 168.93 ± 0.01	70 **Yb** ytterbium 173.05 ± 0.02	71 **Lu** lutetium 174.97 ± 0.01
89 **Ac** actinium [227]	90 **Th** thorium 232.04 ± 0.01	91 **Pa** protactinium 231.04 ± 0.01	92 **U** uranium 238.03 ± 0.01	93 **Np** neptunium [237]	94 **Pu** plutonium [244]	95 **Am** americium [243]	96 **Cm** curium [247]	97 **Bk** berkelium [247]	98 **Cf** californium [251]	99 **Es** einsteinium [252]	100 **Fm** fermium [257]	101 **Md** mendelevium [258]	102 **No** nobelium [259]	103 **Lr** lawrencium [262]

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For notes and updates to this table, see www.iupac.org. This version is dated 4 May 2022.

TSAW—a lifelong challenge or simply an unsolved mystery?

by Thomas Prohaska

The table of standard atomic weights (TSAW) provides of the numbers included in all reprints of the periodic tables of the elements, in all textbooks in schools, high schools and universities, found on the internet, and numerous databases [1]. Whenever one needs to relate masses of an element to molar quantities, standard atomic weights come into the play. They are of fundamental importance in science, education, technology, industries, trade and commerce. It is therefore not surprising that the determination of atomic weights has a central role in chemistry. Also, it is not surprising that it needs a whole commission of experts to set-up such table with highest confidence even though at first sight it seems to be a simple compilation of numbers. That commission of experts is the Commission on Isotopic Abundances and Atomic Weights (referred to as the Commission in the text). (For more information about the Commission visit ciaaw.org).

Before going into more details about how this table is created, let's understand the beauty and also the obviously unsolvable challenge or mystery behind standard atomic weights: standard atomic weights are actually "relative atomic masses of an element". If one reads carefully, one already can imagine the challenge or even the *contradictio in adiecto*.

Before the atomic weight of an element can be estimated, let's first recall that for a single nuclide, a relative atomic mass can be calculated based on measurements. An international group of experts founded by Aaldert Wapstra has collected measurement results of the relative atomic masses of all known nuclides from original publications and has used them to form a full table of estimated (that means professionally assessed) weighted mean values. First published in 2003, such table is regularly reviewed, publishing the latest status of relative atomic masses, and most recently 2020 under the name AME2020 (AME or atomic mass evaluation) [2].

When it comes to the atomic weight of an element in a sample, things become more tricky: the atomic weight $A_r(\mathrm{E, P})$ of an element E in a substance P, is the weighted average of the atomic weights $A_r(^i\mathrm{E})$ of the isotopes (nuclides) $^i\mathrm{E}$ of this element in the substance P:

$$A_r(\mathrm{E, P}) = \sum x(^i\mathrm{E, P})\, A_r(^i\mathrm{E})$$

Therefore, in order to be able to calculate an atomic weight of an element in a sample, its isotopic composition has to be known (analyzed) apart from the relative atomic mass of the isotope retrieved from the AME tables. In the following, the standard atomic weight does not refer to an element in a specific sample but of any provenance possible. This makes things really complicated: "The **standard atomic weight of an element,** $A_r°(\mathrm{E})$, is the recommended value of atomic weight (relative atomic mass) of an element applicable to elements in any normal material with a high level of confidence" [3]. In order to be able to determine a valid standard atomic weight value, one would need to know the isotopic composition of the element averaged wherever it appears in the universe. Mission impossible. Therefore, it was decided to calculate a standard atomic weight for terrestrial material only and for the latter, only for elements which appear in "normal materials":

> "Normal materials include all substances, except (1) those subjected to substantial deliberate, undisclosed, or inadvertent artificial isotopic modification, (2) extraterrestrial materials, and (3) isotopically anomalous specimens, such as natural nuclear reactor products from Oklo (Gabon) or other unique occurrences." [3]

This definition excludes extraterrestrial materials and recognizes that the variation of the standard atomic weight of some elements is caused by isotopic fractionation processes that operate on different time scales. Of 91 naturally occurring elements, 69 have more than one isotope.

It is evident that this definition is a compromise and thus the value itself can only be a compromise: the standard atomic weight strongly depends on the knowledge of the isotopic composition of all elements in as many materials as possible. In addition, the distribution of these materials should be known and considered as well. Therefore, the Commission assesses the existing data on the highest scientific level possible to provide a value which can be expected with the highest confidence in a material which is treated in industry, laboratories or wherever over the world.

Now that the conditions of a compromise have been decided, let's review how the composition is estimated: Laboratories all over the world determine the isotopic composition of different materials. Ideally, starting with a fully calibrated method in order to provide a "best measurement" and establishing a measurement uncertainty. The Commission regularly evaluates these types of measurements. Continuing from there, the distribution of the isotopic composition of an element in various naturally occurring materials is determined and published in literature. Here starts the second

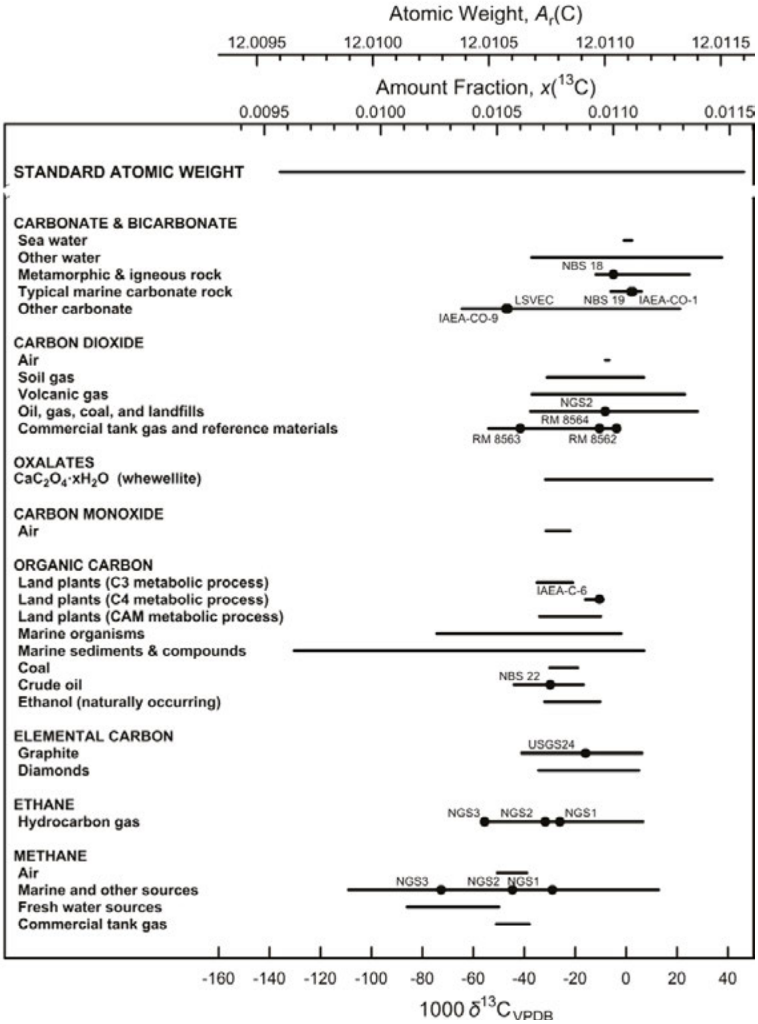


Fig. 1: Variation of the atomic weight based on the variation of the isotopic composition on the example of carbon. (Reproduced from T.B. Coplen and Y. Shrestha. Pure Appl. Chem. 88, 1203-1224 (2017); https://doi.org/10.1515/pac-2016-0302)

duty of the Commission: evaluating the variation of the isotopic composition based on literature data and its transfer into a standard atomic weight including an uncertainty. It goes unsaid that both the improvement of analytical methods and the assessment of the isotopic composition of an increasing number of materials makes a continuous review and, if necessary, revision of the table of standard atomic weights necessary.

To make things even more complicated, a standard atomic weight value which lasts for an extended period of time relies on a stable isotopic composition. Thus, it turns out to be (almost) impossible to determine a standard atomic weight for elements with (only) radioactive isotopes as the isotopic composition is changing continuously both for the parent and child isotope depending on the half-life of these nuclides. Therefore, technetium, promethium and all elements from polonium (except for thorium, protactinium and uranium) have not obtained a standard atomic weight. With elements consisting both of radioactive and non-radioactive elements, things become more critical: radioactive isotopes with a "relatively long half-life" and a characteristic terrestrial isotopic abundance that contributes significantly and reproducibly to the determination of the standard atomic weight of the element in normal materials are considered. For example, the half-lives of ^{144}Nd and ^{150}Nd are 2.1 × 10^{15} years and 1.3 × 10^{20} years, respectively. For uranium, no stable isotope exists, but the half-lives of the naturally occurring isotopes are long enough to allow for calculating a standard atomic weight within a specifically evaluated uncertainty. At a certain point, a decision has to be made if the half-life is long enough to allow for the assignment of a standard atomic weight; these boundaries seem to be blurred but are considered meticulously in the uncertainty of the standard atomic weight.

As there is no value based on measurement without uncertainty, the standard atomic weight requires an uncertainty as well, which comprises both the measurement uncertainty and the natural variation. Uncertainties of standard atomic weights are estimated by the Commission through evaluation of the relevant published literature. The atomic weight of any element is expected to be within the interval indicated by the uncertainty of the standard atomic weight with at least 95 % probability for normal materials which have been investigated at the time of the compilation of the data. (see text box) Sometimes the variation of the isotopic composition is so small that it is hidden in the measurement uncertainty and for some elements, it is so large that it is impossible to provide a single representative value (Fig. 1). Instead, it was decided that an interval within which an element can be expected to have its standard atomic weight is a better representation of a standard atomic weight. In the latest TSAW 2021, it is clearly stated: "The interval notation does not alter the meaning of the standard atomic weight, nor does it constitute "a new definition" of standard atomic weights. Rather, it is an alternative means for expressing the uncertainty of this quantity. Writing the standard atomic weight of carbon as $A_r°(C) = [12.0096, 12.0116]$ indicates that at the current

Expression of uncertainty

The uncertainty of standard atomic weights was expressed in parentheses () for a long time. For example, the standard atomic weight of iridium ($A_{\mathrm{r}}^{\circ}(\mathrm{Ir}) = 192.217$) has an uncertainty of ± 0.002. This was expressed as 192.217(2). This was not in compliance with the GUM (Guide to the Expression of Uncertainty in Measurement) as this format is used to state a standard uncertainty. In the 2021 TSAW, the uncertainty value is delineated with the symbol "±". (e.g., the standard atomic weight of iridium is now expressed as 192.217 ± 0.002).

status of knowledge its atomic weight in any normal material will be greater than or equal to 12.0096 and will be less than or equal to 12.0116." [4]

It is evident that the Commission has had a substantial responsibility ever since to provide the best estimate of reality: the first table of relative atomic masses was published by John Dalton in 1805. He obtained it on the basis of the mass ratios in chemical reactions, where he chose the lightest atom, the hydrogen atom, as the "unit of mass". Further relative atomic and molecular masses were calculated for gaseous elements and compounds on the basis of Avogadro's law. A real pioneer for atomic weights of elements was Jean Baptiste Dumas. He determined the atomic weights of 30 elements very precisely and found that 22 elements had atomic weights that are multiples of the atomic weight of hydrogen. Considering the technical possibilities, these findings were outstanding. Nonetheless, atoms of an element were considered to be uniform but things turned out to become more difficult with the advent of mass spectrometry and the discovery that an element consists of more than one type of atom, the isotopes.

It all started when Joseph John Thomson and Francis William Aston observed different patches of light and correctly interpreted the signal on $m/z = 11$ as the doubly charged particle $^{22}\mathrm{Ne}^{2+}$ at the begin of the 20th century. The mind-blowing conclusion was that neon is composed of atoms of two different atomic masses. In the following years, Aston worked on the improvement of the technique and created an improved version of his mass separator. Thus, he was able to identify the isotopes of mercury and within a few years he could quickly determine isotopes of more than thirty elements. Aston received the Nobel Prize in Chemistry 1922 for his work on isotope studies. The term isotope itself was coined by the Scottish doctor and writer Margaret Todd in 1913 in a suggestion to chemist Frederick Soddy. In 1910, Frederick Soddy had discovered that the element lead differed in mass depending whether it had been formed via the decay of thorium or the decay of uranium.

Formally established in 1899, the Commission on Isotopic Abundances and Atomic Weights remains one of the oldest continuously serving scientific bodies. It was created to introduce uniformity in the atomic weight values used on a global scale. The establishment of the Commission dates back to 1897, when soon-to-be Nobel laureate Hermann Emil Fischer proposed the creation of a working committee to report on atomic weights. The committee consisted of the future Nobel laureate Wilhelm Ostwald (University of Leipzig), Karl Seubert (University of Hanover), and was chaired by Hans H. Landolt (Berlin University). This committee published its first report in 1898. It suggested an International Committee on Atomic

Abridged standard atomic weights

In some cases, the standard atomic weights provide too many details (i.e. a large number of significant digits or are given as interval). For this purpose, abridged atomic weights are quoted to five significant digits (see 2021 TSAW column 7, in Table 1 of ref [4]) unless such precision cannot be attained due to the variability of isotopic composition in normal materials or due to the limitations of the measurement capability. For 14 elements (argon, boron, bromine, carbon, chlorine, hydrogen, lead, lithium, magnesium, nitrogen, oxygen, silicon, sulfur, and thallium) the standard atomic weight is given as an atomic weight interval. In some cases, a single value is needed for these elements, which is provided in column 7, as well. These values do not correspond necessarily to the midpoints of the intervals but to a value which is considered to be most probably found for normal materials or correspond to the $A_{\mathrm{r}}(\mathrm{E})$ values of frequently used reference materials (e.g. NIST SRM 981 for Pb; argon in tropospheric air for Ar). A corresponding conservative +/- value is provided in column 8 which corresponds to the smallest symmetric number in order to cover the standard atomic weight interval. The significant numbers of digits after the decimal point of the abridged atomic weights corresponds to the significant numbers of digits after the decimal point of this value [4].

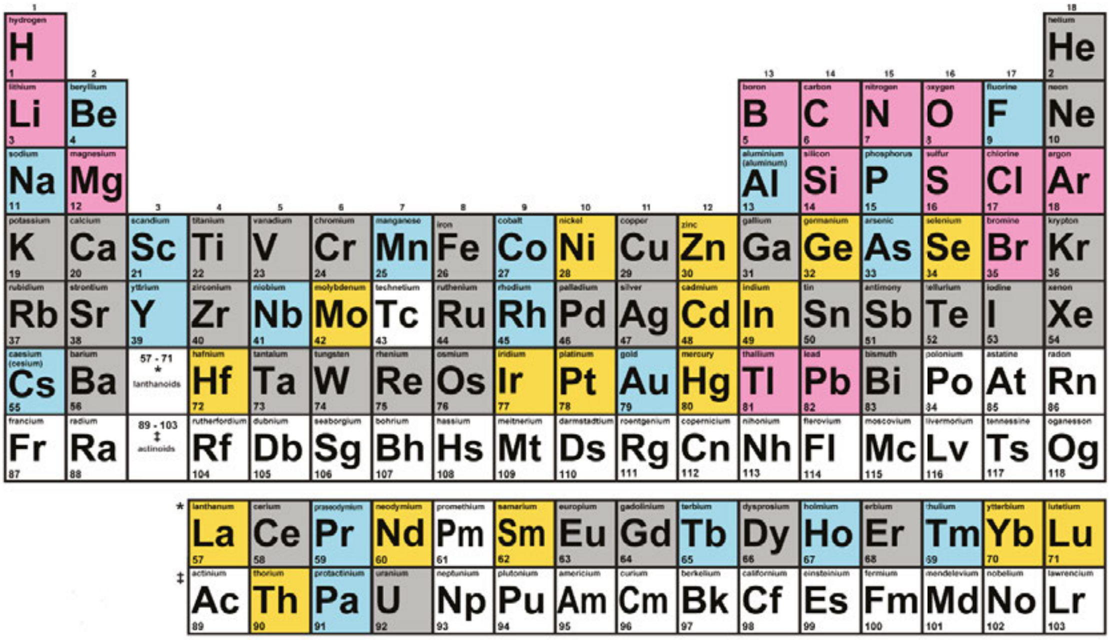
Weights. To this end, on 30 March 1899 the invitation was sent to national scientific organizations worldwide to appoint delegates to the International Committee on Atomic Weights: “The Great International Committee on Atomic Weights”.

Today, the Commission operates under the auspices of the Inorganic Chemistry Division of IUPAC. Members of the Commission are renowned experts in isotopic research who work on a fully voluntarily basis. For the last eight years, the Commission was chaired by Juris Meija, an isotope expert at the NRC Canada and, since this January 2022, has been chaired by Johanna Irrgeher from the Montanuniversität Leoben, Austria.

My own work in the Commission started in 2009. I was impressed at that time by the fact that renowned scientists have one goal: reviewing and possibly revising the standard atomic weight based on isotopic measurements with highest metrological quality. Later, becoming secretary of the Commission, I was appointed to compile the update of the table of standard atomic weights. The table itself is published in a publication in *Pure and Applied Chemistry* providing all necessary details around the values. The previous TSAW 2013 was published in 2016 [5]. Since, substantial scientific exchanges, discussions, updates, voting, fine-tuning the text and weighing each word in meetings and uncountable emails amongst the 21 international authors have taken almost seven years in total with continuous updates until the latest version, TSAW 2021, became reality and gets published in IUPAC journal *Pure and Applied Chemistry* this year [4].

To sum-up, standard atomic weights are a perpetuity compromise to describe nature to the best of our knowledge. We know about the shortcomings, we have

Elements with standard atomic weight updates since 2004



🟥 Element assigned an interval atomic weight value and a single value for use in education and trade following an evaluation of published, peer-reviewed literature by an IUPAC project.

🟨 Element has two or more stable isotopes and is assigned an updated standard atomic weight value based on an evaluation of published, peer-reviewed literature.

🟦 Element assigned an updated standard atomic weight value, which is based on a single isotope and the latest atomic mass evaluation of nuclides.

▨ Element was assigned a standart atomic weight value prior to 2004, and no published, peer-reviewed publications have been identified that justify an updated value.

☐ Element has no standard atomic weight because all its isotopes are radioactive and no isotope occurs with a characteristic isotopic abundance from which a standard atomic weight value can be determined.

to live with a number of assumptions, we need to admit that we do know only little but still we have to judge on expert level with highest confidence. This imperfection of the standard atomic weight comprises its weakness and its beauty: we do know so little but we still have sufficient knowledge to be able to provide substantial and reliable numbers in the table of standard atomic weights.

References and notes

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Thomas Prohaska <thomas.prohaska@unileoben.ac.at> is professor at the Montanuniversität Leoben, Austria. He has been a member of the IUPAC Commission on Isotopic Abundances and Atomic Weights since 2010 and secretary from 2014 to 2021; https://orcid.org/0000-0001-9367-8141

TSAW—An Exercise in Consensus

by Ty Coplen

The Table of Standard Atomic Weights (TSAW) of the chemical elements is perhaps one of the most familiar datasets in science. Many in the scientific public do not have a full understanding of the amount of effort and the processes that occur regularly by the IUPAC Commission on Isotopic Abundances and Atomic Weights (CIAAW) to continuously update standard atomic weight values:

How are new standard atomic weight values determined, and what are the guidelines for updating them?

What are the uncertainties on standard atomic-weight values—standard uncertainties or expanded uncertainties?

Why do 14 elements now have standard atomic weight values expressed as intervals?

When an element has a standard atomic weight value expressed as an interval, what value should be used in education and trade?

Why do 34 elements have no standard atomic weight value?

With leadership from the Commission's Subcommittee on Natural Assessment of Fundamental Understanding of Isotopes (SNAFUI), an article titled “The Table of Standard Atomic Weights—an exercise in consensus” was published by members of the CIAAW to enhance the understanding of the values in the Table of Standard Atomic Weights [1].

Meeting prior to biennial Commission meetings, the Commission's Subcommittee on Isotopic Abundance Measurements (SIAM) reviews published, peer-reviewed literature to search for new isotopic abundance measurements that might lead to revised standard atomic weights. The Subcommittee forwards such measurements to the Commission for discussion according to the guidelines which were created in 1985 [2] and updated in 1995 [3]. A change in a standard atomic weight and uncertainty pair is only adopted if a significant improvement in reliability or precision can be achieved.

Since 2004, the standard atomic weight values of 50 elements have been updated (See table on page 18) Fourteen elements have well-known natural isotopic variation and were assigned standard atomic weight intervals (pink backgrounds in table). The standard atomic weight values of 19 elements, which are based on a single isotope (blue backgrounds) and that of 17 elements having two or more stable isotopes (yellow backgrounds) were also updated. The TSAW fulfills the aim by which scientist, taking any natural sample, can expect their sample atomic weight to lie within the lower and upper bounds of the standard atomic weight with high certainty.

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3. Atomic weights of the elements 1995. *Pure Appl. Chem.* 68, 2339 (1996); https://doi.org/10.1351/pac199668122339


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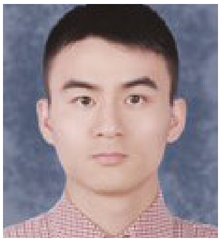
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Winners of the 2022 IUPAC-Solvay International Award for Young Chemists

The International Union of Pure and Applied Chemistry and Solvay announce the winners of the 2022 IUPAC-Solvay International Award for Young Chemists, presented for the best Ph.D. theses in the chemical sciences, as described in 1000-word essays.

The five winners are:

- **Alexander John Cruz** (Belgium), Ph.D., KU Leuven, Belgium
- **Yuyang Dong** (China/Beijing, USA), Ph.D., Harvard University, USA
- **Stefano Ippolito** (France), Ph.D., University of Strasbourg, France
- **Li Jianbin** (China/Beijing, Canada), Ph.D., McGill University, Canada
- **Juliane R. Sempionatto** (USA), Ph.D., University of California San Diego, USA

The winners will each receive a cash prize of USD 1000 and travel expenses to the 49th IUPAC World Chemistry Congress, 20-25 August 2023, in The Hague, The Netherlands. Each winner will also be invited to present a poster at the IUPAC Congress describing his/her award-winning work and to submit a short critical review on aspects of his/her research topic, to be published in *Pure and Applied Chemistry*. The awards will be presented to the winners of the 2022 and 2023 competitions during the Opening Ceremony of the Congress.

The titles of the winners' theses are:

- **Alexander John Cruz:** "Metal-organic frameworks by vapor deposition processes"
- **Yuyang Dong:** "C–H Functionalization Catalysis Mediated by First-Row Transition Metal-Stabilized Ligand-Based Radicals"
- **Stefano Ippolito:** "Defect engineering in 2D semiconductors : fabrication of hybrid multifunctional devices"
- **Li Jianbin:** "Development of novel C-H and C-O functionalization tools in the absence of noble metal"
- **Juliane R. Sempionatto:** "Wearable Electrochemical Sensors for Non-Invasive Health Monitoring"

There were 44 applications from individuals receiving their Ph.D. degrees from institutions in 15 countries. The award selection committee, chaired by Professor Christopher Brett, IUPAC Past President, comprised members of the IUPAC Bureau and a senior science advisor from Solvay, all of whom have a wide range of experience in chemistry. In view of the many high-quality applications, the Committee also decided to award three Honorable Mentions to:

- **Xiang Shi** (China/Beijing), Ph.D., Fudan University, China
- **Anirban Mondal** (Netherlands), Ph.D., University of Groningen, The Netherlands
- **Soraya Learte Aymamí** (Spain), Ph.D., Universidad de Santiago de Compostela, Spain

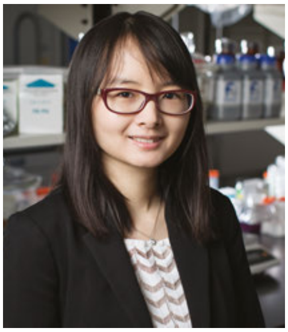
The call for applications for the 2023 IUPAC-Solvay International Award for Young Chemists will open soon. Eligible candidates must have received a Ph.D. or equivalent degree in any of the countries that have National Adhering Organizations in IUPAC during the year 2022.

Hanwha-TotalEnergies IUPAC Young Polymer Scientist Award 2022

The 2022 Hanwha-TotalEnergies IUPAC Young Scientist Award, to be presented at MACRO 2022, has been awarded to Qian Chen and Eric Appel.

The Hanwha-TotalEnergies IUPAC Young Scientist Award (formerly Samsung-Total Petrochemicals–IUPAC Young Scientists Award) is dedicated to outstanding young scientists (not older than 40 years) and is sponsored by a grant from the aforementioned company. The prize was first awarded on the occasion of MACRO 2004 (Paris) and is granted biennially on the occasion of the IUPAC World Polymer Congress. The awardees are selected from the nominees by a Committee of the IUPAC Polymer Division. In the year 2022 the award will be presented at Macro2022 and there are two awardees (ex aequo) namely:

- **Qian Chen,** Department of Materials Science and Engineering, University of Illinois Urbana-Champaign
- **Eric Appel,** Department of Materials Science and Engineering, Stanford University


Qian Chen

Qian Chen is Associate Professor at the Department of Materials Science and Engineering at the University of Illinois Urbana-Champaign (UIUC), and also affiliated to the Department of Chemistry, the Materials Research Laboratory, the Beckman Institute for Advanced Science and Technology, and the Carle Illinois College of Medicine.

Chen received her BS in Chemistry from Peking University (2007), and her Ph.D in Materials Science and Engineering from UIUC with Steve Granick (2012). She then won the prestigious Miller fellowship and worked with A. Paul Alivisatos at UC Berkeley. She joined MatSE at UIUC as an assistant professor in 2015. In 2021, she was promoted to Associate Professor with Racheff Scholarship.

Her research focuses on understanding the organization of complex materials and biological systems in space and time. Specific systems are wide-ranging and ever-expanding from ion-oxide intercalation in batteries, crumpled polymer films for water filtration, phase-changing nanoparticle ensembles as adaptive devices, ion channels gating cells, to amyloid fibril prevention for curing disease. These efforts are all unified by one common framework: deciphering fundamental rules of organization from “seeing is believing,” to resolve the dynamics of the constitutes. The implementation of such framework draws on Chen’s unique expertise in direct in-situ imaging, particularly on the groundbreaking liquid-phase transmission electron microscopy (TEM) that resolves the structure and dynamics of nanoscale entities in a suspending media. https://chenlab.matse.illinois.edu/


Eric. A. Appel

Eric A. Appel is an Assistant Professor of Materials Science & Engineering at Stanford University. He received his BS in Chemistry and MS in Polymer Science from Cal Poly, San Luis Obispo. Eric performed his MS thesis research with Robert D. Miller and James L. Hedrick at the IBM Almaden Research Center in San Jose, CA. He then obtained his PhD in Chemistry working in the lab of Dr. Oren A. Scherman in the Melville Laboratory for Polymer Synthesis at the University of Cambridge. His Ph.D research focused on the preparation of dynamic and stimuli-responsive supramolecular polymeric materials. For his PhD work, Eric was the recipient of the Jon Weaver Ph.D prize from the Royal Society of Chemistry and a Graduate Student Award from the Materials Research Society. Upon graduating from Cambridge in 2012, he was awarded a National Research Service Award from the NIH (NIBIB) and a Wellcome Trust Postdoctoral Fellowship at MIT to work with Robert S. Langer on the development of supramolecular biomaterials for drug delivery and tissue engineering. For his independent work, Eric has been awarded a Hellman Faculty Scholarship, Terman Faculty Fellowship, a Margaret A. Cunningham Immune Mechanisms in Cancer Research Award, and junior faculty awards through the American Diabetes Association, the American Cancer Society, and the PhRMA Foundation. Eric also had the pleasure of participating in the Young Investigator Award Symposium from the Polymeric Materials Science & Engineering division of the American Chemical Society.

The underlying theme of the Eric’s research program integrates concepts and approaches from supramolecular chemistry, natural/synthetic materials, and biology to pursue innovative interdisciplinary science and engineering to tackle two areas of critical importance to society: advanced materials and human health. Eric’s lab focuses on developing materials for immunoengineering applications in infectious disease and cancer, drug delivery applications in the treatment of diabetes, and novel materials for wildfire prevention. http://www.supramolecularbiomaterials.com/

8th Polymer International-IUPAC Award Goes to Zachary Hudson

The Editorial Board of Polymer International and the IUPAC Polymer Division are delighted to announce that Dr Zachary Hudson (The University of British Columbia, Canada) is the winner of the 8th Polymer International-IUPAC award for Creativity in Applied Polymer Science.

The award celebrates the outstanding contributions that Dr Hudson has made to polymers for optoelectronics, as well as in working with industry to develop polymer technologies to confront global plastic waste. Hudson's creative discoveries have disrupted industries and gained international recognition.

Hudson's research develops light-emitting materials for the electronics, healthcare, and pharmaceutical industries. He develops luminescent polymer nanoparticles, or 'Pdots', for bioimaging and analysis, with sufficient brightness to be detected by a handheld smartphone camera. This technology has the potential to improve healthcare in remote or low-income communities, where smartphones are ubiquitous but lab equipment is scarce. He has also developed technology for photopatterning thin films for polymer electronics at extremely low cost, creating multilayer device structures in a beaker on the benchtop.

A rising leader in the field of polymer science, Dr Hudson's work has been featured in prominent peer-reviewed journals. He has also worked with local industry to help confront the global crisis caused by single-use plastic. He served as Chief Scientific Officer of NEXE Innovations, developing fully compostable single-serve coffee pods for commercial brewers. In 2020, he worked with CTK Cosmetics (Korea) to develop biodegradable materials for cosmetics packaging. [Link to Hudson's homepage @ubc.ca]


Dr Zachary Hudson, winner of the 8th Polymer International-IUPAC Award

Hudson will give a lecture and receive this award at the World Polymer Congress, which will be held in Winnipeg, Canada from July 17 to 21, 2022. The award includes $5,000, plus up to $3,000 travel and hotel accommodation expenses to attend MACRO 2022.

The winner was selected by members of the scientific committee representing Polymer International and the IUPAC Polymer Division:

- Professor (Melissa) Chin Han Chan (Polymer International/IUPAC)
- Dr Dick Dijkstra (Polymer International/IUPAC)
- Professor Jiasong He (Polymer International/IUPAC)
- Professor Igor Lacik (IUPAC)
- Professor Tim Long (Polymer International)
- Professor Christine Luscombe (Polymer International/IUPAC)
- Dr Carmen Scholz (Polymer International)
- Professor João Soares (IUPAC)

The selection committee and the Editorial Board of Polymer International extend their congratulations to Dr Hudson!

Announcement published in Chem Int July 2022,

See originating call or link to PI https://onlinelibrary.wiley.com/journal/10970126

reprinted fom <https://onlinelibrary.wiley.com/journal/10970126/8thpiiupacaward>

2023 Distinguished Women in Chemistry/Chemical Engineering Award—Call for Nominations

IUPAC is pleased to announce the call for nominations for the IUPAC 2023 Distinguished Women in Chemistry or Chemical Engineering Awards. The purpose of the awards program, initiated as part of the 2011 International Year of Chemistry celebrations, is to acknowledge and promote the work of women in chemistry/chemical engineering worldwide. In 2011, 23 women were honored during a ceremony held at the IUPAC Congress in San Juan, Puerto Rico, on 2 August 2011. At each of the subsequent IUPAC Congresses, 12 women received this recognition; in Istanbul, Turkey in 2013, in Busan, Korea in 2015, in Sao Paulo, Brazil in 2017, in Paris, France in 2019, and virtually (in Montréal) in 2021. A similar award ceremony will take place during the 2023 IUPAC Congress in August 2023 in The Hague, The Netherlands.

Awardees will be selected based on excellence in basic or applied research, distinguished accomplishments in teaching or education, or demonstrated leadership or managerial excellence in the chemical sciences. The Awards Committee is particularly interested in nominees with a history of leadership and/or community service during their careers.

Nomination: Each nomination requires a primary nominator and two secondary nominators who must each write a letter of recommendation in support of the nomination. A CV of the nominee is required. Self-nominations will not be accepted. Nominations should be received by 1 November 2022.

Presentation: Awardees will be honored at the 2023 IUPAC World Chemistry Congress in The Hague, The Netherlands during a celebration in their honor and a symposium.

For additional information on the IUPAC 2023 Distinguished Women In Chemistry Awards, contact Fabienne Meyers at <fabienne@iupac.org>.

https://iupac.org/2023-women-in-chemistry/

GWB2023 Sponsorship Opportunities

IUPAC is seeking organizational, corporate, and individual sponsors for the 2023 IUPAC Global Women's Breakfast to be held 14 February 2023. A wide range of sponsorship opportunities are available from Platinum level (at $10000 USD) to Bronze ($1000 USD).

Highlights from GWB 2022 event: https://iupac.org/gwb/highlights-from-gwb2022/

With a theme of "Breaking Barriers in Science", the Global Breakfast is designed to support the United Nations Day of Women and Girls in Science. In 2023, the GWB will also be a key part of the Celebration of the International Year of Basic Sciences for Sustainable Development. In 2022 more than four hundred events in 75 nations/territories were included in the GWB touching more than 30000 participants from high school to university to industry organizations.

See details at https://iupac.org/gwb2023-sponsorship-opportunities or https://iupac.org/gwb/

Benefits	**Bronze $1000**	**Silver $2500**	**Gold $5000**	**Platinum $10000**
Your logo on GWB website with back link to your site	Fourth Row	Third Row	Second Row	Top Row Large
Coupon for IUPAC Merchandise	$25	$50	$100	$200
Your logo with back link in all GWB email newsletters	√	√	√	√
Your logo included at end of GWB Welcome Video	√	√	√	√
Highlighted Social Media Posts on IUPAC channels or link to your company video		1 post	2 posts	3 posts
One-year IUPAC Company Associates Membership			√	√
Opportunity to place ad in Chemistry International			Half Page	Full Page
Opportunity to include story or video in GWB Email Newsletter				√

Scientific Editor for *Pure and Applied Chemistry*—Call for Nominations

Professor Hugh D. Burrows, Scientific Editor of *Pure and Applied Chemistry*, is stepping down at the end of 2022 after serving as Scientific Editor since 2014. IUPAC requests nominations and/or applications to succeed Professor Burrows in this position. The mandate for the Scientific Editor will be to maintain the scientific standards, focus on the international profile of the journal, and explore creative ways to engage with the IUPAC community in the digital 21st century. *PAC* is published monthly and includes recommendations, reports, as well as lectures from conferences.

Nominations will be accepted from NAOs as well as from individual scientists. In either case, a CV, a brief statement of interest, and an outline of thoughts on the journal should be submitted to the Secretary General Richard Hartshorn <rhartshorn@iupac.org>. If an NAO is making the nomination, a letter of nomination from the NAO should also be included. The deadline for nominations is 31 July 2022.

https://iupac.org/scientific-editor-for-pac

IUPAC Centenary Endowment Board—Call for members

In August 2021, the IUPAC Council approved the establishment of the Centenary Endowment Board to provide a mechanism through which Fund Donors can support and engage in IUPAC's international work. Among other responsibilities, the Board shall be responsible for and administer IUPAC's funds solicitation efforts and the development of the Fund and recommending disbursement in accordance with the Fund Mission and, where relevant, specific designations by Donors.

The purpose of the fund will be to finance projects and activities in support of:

- the establishment of IUPAC nomenclature and standards in the digital domain to enable advances in Big Data relevant to chemistry and chemistry related research and development,
- the Union's unique international role in the critical evaluation of chemical data and establishment of standards that will be necessary to underpin the achievement of Sustainable Development and the UN millennium goals, and
- the setting of chemistry education and capacity building in emerging regions to promote their economic development whilst helping to ensure the safe and environmentally sensitive application of chemical technologies in these countries.

IUPAC is now recruiting individual volunteers with significant experience in fund raising and connected to a large network of funders to start this venture. Having a background in Chemistry is desirable, as there are many activities and programs running in IUPAC that would appeal to a diverse group of potentially interested donors.

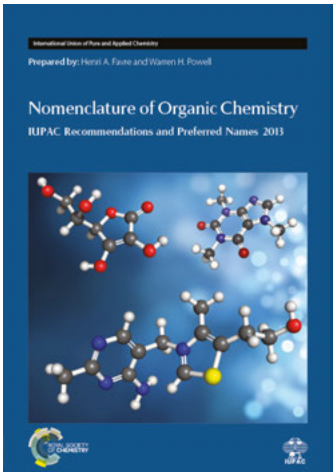
The initial objective of the Fund is to provide endowment investment earnings of at least $100,000 per annum for IUPAC activities consistent with the Fund Mission, net of the operational costs of the fund, including those of the Centenary Endowment Board.

Interested individuals are encouraged to contact IUPAC Executive Director, Lynn Soby <lsoby@iupac.org>

https://iupac.org/body/070

IUPAC Blue Book

When the so-called IUPAC Blue Book "Nomenclature of Organic Chemistry (IUPAC Recommendations and Preferred IUPAC Names 2013)" was last published in 2014, it greatly expanded the coverage of the previous edition (1979) and included for the first time recommendations for a preferred IUPAC name (PIN) for those needing a consistent name. Still and for use in general nomenclature, alternative unambiguous names were included. A html version of the whole book including all corrections, changes, and modifications is now available.



International Union of Pure and Applied Chemistry

Prepared by: Henri A. Favre and Warren H. Powell

Nomenclature of Organic Chemistry

IUPAC Recommendations and Preferred Names 2013

That edition of the Blue Book was prepared over many years and inevitably was not totally consistent. Since its publication, corrections, changes and modifications have been listed on the following webpage: https://

iupac.qmul.ac.uk/bibliog/BBerrors.html. A html version of the whole book including all corrections, changes, and modifications has been prepared; it also includes a PDF of each chapter and a combined PDF of the whole book. Version 2, released on 1 April 2022 is available at https://iupac.qmul.ac.uk/BlueBook/PDF/

The web version has been prepared and is maintained by G. P. Moss, School of Physical and Chemical Sciences, Queen Mary University of London, UK. Please return questions to g.p.moss@qmul.ac.uk

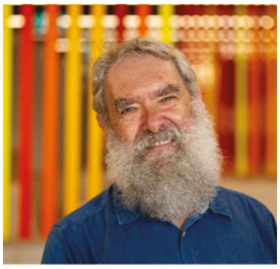
IUPAC Emeritus Fellows

Emeritus Fellows are former members of IUPAC Divisions and erstwhile Commissions and Subcommittees, who have made outstanding contributions to IUPAC and, through chemistry, to the chemical sciences in general.

Emeritus Fellows may be appointed during each Biennium, the number of appointments reflect the current Subcommittee structure of the Division. Fellows are kept abreast of Division activities and are encouraged to remain active with the Divisions as ad hoc consultants.

The Emeritus Fellows awarded earlier this year are:

Analytical Chemistry Division (Div V)



D. Brynn Hibbert (Australia); Member since 2002; Member, Secretary, Vice President, President (2014-15), and Past President of Div V, representative on ICTNS and National Representative

Chemistry and the Environment (Div VI)

Ken Racke (USA; Active IUPAC Member since 1992, Division VI President (2004-2007), Chair of the Commission on Agrochemicals and the Environment (1995-2001), Chair of the Advisory Committee on Crop Protection Chemistry (2002-2010), Chair of the IUPAC Delegation to the Codex Committee on Pesticide Residues (1998-2010)

Nicola Senesi (Italy); Active IUPAC Member since 1994, Division VI President (2008-2011), Chair of the Subcommittee on Chemical and Biophysical Processes in the Environment (1998-2013), Co-Editor of IUPAC Book Series "Analytical and Physical Chemistry of Environmental Systems" (1998, 2002, 2008), Co-Editor of IUPAC Book Series "Biophysico-Chemical Processes in Environmental Systems" (2009, 2011, 2016, 2022)

Willie Peijnenburg (Netherlands); Active IUPAC member since 1989, Division VI Secretary (2006-2013), Secretary of IUPAC Commission on Soil and Water Chemistry (1996-2001)

Chemistry and Human Health (Div VII)

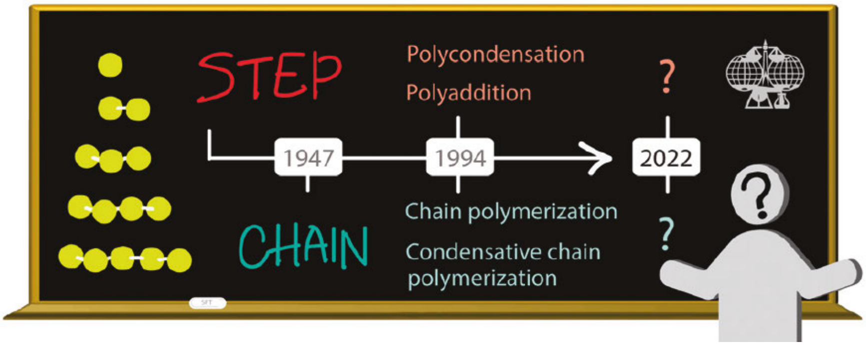
János Fischer (Hungary); Active IUPAC member since 1998, National Representative, Associate and Titular Member on the Chemistry and Human Health Division and on its Subcommittee on Drug Discovery and Development, also member of the Committee and Chemistry and Industry (2008-15) and on CHEMRAWN (2016-19)

Links to their biographical record are available online. <https://iupac.org/who-we-are/emeritus-fellows/>

Project Place

Information about new, current, and complete IUPAC projects and related initiatives.
See also www.iupac.org/projects

Terms for Mechanisms of Polymer Growth



The Subcommittee on Polymer Terminology (SPT, Division IV) has recently published a paper in *Polymer Chemistry* (https://doi.org/10.1039/d2py00086e) outlining their concerns with terms describing basic classification of mechanisms of polymer growth. The terms "step-growth" and "chain-growth," and a variety of related terms, are used widely by the polymer community. In brief, "step-growth" typically refers to polymers that are synthesized from one (or more) type(s) of multifunctional monomer(s) where at least bifunctionality is required, with growth occurring between monomers, oligomers, or polymers of any length. An example is the synthesis of linear polyamides from diamines and dicarboxylic acids. "Chain-growth" generally describes polymers that increase in molar mass by a chain reaction process of monomers adding to polymeric active sites, which are typically created through inclusion of an external initiator in the polymerization reaction. An example is the synthesis of polystyrene from styrene and a radical initiator.

IUPAC has never endorsed the terms "step-growth" and "chain-growth," in part because they do not clearly distinguish between these two mechanisms of polymer growth—all polymers grow in a series of steps to form polymer chains. SPT therefore recommended four terms in 1994: These included *polyaddition* and *polycondensation* for polymers that grow in a "step-growth" mechanism, and *chain polymerization* and *condensative chain polymerization* for polymers that grow following a "chain-growth" mechanism. An analysis of various textbooks in general chemistry, organic chemistry, and polymer chemistry and related field revealed that these recommended terms have not been taken up by the polymer community. In fact, there is no consensus among textbook authors to distinguish between these two fundamentally different mechanisms of polymer growth. The paper details several reasons for why this may be the case, including the lack of generic, umbrella terms covering the condensative and non-condensative versions of the mechanisms of polymer growth.

The paper also details a short history of various terms used, revealing the circuitous path that led to the position we are in today, where "step-growth" and "chain-growth" persist alongside the related terms *polyaddition*, which is different from the deprecated term "addition polymerization," and *polycondensation*, which is different from the deprecated term "condensation polymerization." This lack of clear and consistent terminology leads to confusion among practitioners of polymer science and students learning polymer science, as well as difficulties in translating these terms to other languages.

This paper does not recommend new terms. Instead, the members of SPT working on this project seek suggestions from the community on how to provide clear, simple, and consistent terms to describe the two major mechanisms of polymer growth and their subclasses. They ask that ideas, concerns, and suggestions be sent to polymer.terminology@iupac.org.

For more information and comments, contact Task Group Chair John B. Matson <jbmatson@vt.edu>
https://iupac.org/project/2019-027-1-400

Digital Representation of Units of Measurement

The objective of this CODATA Task Group on Digital Representation of Units of Measurement (DRUM) is to work with the International Science Unions to raise awareness of, educate, and enable their communities in the understanding and implementation of digital unit representation. This will be done with reference to each of the three objectives of the CODATA Decadal Programme, namely:

- Enabling Technologies and Good Practice for Data-Intensive Science
- Mobilising Domains and Breaking Down Silos
- Advancing Interoperability Through Cross-Domain Exemplary Case Studies

Each of the above objectives can be addressed by awareness of the different units of measurement representations that are currently available This, coupled with the movement toward FAIR data, will be used to promote the idea that units of measurement are not second class citizens in science, but rather the most important aspect of what is needed to make data FAIR.

The DRUM Task Group and with colleagues from the CIPM's Digital SI Task Group have recently published a comment article in *Nature* 'Stop squandering data: make units of measurement machine-readable' describing some of the pervasive challenges caused by "sloppy or missing units" (https://doi.org/10.1038/d41586-022-01233-w).

The article provides an overview of current activities globally, the role of DRUM and the Digital SI Expert Group. It also includes a Call for Action 'to create interoperable data with machine-readable quantities and units of measurement' and invites colleagues to contact the Task Group to get involved.

This IUPAC project ties directly into the ongoing work to develop a 'digital first' 5th edition of the Green Book on quantities and units in Chemistry (project 2019-001-2-100).

For more information and comments, contact Task Group Chair Jeremy Frey <j.g.frey@soton.ac.uk>
https://iupac.org/project/2022-009-1-100

IUPAC Green Book—Update and More

The so-called IUPAC Green Book: Quantities, Units, and Symbols in Physical Chemistry, provides a readable compilation of widely used terms and symbols from many sources together with brief understandable definitions. The 4th edition has been updated with the new SI and will be published soon along with an abridged edition. Its content has been reviewed in consultation with the IUPAC divisions and committees, to identify which aspects should be retained (*e.g.* should all the data tables be retained), what areas needed revision, shall be enhanced or deleted, and which topics needed to be added (*e.g.* perhaps less emphasis on data tables, and more information on NMR, nanoscience, computational chemistry and simulations, non-equilibrium thermodynamics and statistical mechanics *etc.*). That edition is being finalized and shall be available later this year.

The following edition is now being conceived as a Digitally Native Book. The task group plan to carefully evaluate the methodology used with the preparation of earlier traduction (*e.g.* the Portuguese version) which created an XML version and tested the software infrastructure to derive the print versions. This would in principle enable the production of more versatile Web based versions of the Green Book in addition to the printed book. This would also facilitate semantically marked up content very suitable to link to the evolving Gold Book and provide and online resource to be used by others in generating correct text for other publications which use the material in the Green Book (*i.e.* symbols and units).

The task group is now seeking input from the community at large while examining the possible content of the 5th edition of the Green Book and is inviting everyone to fill in a survey to help gather community views on what should be included in the 5th edition. The survey will remain open until September 2022, but early replies will be very useful in planning the 5th edition project.

For access to the survey and more information and comments, contact Task Group Chair Jeremy Frey <j.g.frey@soton.ac.uk>
https://iupac.org/project/2019-001-2-100

Call for Proposals

Any individual or group can submit a project proposal to IUPAC, with or without current affiliation with an IUPAC body. Projects can be submitted at any time. For detailed information, see the Guidelines for Completion of the Project Submission Form. Frequently Asked Questions on Project Submission and Approval Process are also available on the Union's website at www.iupac.org/projects. The proposal template is straightforward and is arranged so that it presents "up front" the project's intended impact (purpose), the intended stakeholders and beneficiaries, the dissemination plan, and how the effectiveness of that plan can be evaluated. More recently, specific guidelines have been added for the management of scientific data and digital outputs.

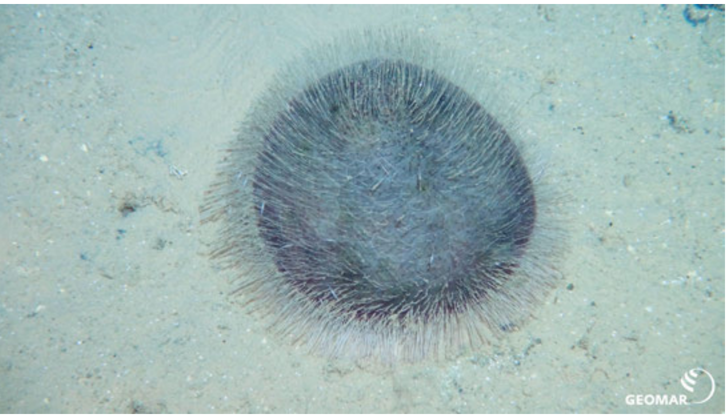
The revised form and guidelines are available at https://iupac.org/projects/project-submission-form-and-guidelines/


photo by Diego PH/Unsplash

Seabed mining and blue growth: exploring the potential of marine mineral deposits as a sustainable source of rare earth elements (MaREEs) (IUPAC Technical Report)

Fani Sakellariadou, *et al.*
Pure and Applied Chemistry, 2022
Vol. 94, no. 3, pp. 329-351
https://doi.org/10.1515/pac-2021-0325

The expected growth of the global economy and the projected rise in world population call for a greatly increased supply of materials critical for implementing clean technologies, such as rare earth elements (REEs) and other rare metals. Because the demand for critical metals is increasing and land-based mineral deposits are being depleted, seafloor resources are seen as the next frontier for mineral exploration and extraction. Marine mineral deposits with a great resource potential for transition, rare, and critical metals include mainly deep-sea mineral deposits, such as polymetallic sulfides, polymetallic nodules, cobalt-rich crusts, phosphorites, and rare earth element-rich muds. Major areas with economic interest for seabed mineral exploration and mining are the following: nodules in the Penrhyn Basin-Cook Islands Exclusive Economic Zone (EEZ), the Clarion–Clipperton nodule Zone, Peru Basin nodules, and the Central Indian Ocean Basin; seafloor massive sulfide deposits in the exclusive economic zones of Papua New Guinea, Japan, and New Zealand as well as the Mid-Atlantic Ridge and the three Indian Ocean spreading ridges; cobalt-rich crusts in the Pacific Prime Crust Zone and the Canary Islands Seamounts and the Rio Grande Rise in the Atlantic Ocean; and the rare earth element-rich deep-sea muds around Minamitorishima Island in the equatorial North Pacific. In addition, zones for marine phosphorites exploration are located in Chatham Rise, offshore Baja California, and on the shelf off Namibia. Moreover, shallow-water resources, like placer deposits, represent another marine source for many critical minerals, metals, and gems. The main concerns of deep-sea mining are related to its environmental impacts. Ecological impacts of rare earth element mining on deep-sea ecosystems are still poorly evaluated. Furthermore, marine mining may cause conflicts with various stakeholders such as fisheries, communications cable owners, offshore wind farms, and tourism. The global ocean is an immense source of food, energy, raw materials, clean water, and ecosystem services and suffers seriously by multiple stressors from anthropogenic sources. The development of a blue economy strategy needs a better knowledge of the environmental impacts. By protecting vulnerable areas, applying new technologies for deep-sea mineral exploration and mining, marine spatial planning, and a regulatory framework for minerals extraction, we may achieve sustainable management and use of our oceans.



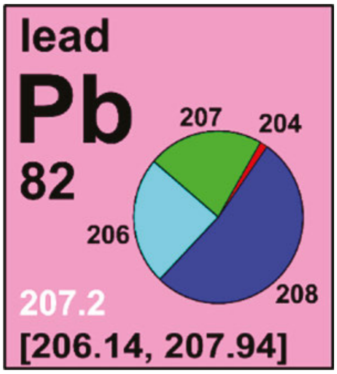
The photo was taken with the cameras of ROV KIEL 6000 during expedition SO268 at the seafloor of the Clarion Clipperton Zone (CCZ). The expedition was part of the JPIO MiningImpact project. It investigates the impact that potential manganese nodule mining in the deep sea would have on ecosystems there. The photo shows a sea urchin Urechnidae on the sea floor. Copyright ROV Team/GEOMAR (CC-BY 4.0)

https://iupac.org/project/2018-039-3-600

Standard atomic weights of the elements 2021 (IUPAC Technical Report)

Thomas Prohaska, *et al.*
Pure and Applied Chemistry, 2022, AOP 4 May 2022
https://doi.org/10.1515/pac-2019-0603

Following the reviews of atomic-weight determinations and other cognate data in 2015, 2017, 2019 and 2021 by the IUPAC Commission on Isotopic Abundances and Atomic Weights (CIAAW), an update of the Table of Standard Atomic Weights (TSAW) has been released 4 May 2022. The CIAAW has changed the values of the standard atomic weights of five elements based on recent determinations of terrestrial isotopic abundances: Ar (argon), Hf (hafnium), Ir (iridium), Pb (lead), and Yb (ytterbium). The standard atomic weight of



argon and lead have changed to an interval to reflect that the natural variation in isotopic composition exceeds the measurement uncertainty in a specific substance. The standard atomic weights and/or the uncertainties of fourteen elements have been changed based on the Atomic Mass Evaluations 2016 and 2020 accomplished under the auspices of the International Union of Pure and Applied Physics (IUPAP): Al (aluminium), Au (gold), Co (cobalt), F (fluorine), Ho (holmium), Mn (manganese), Nb (niobium), Pa (protactinium), Pr (praseodymium), Rh (rhodium), Sc (scandium), Tb (terbium), Tm (thulium), and Y (yttrium).

See "TSAW —a lifelong challenge or simply an unsolved mystery?" on page 18.

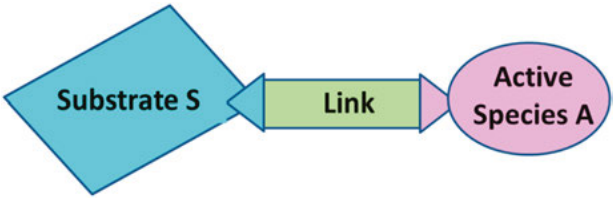
https://ciaaw.org

Terminology and the naming of conjugates based on polymers or other substrates (IUPAC Recommendations 2021)

Michel Vert, Jiazhong Chen, Andrey Yerin, Karl-Heinz Hellwich, Roger C. Hiorns, Richard Jones, Graeme Moad, and Gerard P. Moss

Pure and Applied Chemistry, 2022, AOP 17 March 2022
https://doi.org/10.1515/pac-2020-0502

A number of human activities require that certain complex molecules, referred to as active species (drugs, dyes, peptides, proteins, genes, radioactive labels, *etc.*), be combined with substrates, often a macromolecule, to form temporary or permanent conjugates. The existing IUPAC organic, polymer, and inorganic nomenclature principles can be applied to name such conjugates but it is not always appropriate. These nomenclatures have two major shortcomings: (1) the resulting names are often excessively long and (2) identification of the components (substrate, active species, and link) can be difficult. The new IUPAC naming system elaborates rules for unambiguous and facile naming of any conjugate. This naming system is not intended to replace the existing nomenclature but to provide a suitable alternative when dictated by necessity. Although the rules are intended to be primarily applicable to the naming of polymer conjugates, they are also applicable to naming conjugates with other substrates, which include micelles, particles, minerals, surfaces, pores, *etc.* The naming system should be used when recognition of the substrate and active substance is essential and will also be useful when constraints of name length make the otherwise preferred IUPAC nomenclatures untenable. The proposed rules for the new naming system are complemented by a glossary of relevant terms.



https://iupac.org/project/2014-034-2-400

Glossary of terms used in physical organic chemistry (IUPAC Recommendations 2021)

Charles L. Perrin, *et al.*

Pure and Applied Chemistry, 2022
Vol. 94, no. 4, pp. 353-534
https://doi.org/10.1515/pac-2018-1010

This Glossary contains definitions, explanatory notes, and sources for terms used in physical organic chemistry. Its aim is to provide guidance on the terminology of physical organic chemistry, with a view to achieving a consensus on the meaning and applicability of useful terms and the abandonment of unsatisfactory ones. Owing to the substantial progress in the field, this 2021 revision of the Glossary is much expanded relative to the previous edition, and it includes terms from cognate fields.

The first Glossary of Terms Used In Physical Organic Chemistry was published in provisional form in 1979 and in revised form in 1983, incorporating modifications agreed to by IUPAC Commission III.2 (Physical Organic Chemistry). A further revision was undertaken under the chairmanship of Paul Müller, which was published in 1994. The work was coordinated with that of other Commissions within the Division of Organic Chemistry. In 1999, Gerard P. Moss, with the assistance of Charles L. Perrin, converted this glossary to a World Wide Web version. This Glossary has now been thoroughly revised and updated, to be made available as a Web document. The general criterion adopted for the inclusion of a term in this Glossary has been its wide use in the present or past literature of physical-organic chemistry and related fields, with particular attention to those terms that have been ambiguous. It is expected that the terms in this Glossary will be incorporated within the online version of the IUPAC Gold Book, which is the merged compendium of all glossaries.

See recent feature by Ian H. Williams. “Physical Organic Chemistry in the 21st Century: A Q1 Progress Report”, *Chem. Int.* vol. 44, no. 2, 2022, pp. 10-13. https://doi.org/10.1515/ci-2022-0203

https://iupac.org/project/2009-002-1-300

Synthesis design using mass related metrics, environmental metrics, and health metrics

Marco Eissen

Pure and Applied Chemistry, 2022
Vol. 94, No. 2, pp. 215-245
https://doi.org/10.1515/pac-2021-0326

The efforts to integrate environmental aspects, health aspects as well as safety aspects into chemical production has led to the development of measurable and thus objectifying metrics. The application of these metrics is considered to be most promising, especially during the earliest phases of synthesis design. However, the operability in daily work suffers from the lack of available data, or a large variety of data, and the complexity of data processing. If a life cycle assessment is not practical in the early development phase, environmental factor and process mass intensity can give a quick and reliable overview. The author shows that this often says the same in advance as a subsequently prepared life cycle assessment. Readers will realise that, based on preparative descriptions, they can quickly determine these metrics for individual syntheses or extensive synthesis sequences applying the available software support. Environmental relevance in terms of persistence, bioaccumulation and toxicity (PBT) can be presented using a modification of the European ranking method “DART” (Decision Analysis by Ranking Techniques). Based on corresponding PBT data, one can determine a hazard score between 0 and 1 for any substance using the spreadsheet file provided, with which the mass of (potentially emitted) substances can be weighted. Occupational health can be represented using a modification of the recognized “Stoffenmanager.” Both concepts are presented and spreadsheet files are offered.

This special topic paper published in PAC is based on a presentation made at the Green Chemistry Postgraduate Summer School in Venice, 6-10 July 2020, and pertinent to the current IUPAC project 2017-030-2-041, titled “Metrics for green Synthesis.”

Highlights *from* GWB2022

407
Events

78
Countries

~30K
Attendees

Average attendance per event

80 people

Overall rating of GWB by organizers

4,6/5 out of 5

Who attended? Reported by Organizers

80% of events included University Students and faculty

20% of events included Government Scientists

29% of events included Industry Scientists

18% of events included Non-Profit Organization Scientists

26% of events included High-School Students

16% of events included other organizers

Breakfast Event Formats

54%
Virtual

24%
In Person

22%
Hybrid

How are we strengthening a global network?

>50%

of organizers reported that the GWB has led to new connections within their organization and externally.

How are women benefiting?

>40%

of organizers reported that the GWB provided leadership development opportunities for women in their organization.

How are we moving the needle on diversity?

>60%
of organizers

reported that the GWB has increased attention to diversity issues and allowed for more open discussions on diversity in their organizations.

Bookworm

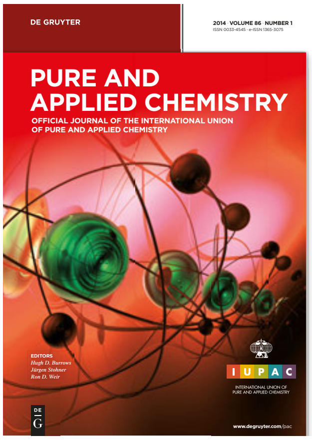
Books and publications hot off the press.
See also www.iupac.org/what-we-do

Cheminformatics: Data and Standards

A Pure and Applied Chemistry Special Issue

Vol 94, Issue 6, June 2022

by Vincent F. Scalfani (Guest editor)



Many readers of *Pure and Applied Chemistry* and *Chemistry International* are likely familiar with the IUPAC Color Books. The current collection of IUPAC Color Books is comprised of eight volumes, and includes authoritative descriptions of chemical units, nomenclature, terminology, and symbols [1]. IUPAC standards and recommendations exist outside of the Color Books as well, for example, in individual publications and reports from IUPAC Project task groups. Relevant to cheminformatics, two longstanding IUPAC standards and recommendations include the InChI for chemical identification [2], and JCAMP-DX for spectral data exchange [3,4]. In addition to continued development of InChI and JCAMP-DX within IUPAC, the IUPAC Committee on Publications and Cheminformatics Standards (CPCDS) along with numerous IUPAC task groups have been engaged with advancing cheminformatics, or more broadly, digital chemistry standards over the last two decades. For example, a basic search in the IUPAC Project database [5] for the words 'cheminformatics' or 'digital' resulted in 26 projects, with 15 of the projects still active. Some examples of current projects include enhancements to the Gold Book, metadata schema for solubility data, FAIR data projects, and efforts to enhance molecular representations (*e.g.,* SMILES and InChI). Clearly, digital standards and cheminformatics are active areas of interest to IUPAC, the contributing volunteers, and the broader chemistry community. Readers are encouraged to visit the IUPAC Digital Standards webpage and submit feedback on current projects or ideas for new standards projects [6].

While the current IUPAC Color Books, publications, and task group reports contain some digital and cheminformatics standards, a need for a dedicated IUPAC Cheminformatics Color Book was recognized by a task group in 2017 [7]. The task group completed a review of the current cheminformatics community needs and began preliminary planning for a new Cheminformatics Color Book. In late 2020, the IUPAC Subcommittee on Cheminformatics Data Standards (SCDS) aims were updated to focus on the digital dissemination of IUPAC cheminformatics data standards:

> "The Subcommittee on Cheminformatics Data Standards (SCDS) coordinates and leads the digital dissemination of IUPAC cheminformatics data standards. SCDS works collaboratively with relevant IUPAC Divisions, IUPAC Committees, publishers, external scientific organizations, and the chemistry community to manage source reference material for IUPAC outputs related to cheminformatics and data standards. Such outputs may include cheminformatics related theory, policy around digital data/metadata exchange, standards, recommendations, validation data, and community engagement. SCDS maintains a vision for the dissemination of IUPAC cheminformatics standards and works closely with contributors and the community to share and maintain this information."

In 2021, SCDS was then tasked with continuing the planning and development of a new IUPAC Cheminformatics Color Book. These new goals for SCDS and discussions within the Committee led to this *Pure and Applied Chemistry* special issue on Cheminformatics: Data and Standards as a first step towards a Cheminformatics Color Book. A call for papers was published in May 2021, with the aim of discussing cheminformatics standards and future needs. The proposed topics for the issue were as follows [8]:

- Cheminformatics standards use-cases and workflows across disciplines.
- Discussions around how cheminformatics standards advance research and teaching.
- Perspectives related to current cheminformatics standards and future needs, for example interoperability and metadata considerations.
- Cheminformatics datasets useful for teaching and/or validation.
- Standardization needs related to infrastructure (*e.g.,* repositories), cheminformatics toolkits, or data sharing.
- Conference, symposia, or workshop based outcomes related to cheminformatics standardization.

How would a *Pure and Applied Chemistry* special issue on Cheminformatics: Data and Standards lead to an official IUPAC Color Book? Discussions are ongoing within IUPAC. One potential strategy is for the Cheminformatics: Data and Standards special issue to become a virtual "rolling" issue; in other words, articles are continually added. From the collection of cheminformatics articles in *Pure and Applied Chemistry*, selected articles could then be adapted into a cheminformatics Color Book chapter in collaboration with the author(s) and relevant IUPAC committees. This model for the Cheminformatics Color Book would be similar to an "overlay" journal [9]. Determining which articles would be appropriate for inclusion into the Color Book could be made through a combination of input from the community, IUPAC committees (e.g., SCDS) and related IUPAC task groups. Selected articles would then go through a similar approval process as other IUPAC Color Books. This workflow of completing the Cheminformatics Color Book piece-wise would spread the work across many contributors, while also serving to more quickly disseminate authoritative cheminformatics standards and recommendations to the global community.

Having now described the history and thought behind this special issue and future ideas for an IUPAC Cheminformatics Color Book, let me summarize the content within this issue.

There are four main themes of the contributed articles. The first theme is **education** with a contributed article on experiences with the Royal Society of Chemistry Chemical Information and Computer Applications interest Group's open source chemical data and cheminformatics virtual workshops (Swain, see also box on next page), and another contributed article with a detailed account of experiences related to launching a materials informatics program (Lipscomb). The second theme is **cheminformatics file formats** and use cases. This includes an article on a proposed data model for compounds and assays (Kappler), an article describing a big data use case with RInChI (reaction InChI) (Blanke), and an article on the Reaction Structured Product Labeling format and associated use-cases (Nicklaus). The third theme is **spectroscopic data** and includes an article with an overview of the JCAMP-DX file format (Davies), and another article describing a proposed IUPAC specification for the FAIR management and sharing of spectroscopic data (Hanson). And the fourth theme was **surveying the landscape**, including an article reviewing chemical ontologies (Koepler) and a review of analytical data standards (Rauh). I expect that there will be many more contributions and themes that emerge with new submissions. As more machine-readable chemical data is continuing to be shared, standardization efforts will become even more important, and I hope articles collected within this *rolling* special issue can serve as a starting point toward identifying key chapters for a Cheminformatics Color Book, as well as identifying new IUPAC projects that are needed to advance cheminformatics standardization efforts.

Thank you for reading this special issue. And thank you to the contributing authors, reviewers, and Hugh Burrows, Editor of *Pure and Applied Chemistry*, for his enthusiasm and help making this issue a reality. Finally, thank you to my colleagues within IUPAC for their encouragement and feedback during the planning of this special issue on Cheminformatics: Data and Standards.

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https://www.degruyter.com/PAC ; keyword: Cheminformatics
https://www.degruyter.com/journal/key/pac/94/6/html

Promoting Open Chemical Science Online

by Christopher J. Swain, Jeremy G. Frey and Jonathan M. Goodman

What is the state of open science in chemistry? What are the scope and limitations of the current chemistry situation in data, in publishing and in scientific software? How is it possible to run meetings without meeting in-person?

These questions were addressed during a meeting of the Royal Society of Chemistry's Chemical Information and Computer Applications interest group (RSC CICAG) organised in Nov 2020, by Christopher Swain, Jeremy Frey, and Jonathan Goodman. The five-day online meeting entitled *Open Chemical Science* (https://www.rsc.org/events/detail/42090/open-chemical-science) had three interwoven themes: Open Data, Open Access publishing and Open-Source tools. One of the advantages of an online event was it could be attended by people from 45 different countries. The challenges involved in converting what was planned as a three-day physical event into a five-day virtual event with three intertwined strands.

Open science is flourishing in chemistry, but the current infrastructure of both academic and commercial research developed mainly with closed science in mind. A transition to an open infrastructure represents a significant shift. How open science is best funded and assessed is not clear, and researchers are reasonably concerned that their work may not receive all of the recognition that it deserves. However, the move in this direction may be unstoppable.

Publishing data is increasingly coming into focus as a major challenge. Open data is central to current chemical science, but how can this be funded and sustained? The benefit of everyone else's data being open accessible long term is obvious; the driver for making your own data available can be less clear.

Open access publishing is becoming more accepted as a normal way of publishing research. However, a large number of important publishing resources are not open-access, and it is not clear when or if this will change. The Declaration on Research Assessment (DORA https://sfdora.org) is important, but it is not clear that members of institutions which have committed to DORA are not always aware of the obligations that this entails.

Open software for chemistry is thriving. People learned about examples and best-practice in open data from the meeting. This section of the meeting generated more immediate data and feedback than the other two sections. Open software is a key component of open chemistry. Feedback from software users may provide a more immediate link to the developers than a publication.

The organizers initial apprehension about the success of the meeting, as the date approached and the pandemic did not subside, turned out to be unfounded. The meeting almost certainly had a higher and more diverse attendance than it would have done had it been a traditional in-person meeting. Informal interactions over a video conference, however, were more stilted than actually meeting people in person. In planning future meetings, the CICAG committee will balance the benefits of a more international, economical and environmentally-friendly on-line meeting with a more intense but smaller in-person meeting.

The online meeting was recognised by the RSC with the award of the "2021 Inspirational Committee Award" (https://www.rsc.org/prizes-funding/prizes/2021-winners/rsc-chemical-information-and-computer-applications-group/). The conference has led to a continuing series of workshops.

All the workshops are available on the RSC CICAG YouTube channel https://www.youtube.com/c/RSCCICAG

See full account in PAC: Swain, Christopher J., Frey, Jeremy G. and Goodman, Jonathan M.. "RSC CICAG Open Chemical Science meeting: integrating chemical data from two symposia and a series of workshops" *Pure and Applied Chemistry,* AOP 21 Apr 2022; https://doi.org/10.1515/pac-2021-1003.

Systematic Nomenclature of Organic, Organometallic and Coordination Chemistry. Chemical-Abstracts Guidelines with IUPAC Recommendations and Many Trivial Names

by Ursula Bünzli-Trepp

Logos Verlag Berlin 2021; 685 pp.

reviewed by Molly Strausbaugh, Edwin Constable, Andrey Yerin, and Ture Damhus, all of IUPAC Division VIII.

Accuracy and unambiguity are at the heart of good science communication, and the publication of the second edition of Ursula Bünzli-Trepp's book on chemical nomenclature is a significant contribution toward achieving these standards. The title of the book is self-explanatory, and the author presents the topic in an encyclopedic manner. The book comprises six chapters: *Directions for the use of this book*, *Fundamentals*, *Guide to name construction and name interpretation*, *Molecular-skeleton parents*, *Substituent prefixes*, and *Compound classes,* together with appendices and tables. The coverage of organic compounds is more comprehensive than that of coordination and organometallic species, which is confined to 55 pages in the chapter entitled *Compound classes*. The text is an overview of the major nomenclature systems used in the Anglophone world but cannot be considered a complete guide to any of them. The liberal approach to nomenclature found in the primary literature is a justification for a book that shows what could (and could not) be considered an appropriate name.

The text usually emphasizes the differences between IUPAC and Chemical Abstracts Service (CAS) nomenclatures and occasionally gives value judgements of the approaches (see below on anionic ligands). Very often, the author lands on the side of the CAS name. Much of the book comprises loose paraphrases of IUPAC and CAS documents, making it a good reference work but does not necessarily enhance the readability. The organization of the sections might not be obvious to all readers, and it is not always simple to determine the hierarchical level of nomenclature to which a particular section belongs.

It is useful to consider what readers might expect to gain from this book:

1. An understanding of the basics of CAS and IUPAC nomenclature
2. The ability to convert an "official" CAS or IUPAC name to a structure
3. A feeling for the most appropriate nomenclature system to use for their compounds of choice
4. All of the above in an accessible and readable form that, at the same time, would serve as a single point of reference.

The structure of this review will center upon these four aspects.

In the first aspect, the author succeeds in giving a broad understanding of the principles of the two major systems of nomenclature, although the approach of dealing with them together has an inherent danger of leaving the reader confused and adopting hybrid nomenclature schemes (which probably is a fair assessment of the general approach to nomenclature by most practicing chemists). The author probably over-estimates the level of knowledge in the general community regarding the nuances and similarities of, as well as the differences in, the CAS and IUPAC systems. The 520 pages of main text are information-rich and contain numerous chemical structures which clearly illustrate the nomenclature principles. The author has had to base herself on the 2013 IUPAC *Blue Book* [1], which was, however, revised in the 2021 html online version [2]. The reader should refer also to the latter version. The present book fills a gap between the very short IUPAC publications, *Brief Guide to Polymer Nomenclature* [3], *Brief Guide to the Nomenclature of Organic Chemistry* [4] and *Brief Guide to the Nomenclature of Inorganic Chemistry* [5], the broader *Principles of Chemical Nomenclature: A Guide to IUPAC Recommendations* (2011) [6], and the full documentation in the IUPAC *Red* (2005) [7], *Purple* (2008) [8] and *Blue* (2013, 2021) [1,2] Books and the *CAS Index Guide* [9].

The emphasis of the book is on the construction of accurate and unambiguous names for compounds of known structure. In reality, the opposite process is equally important for a chemist and the need to deconvolute a systematic, semi-systematic or trivial name in a chemical catalog or publication to a chemical structure is one of the most common ways in which nomenclature impinges on our everyday life. Despite the title of Chapter 3 mentioned above, this deconvolution aspect, as found in other general texts dealing with nomenclature, is not explicitly addressed in the current book. Although the process is relatively straightforward if IUPAC names are used, a degree of familiarity with the rules is essential. In a future edition, a flow chart illustrating this reverse procedure for both CAS and IUPAC names would considerably benefit the reader.

Although we like to think that chemists want to invest time in constructing accurate and unambiguous names for their compounds using one of the commonly accepted (*i.e.*, CAS or IUPAC) systems, we know this is not the case. This book presents strategies for naming most of the types of compounds likely to be encountered in molecular chemistry. The author often prefers the CAS name over IUPAC, but usually gives justification for the choice. In many cases, the author only gives CAS names arguing that the CAS guidelines are simpler to apply than the IUPAC recommendations. This is a personal choice, and many readers may prefer the IUPAC system.

A particularly debatable subject is the naming of esters (Section 6.14). The functional class names preferred by IUPAC ("ethyl acetate" type) constitute a uniform system, while the CAS system is more complicated with different name constructions depending on the complexity of alcohol and acid components (*e.g.,* "acetic acid ethyl ester" but "2-chloroethanol acetate"), and the book requires considerable space to describe the system.

Another example could be the discussion of anionic ligands on p. 465 and pp. 476-477. The IUPAC selection of "ido" endings for anionic ligands, such as chlorido, oxido and cyanido, was made to ensure a simple general and pedagogical procedure for generating ligand names from anion names. These names also distinguish these species when acting as ligands rather than as substituents, when they are notated chloro, oxo and cyano. These aspects do not seem to be appreciated by the Author.

The final question relates to accessibility and readability and whether the book can serve as a single point of reference. The book is not entirely successful in this respect. The text is attractively presented, although the font is relatively small. Colors are used sensibly and will be helpful, except to readers who are color-blind. Molecular structures are nicely drawn, although the hashed lines representing bonds pointing below the plane are ambiguous and have been replaced with hashed *wedges* by *both* CAS and IUPAC. Structures are generally placed where they are named in the text; Table 6.4 with the structural diagrams on the opposite page from the table of ligand abbreviations is much more user-friendly than the combination of two tables needed in IUPAC's *Red Book* 2005 [7].

There is a genuine question of whether a 680-page book can really be readable. It is certainly more reader-friendly than the *Blue Book*, but in this respect, *Principles of Chemical Nomenclature* mentioned above probably succeeds better, although with less comprehensive coverage. The real question is who the target audience is and whether it can serve as a single point of reference. This is very difficult to answer. On the one hand, the book is too detailed for doctoral and pre-doctoral workers and, on the other hand, does not contain enough detail for the established researcher who really wants to find the "correct" name for a compound. So, in this sense, the text successfully reaches the "normal" audience of chemists who want to use names that other scientists will understand without recourse to IUPAC's color books or the CAS guidelines. Paradoxically, however, the concept of the book in presenting all of IUPAC, CAS and trivial names might deter this audience if they are seeking "*the* name".

The book does not properly address the future and pragmatic reality of nomenclature. We all know that in the laboratory, fully systematic names such as the book's example 231 on p. 490, [1,1′-methylenebis[1,1-diphenylphosphine-κ*P*]]bis(triphenylphosphine)palladium(2+) tetrafluoroborate(1–) (1:2), are not used, but rather short code-like names such as Pd-phosp or BJ219. Correct nomenclature is important for the precise identification of compounds in print and in electronic records. The future of nomenclature will increasingly involve machine-readable scripts, with a resultant drift away from plain text to precise code, which is not necessarily human-friendly. This omission from the book is all the more surprising considering that industry standard software such as ChemDraw can efficiently generate SMILES, InChI, and InChIKey descriptions for the vast majority of organic structures.

It would be surprising if a work of this length and with this large scope were completely free of errors, inaccuracies and omissions, but true typographical errors such as "bis(chlorate) (2 ClO_4^-)" on p. 477 seem to be rare.

There are issues of terminology, however. The introductory list of nomenclature terms under "Additive name" does not mention the use of additive procedures in coordination names and names of addition compounds—this is a significant omission. Under "Affix" in the same list, it says, “IUPAC uses the term affix as a collective term for prefixes and suffixes” (as if IUPAC does not include infixes). However, the wording in Section P-14.2 in the *IUPAC Blue Book* (1) is clear: “affixes (suffixes, **infixes**, and prefixes)”. Still further down, the definitions of “characteristic group” and “isolated group” are slightly surprising. For the less common term *heterochains*, one notes that there are homogeneous heterochains! A definition of “nonfunctional compound” is absent or at least difficult to find. The term “ending” is used differently from IUPAC, but the difference is explicitly acknowledged. In Table 3.2 and other places it seems that there is a seniority order of entire compounds of various kinds. It is not clear what this has to do with the choice of principal groups.

Bunzli-Trepp chooses to use “proton” generally instead of “hydron.” Just a matter of taste or convenience? The general name (from IUPAC) has officially been “hydron” since 1988, as opposed to “proton” specifically for $^1H^+$.

Being very brief when referring to alternative names may lead to inaccuracies. On p. 508 for Cp it says “IUPAC: cyclopentadienyl” as if IUPAC does not use cyclopenta-2,4-dien-1-yl (which IUPAC does, but cyclopentadienyl is given as an acceptable short form). We also note that the forms cyclopentadienido or cyclopenta-2,4-dien-1-ido are recommended by IUPAC in the names of coordination and organometallic entities.

The title of the book refers also to *trivial names*, *i.e.*, names containing no parts with a systematic meaning. Examples are given together with the definition of this term, but a couple of them (like D-glucose) contain stereodescriptors and may not be seen to fulfil the criterion. Further appearances of trivial names seem to be primarily those that have been adopted into systematics as names for parent hydrides or functional parents. Also, examples of various current systematic names are accompanied by notes giving alternatives, for example “trivially diethyl azodicarboxylate” or “trivially methylene chloride”. It may be debated whether these are true trivial names or just belong to older, more traditional, systematics.

The question is what expectations the title’s use of “trivial names” creates in the reader’s mind. One will not find a broad collection of daily-life trivial names like alum, borax, calomel, carborundum, caustic soda, ferroin, laughing gas, magnesia, nicotine, red lead, *etc.*, not to speak of common international non-proprietary names like amfetamine and triclosan or eponyms like Caro’s acid and Zeise’s salt or toponyms like Epsom salt. At least these names are not in the index, which appears to be otherwise very comprehensive, although IUPAC variants mentioned in small print in the main text may not be included in the index (*e.g.*, borinine, arsinine, phosphinane).

The author frequently uses the heading “Instructions” to introduce the principles of naming a specific compound, although these are actually “Descriptions” rather than “Instructions.” There are several mistaken usages of “principals” for “principles.” Some classes of compounds are dealt with by what is called “Specialist nomenclature,” although compounds like carbohydrates and polymers are important to many of us who are not specialists within these classes.

In conclusion, despite the specifics discussed above and some inconsistencies, this book provides a comprehensive and detailed summary of current systematic CAS and IUPAC nomenclature systems. The inclusion of a great number of chemical structures with their various systematic and trivial names makes it a very useful handbook for the nomenclature of many classes of chemical compounds.

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InChI Open Meeting

by Jonathan Goodman, Gerd Blanke, Rudy Potenzone, and Steve Heller

An open meeting on the InChI chemical identifier was held on-line on 5-6 April 2022. Eleven working groups reported on their work developing the InChI standard and its applications. Sixty-five people attended the meeting, questioned the speakers and contributed to vigorous discussions in the on-line chat. The slides for the meeting are available on: https://www.inchi-trust.org/decks-open-inchi-days-2022/

Jonathan Goodman and Gerd Blanke introduced the meeting. The InChI Trust and IUPAC look after the InChI standard: https://www.inchi-trust.org & https://iupac.org/body/802

The latest release of the InChI is version 1.06 [1]. One of the key challenges for the InChI, its possible extensions and its derivatives is deciding when two systems are sufficiently similar to use the same InChI. The layered structure of the InChI is helpful for this: two InChI may be the same in the first layers and differentiated in later layers, by stereochemistry for example. The current standard InChI and InChIKey strikes a good balance between the need to connect and the need to differentiate. We know this because they are very widely used. Pre- or post-processing may be an effective strategy to tune discrimination. The right balance for the future must be chosen carefully, based on data whenever possible.

Extended Stereochemistry

Andrey Yerin (ACD labs)

The InChI describes stereochemistry well, but this can be improved further. Andrey outlined how extended cumulenes, atropisomers and advanced stereochemistry can all be added to the InChI fairly readily and how the interpretation of different representations of molecules can be improved. Polyhedral stereochemistry will become important as the working group on organometallics and coordination compounds develops its recommendations. InChI are generated from molfiles. Interpreting molfile information can be challenging, particularly when Haworth, Fischer and other representations are used.

Polymers

Gerd Blanke (InChI Trust Technical Director; StructurePendium Technologies)

Major enhancements to polymer representation became available in 2020 with InChI v1.06 [1]. These are not (yet) a part of the standard InChI, although they make possible the canonical representation of many polymers. There are challenges ahead, particularly with non-linear polymers and the composition of co-polymers. How similar should polymers be to be given the same InChI?

Markush/Variable

Jonathan Goodman (University of Cambridge)

InChI which can describe large groups of molecules may be very useful for precisely describing claims in patents, for monitoring multi-parallel syntheses, and for many other purposes. The working group is approaching this problem from two directions: first, compressing lists of molecules using chemically-intelligent algorithms; second, encoding Markush-like structures in InChI strings. Experimental programs are now available for both approaches. The working group is also discussing exactly how such identifiers might be most useful for patent experts.

Education and Outreach

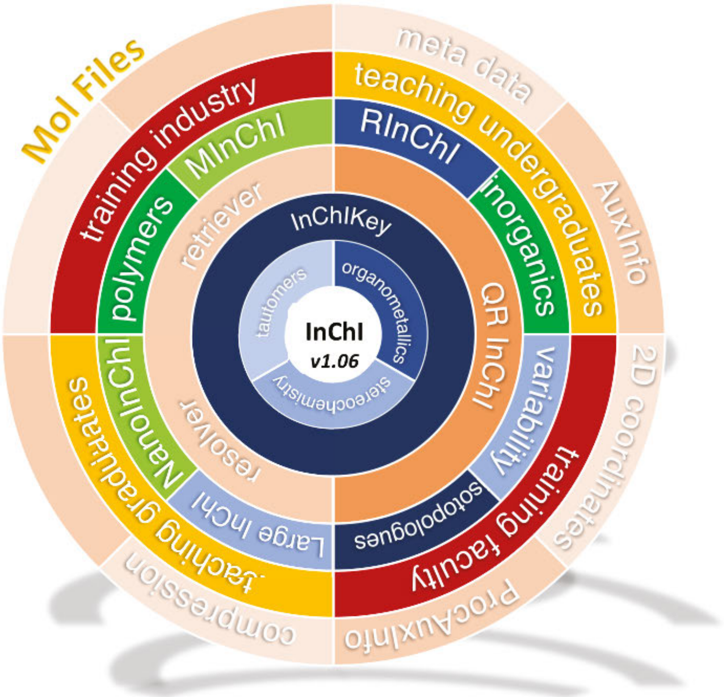
Bob Belford (University of Arkansas at Little Rock)
Rudy Potenzone (InChI Trust)

Bob Belford described the InChI Open Education Resource which is available on the InChI Trust website: https://www.inchi-trust.org and surveyed the conference for its views on InChI education resources. There was enthusiasm for including InChI in the chemistry curriculum, although adding new information to courses would necessitate removing some current information. Rudy Potenzone outline the outreach activities that focus on the InChI Trust website and include a newsletter, information about the working groups, and a list of papers which cite the InChI.

Large Molecules

Evan Bolton (National Center for Biotechnology Information, NLM, NIH))

How best to handle molecules with more than a thousand atoms and bonds? Such molecules are becoming increasingly important. The current standard InChI might be used, but would require a lot of computer time and generate very long strings. It may be possible to design a layered large-molecule specification on top of the InChI code base. The working group is interacting with HELM project for macromolecules, which is run in a partnership between IUPAC and the Pistoia Alliance. Expertise and use-cases are needed.



Tautomers

Marc Nicklaus (NCI)

The working group has completed its analysis [2]. It is not completely clear how best to incorporate these results into the InChI. A few tautomer rules are already encoded in the standard InChI. Incorporation of all of the rest would change the standard InChI for a large proportion of molecules. Pre-processing or post-processing could be used to address this. What choices for the standard will lead to the widest use of the InChI?

FDA Challenge

Yulia Borodina (Office of Data, Analytics and Research)

The FDA is planning a crowdsourced evaluation of InChI-based tautomer identification. What tautomer rules are most helpful for current databases? The data generated should inform choices about the best defaults for the InChI.

Organometallics, Coordination Compounds and Inorganics

Hinnerk Rey (Elsevier)

Sonja Herres-Pawlis (RWTH Aachen University)

The current standard InChI does not describe organometallic and inorganic compounds very precisely, as bonds to metals are disconnected by the InChI algorithm. Bonds to metals are critical to identifying these structures, and the working group is going though many examples considering the best ways to express them in an InChI. When should structures be differentiated and when do different representations relate to the same substance? Bonding and stereochemistry is more complex than for organic molecules, but it should be possible to extend the InChI approach for these systems. A number of views were expressed in the on-line chat about the best rules for this, as well as the suggestion that the only rule for inorganic chemistry is that there are no general rules.

Reactions

Gerd Blanke (InChI Trust Technical Director; StructurePendium Technologies)

Reaction descriptions with the RInChI are becoming more sophisticated, including atom mapping. Stereochemistry remains challenging with the current standard InChI. Enzymatic reactions are now being addressed by the working group. Auxiliary information is used to record data about reactions which is not suitable for the canonical RInChI. The RInChI working group is leading the way amongst the InChI working groups by developing its code on GitHub.

Mixtures

Leah McEwen (Cornell University)

The MInChI working group is developing ways of using the InChI in the description of mixtures: “Mixtures Informatics” (https://github.com/IUPAC/

MInChI). The multi-layered approach can order much information about mixtures, even in very demanding cases such as UVCBs (unknown variable composition or biological substances) which are necessarily difficult to characterise. The working group has developed a specification and is looking for more use-cases with real data.

Nanomaterials

Iseult Lynch (University of Birmingham)

The nanomaterials working group is the newest of the InChI working groups and is tackling the most complex systems. Building on the work of other working groups, it is building international collaborations to work out what is essential for an InChI describing nanomaterials, and what is best held in auxiliary information. When are two nanomaterials sufficiently similar that they should have the same InChI? The working group is taking a pragmatic approach to the vast space of nano and advanced materials.

QR Codes

Jeremy Frey (University of Southampton)

A proposal for encoding InChI as QR codes has been finalised and the period of IUPAC public review ended on 31 May 2022. A label that includes a standard QR code with chemical information would be very useful. An unofficial QR InChI generator is available on http://www-rinchi.ch.cam.ac.uk/qrinchi/

Isotopologues

Hunter Moseley (University of Kentucky)

The working group has developed an extension to the InChI which can describe isotopologues: molecules which differ only in their isotopic composition. Implementation of the extension is a challenge because molfiles do not describe isotopologues well.

InChI Future

Gerd Blanke

The InChI code requires some re-architecture, but how far should this go? The future of the InChI will include community development. To what extent is backwards compatibility important? The aim is to transfer the code to an open-source repository such as GitHub. These changes will require both a technical working group to consider software architecture, and a context working group to consider prioritization and deliverables.

Conclusions

The open days demonstrated the breadth and energy of the many InChI working groups, both in addressing current issues and in developing new InChI applications. The enthusiasm of the participants showed that the InChI has many exciting advances ahead. If you would like to contribute to the development of the InChI standard by joining a working group, please get in touch.

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In Memoriam

The InChI Trust noted the passing last November of Igor Pletnev, the developer and caretaker of the InChI software algorithm for over 15 years, first at NIST and then at the InChI Trust. Over the years Igor made great contributions to the InChI project. His knowledge of both chemistry and computer programming made him a unique person to carry out all these tasks while interacting with chemists around the world on an almost daily basis. While there were many demands on his work efforts with the InChI algorithm, Igor always was calm and friendly to all, a true professional at all times. He will be missed and dearly remembered for all of his outstanding work by all of us at InChI Trust and the global community of InChI developers and users.

The International Union of Pure and Applied Chemistry is the global organization that provides objective scientific expertise and develops the essential tools for the application and communication of chemical knowledge for the benefit of humankind and the world. IUPAC accomplishes its mission by fostering sustainable development, providing a common language for chemistry, and advocating the free exchange of scientific information. In fulfilling this mission, IUPAC effectively contributes to the worldwide understanding and application of the chemical sciences, to the betterment of humankind.

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