History Come Alive: The Nozoe Autograph Books and IUPAC
Guest Editorial

This issue features an entertaining insight into the human face of IUPAC history (See Jeffrey Seeman’s feature, page 4), and also offers an opportunity to celebrate the life of Carl Djerassi, who passed away this January at the age of 91. Much has been written by and about him, and it seems superfluous to add to the abundant evidence of his extraordinary life other than to pay tribute through footprints in the IUPAC record (see www.iupac.org/publications/pac/authors/CarlDjerassi/)

The Union launched Pure and Applied Chemistry as its official journal in 1960. A founding policy was to publish topical critical reviews arising from the then-nascent program of IUPAC-sponsored international scientific conferences. The ensuing decades coincided happily with an astonishingly productive phase of Djerassi’s chemistry career, and have furnished the opportunity to serialise the history of some of his major research achievements. The IUPAC series of International Symposia on the Chemistry of Natural Products was inaugurated August 1960 in Australia, setting the scene for the publication of numerous works by Djerassi in Pure and Applied Chemistry between 1961 and 1982 on methodologies that revolutionised structural organic chemistry during that era.

The Djerassi school dominated this period of advances in interpretive mass spectrometry and chiroptical diagnostics as indispensable aids for structural elucidation of complex natural products. His final contributed work to the Journal in 1982 heralded the beginnings of an age of computer-aided deconvolution of molecular complexity. During the 80s, Djerassi’s interests broadened increasingly into formerly unexplored areas of creativity, but were unfailingly guided by a desire to enrich, explain, and humanise science in his inimitable way.

Please indulge a footnote arising from personal reminiscences. I attended a Djerassi lecture for the first time as an impressionable student delegate at the 2nd IUPAC Symposium on the Chemistry of Natural Products (Prague, 1962), and for the last time in my capacity as organising Chair of the 13th event in that series ( Pretoria, 1982). My intervening years were punctuated by a post-doctoral period at Stanford University in 1964-1965, and by attendance at four more Natural Products Symposia in which Djerassi featured prominently and persuasively on the plenary programme. I vividly recall the passion and energy, tempered by accessibility, which characterised his academic presence, and which surely influenced an entire generation of former students and collaborators whose careers were founded upon his inspirational leadership. It is a privilege to salute a colossus, and gratifying to note that IUPAC can claim some credit for a small part of his indelible legacy.

James R. Bull
University of Cape Town, South Africa

Pure and Applied Chemistry Scientific Editor 2000-2013

Cover image: Carl Djerassi’s 1964 entry in the Nozoe Autograph Books. As described in Jeffrey Seeman’s feature (page 4), the Nozoe Autograph Books offer an unique historical perspective on international communication among chemists. In his essay, Seeman gives a brief retrospective on how the Books came about. He then shows how in 1963, at the occasion of the 3rd IUPAC Symposium on Chemistry of Natural Products, many of the plenary lecturers, which scientific presentations are published in the IUPAC journal Pure and Applied Chemistry, have contributed along with many symposium participants, to a unique account of the event by signing the Nozoe Autograph Books.

Cover design by Purple Zante, Inc.
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Where 2B & Y

Mark Your Calendar

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January 2015 was a momentous time for the IUPAC Secretariat—at the end of the month it moved from 104 T.W. Alexander Drive, Building 19, Research Triangle Park, North Carolina 27709 after 17 years in what was actually a spacious, but nevertheless temporary, wooden building. Some referred to it as a trailer, Europeans would probably call it a large porta-cabin. Most volunteers will have had dealings with the Secretariat, but few actually enjoyed a visit.

This was the time of former Executive Directors John Jost and Terry Renner, a time of stories of spiders and snakes and the need to reinforce the floor given the huge weight of books stored there. An audit conducted just before the move showed a stock of about 7400 IUPAC publications. We are currently finding good homes for these, while old records will be archived at the Chemical Heritage Foundation.

I had always understood that the great advantage of Building 19 was that we paid a ‘peppercorn’ rent of $1 a year. This was indeed the case, but the full occupation costs for the building were actually much higher—close to $20,000 in 1997 and rising to approximately $45,000 in 2014. In this regard the accommodation was sub-standard, with poor safety and security; poor heating, cooling and plumbing; a leaking roof; and 1990s IT infrastructure.

Last year it became clear that the time was up for Building 19. A lease renewal was not an option, as the building stood in the way of a new development. Without the books to hold it up I don’t expect that demolition will be too tricky!

Our new home is 79 T.W. Alexander Drive, Research Commons Building 4201, Suite 260, Research Triangle Park, NC 27709. This is class ‘A’ office accommodation offering modern standards of safety and security, as well as services including state of the art broadband IT.

Located in the building will be Executive Director Dr. Lynn Soby, Accounting Manager Linda Tapp, and Administrative Assistant Enid Weatherwax. Associate Director Dr. Fabienne Meyers continues to be based remotely at Boston University.

So what does the Secretariat actually do?

The Secretariat’s primary roles are to:
- assist the officers in the administration of the Union
- facilitate the work of the many hundreds of volunteers within the divisions, committees and projects working on behalf of the Union
- communicate our activities through our journals and the website

To do this, the Secretariat prepares and manages against the biennial budget recommended by the Treasurer and approved by the Council. It has to achieve a balance as money comes in and goes out, given the difficulty of managing the timing of these cash flows. Income arises primarily from National Adhering Organisation (NAO) subscriptions, from publishing, and from our investments. This is why the timing of subscription payments is so critical; the later they are left the more difficult things become for the Union. Expenses include the running of the office and approximately 1000 expense claims from volunteers checked and settled, totaling some $900,000 in 2014. We can be expected to settle these claims in up to 50 different currencies, reflecting our international membership of over 60 countries.

The Secretariat maintains the books and accounts to provide management information for the Officers and Finance Committee and ensures the information required for statutory U.S. accounting of payroll and taxes is provided. It also stores data on all the categories of
membership, contacts, and customers of IUPAC, both in current and historical records. Much of the membership data is displayed on our website. The information on the website must be kept up to date and relevant.

The Secretariat is responsible for the administration of both the IUPAC project system and the endorsement or support given to IUPAC conferences. It administers General Assemblies and the associated elections, Bureau and Executive Committee meetings, edits Chemistry International, and facilitates the content of Pure and Applied Chemistry. It also manages the day-to-day business relationship with De Gruyter for publishing and distribution of the journals.

I undertook a review of our processes and systems early in 2014, including consideration of those we should handle ourselves and those we might better outsource. We had already outsourced publishing to De Gruyter and were learning how to manage that relationship and the fit with their processes and deadlines.

The process of change really accelerated with the appointment of Dr. Soby as our Executive Director in July 2014. The Secretariat payroll is now outsourced. We have reconstructed our financial accounting systems to make them compliant with General Accounting Practices and Principles (GAPP) and moved to Cost Accounting methods which will improve budgeting, financial management and enable handling and tracking with multiple currencies. Management financial information will be available to the officers in a more timely manner to help with decision making. Our investment portfolio is now actively managed by BB&T Scott & Stringfellow with the objective of improving returns.

A major source of frustration has been the structure of our databases, the accuracy of the stored information, and persistent difficulties with the link between the databases and the website. Many of you contributed to the web task group survey. One of the top five recommendations for a new website was improving the ease of uploading, updating, and editing content. There was also a recommendation that we move from the current platform, TYPO3, to one that is easier to use and for which support will be more readily available. We are on course to demonstrate new web capabilities at the upcoming General Assembly. At the same time, our databases are under review to improve accuracy and ease of access. Watch this space—we need to get it right this time. Our approach will be to outsource IT services rather than to employ a web manager, given the diversity of skills needed today.

Many of you will have responded to the survey on Chemistry International. We are seeking to better understand member needs in terms of content and delivery and the possible future for IUPAC.org as our web presence and communication channel.

All in all, as an officer, I can say that these are exciting times, but for the Secretariat it is really hard work that we should all recognize and appreciate. At least this work will be undertaken in more appropriate office surroundings.

Photos above, left to right: Executive Committee “time out” in the old conference room, packing up the files, end of the Road for No. 19, Linda and Enid on moving day, leaving our home for the last 17 years, and the wing of the new building. Below: The entrance to the new building.
An International Union of Pure and Applied Chemistry

by Jeffrey I. Seeman
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This essay brings together two of the fundamental products of IUPAC, namely its international symposia and its official journal, Pure and Applied Chemistry, as well as the consequential comradeship and documentation from such unions. Some of this sharing is illustrated in the Tetsuo Nozoe Autograph Books, including well-wishes and chemical pictography provided by meeting attendees and IUPAC officers.

1964 was an uplifting, transformative year in Japan. It was the year of the Summer Olympics, the opening of the super-high speed Tōkaidō Shinkansen train line and the Tokyo Monorail, and the end of the ban on overseas travel for Japanese citizens. To many Japanese, it was the beginning of the time of the Shinjinrui [1]. It was also the year of the Third IUPAC Symposium on the Chemistry of Natural Products, held in Kyoto in April.

Over 1500 scientists from around the world attended this chemistry symposium, one of the very first international chemistry symposia to be held in Japan. As described by one of the meeting organizers, Tetsuo Nozoe, who himself became one of Japanese chemistry’s most beloved senior figures,

The Symposium organized in Kyoto by Professor Munio Kotake and Kyoosuke Tsuda was a big event, which very much contributed to the development of Japanese organic chemistry. Many major chemists attended from all over the world and inspired young Japanese chemists; the meeting also made overseas participants appreciate the level of Japanese organic chemistry [2].

The International Symposia on the Chemistry of Natural Products (ISCNP), which continue to this day, were initiated by the International Union of Pure and Applied Chemistry in Sydney in 1960. The second symposium was held in Prague in 1962, and the third in Kyoto in 1964. The organizers for the 3rd ISCN prepared their work four years earlier, before even the 1st ISCN was held. Koji Nakanishi recalled that,

In preparation for the Kyoto symposium, I was sent [to the 1st and 2nd ISCN in Sydney and Prague] by the seniors to study how symposia are organized and to check the names of active chemists in this field in each country. Thus in 1960, while in Tokyo, I was sent by the Science Council of Japan to attend the Sydney meeting, my first travel abroad since I returned from the United States. On the plane on the way to a pre-symposium meeting in Alice Springs, I was seated next to a middle-aged person reading a novel, who I guessed might be a British Bank Clerk; another passenger in the small plane, I guessed, was a German farmer. The former was Derek Barton, and the latter, Hans Brockmann! . . . With whom ever I met, I asked for the names of the younger generation of natural products chemists so that they could be invited to the Kyoto meeting [3].
Table 1 lists the 11 plenary speakers at the Kyoto meeting, the titles of their papers, which appeared almost immediately after the symposium in the September 1964 issue of Pure and Applied Chemistry, along with the Chair of their session. All 11 papers are available open access on the IUPAC website [4]. From a historical perspective, the paper by Shigehiko Sugasawa [5] is a rich summary of Japanese natural product research up to the early 1960s.

The gathering of participants in Kyoto was prestigious. One measure, illustrative but not completely reflective, is that three of the plenary speakers and at least one other participant would become Nobelists: they are Robert Burns Woodward (Nobel Prize 1965), Derek H.R. Barton (1969), Vladiir Prelog (1975), and Donald Cram (1987). A listing of the discussion leaders is found on page 48 of Nakanishi’s autobiography [3]. Nakanishi reflected on the meeting’s success:

Because the Kyoto meeting was one of the very first international symposia to be held in Japan, great care was taken by the organizing committee with all details, and a huge budget was made available by generous donations from companies. We asked all foreign guests to mingle with the younger generation, including the graduate students. The discussions, conversation, and excursions with overseas participants were very stimulating for us. The simultaneous announcement of the tetrodotoxin structure by Hirata, Tsuda, Woodward and their coworkers was one of the highlights of the meeting. The various lectures given by visitors around the world gave us an opportunity to evaluate our level. There is a Japanese saying, ’Seeing once is better than hearing 100 times.’ The young Japanese chemists not only saw these distinguished foreign scientists but also discussed, ate, and drank with them. We also found that, although lagging, Japanese natural products chemistry was not that far behind. To see the gap narrowing gave us confidence, a factor that is very important for research, and I think the guests also went home with the same message. The

Dancing and singing at the Sakunami spa. Guy Ourisson is second from the left.

Table 1. Speakers, titles of papers as they appear in Pure and Applied Chemistry (open access) [4], and session chairs for the plenary lecturers at the 3rd ISCNP, Kyoto, 1964.
Taking IUPAC Literally

The majority of the Japanese natural product chemists agree this symposium was a turning point [3].

Tetuso Nozoe hosted one of the three post-symposia at the Sakunami spa outside of Sendai. The events included a special banquet in which everyone wore kimonos, sat on tatami mats, and enjoyed sake, singing, and other jovial activities. Several photographs of the event are shown which clearly testify that the Sakunami post-symposium event was a memorable experience!

Nozoe, himself, was an eminent chemist. He discovered and identified the first non-benzenoid aromatic compound, hinokitiol, in Taipei in the 1940s, simultaneous with related research by Holger Erdtman in Sweden and Michael J. S. Dewar in England. And for several decades, Nozoe and his co-workers investigated the chemistry of the tropolones, leading the research in the field that he had discovered [2, 6, 7]. The field of aromaticity was never the same [8].

The Nozoe Autograph Books

As word of non-benzenoid aromaticity spread, Nozoe began to receive invitations to lecture in Europe and the United States. Beginning in 1953 and continuing almost to his death in 1996, Nozoe carried an autograph book with him on his many trips to scientific meetings, as well as to chemistry departments and centers of industry around the world. The autograph books—ultimately nine in all, containing 1179 pages of autographs, chemical pictography [9, 10], well wishes, poetry and puzzles [11]—have now been published in their entirety in The Chemical Record [12]. These autograph books must be viewed as a primary historical resource, in that they document both the nature of international communication among chemists [13], as well as the chemistry of many of the signatories.

Nobelist Vladimir Prelog’s entry on 7 April 1964 in Sendai (on page 149 of the Nozoe Autograph Books) is the first autograph attributable to the IUPAC symposium discussed herein. Roger Adams’s entry on 28 April 1964 (page 159) appears to be the last entry from this symposium. Adams—the recipient of the US National Medal of Science, the Priestley Medal of the American Chemistry Society, and for whom the Roger Adams Award is named—was one of chemistry’s preeminent scientists in the 1930s and 1940s. In between Prelog and Adams can be found many notable signatories. Entries from five plenary lectures and two others are reproduced herein.
An unusual steroid (I) was recently synthesized at Tohoku University, when bombarded with electrons the molecular ion underwent an unusual fragmentation-comb-rearrangement including the unprecedented incorporation of a new element Z into the most abundant fragment ion. High resolution measurements established the trans-symmetry of the resulting species as well as its elemental composition: CaZ48.

4/23/64

Carl Djerassi

Many entries in the Nozoe Autograph Books are creative. Gunhild Aulin-Erdtman’s entry to the left is a touching summary of the event, including, perhaps, a pictograph of Tetsuo Nozoe himself with his glasses. Aulin-Erdtman’s entry captured the general mood of the meeting with the timeless happy face while ‘coming to Japan’ and sad face while ‘leaving again’. The phrase “Domo arigato” means “Thanks a lot” in Japanese.

Gunhild Aulin-Erdtman

Enfin, je penserai ce livre à Sendai, avec un groupe de vieux amis, et en compagnie du Professeur Nozoe. Avec mes remerciements pour votre invitation.

Guy Ourisson
Taking IUPAC Literally

Other IUPAC-related entries in the Nozoe book

Within the Nozoe Autograph Books are many entries having to do with IUPAC—not surprising, given that thousands of chemists participate in IUPAC activities as officers, organizers and participants [14, 15]. In 1953 and 1957, on Nozoe’s first two travels to Europe, Arthur Stoll, President of IUPAC from 1955-1959, signed the autograph books. The 1957 entry was recorded during the IUPAC Congress in Paris and is signed by Stoll as IUPAC President. Nozoe was a plenary lecturer at the 1957 IUPAC Congress [16].

Guy Ourisson—IUPAC Secretary General from 1975-1983—signed the Nozoe Autograph Books in 1964 while participating in the 3rd ISCNP in Kyoto (see above). Rudolf Morf, Secretary General of IUPAC from 1955 to 1971, made two entries in the Nozoe Autograph Books. The first, on 10 October 1966, marks the occasion when Tetsuo Nozoe visited Morf at his IUPAC office in Basle (below). According to Ted Becker, himself IUPAC Secretary General from 1996 to 2003, “Morf was the last Secretary General to handle all IUPAC ‘business’ himself before a full time Secretariat was set up at Oxford in 1968.” [17] The second entry by Rudolf Morf came 11 years later in September 1977 (page 582 in the Nozoe Autograph Books) and was recorded during the 26th IUPAC Congress in Tokyo. Morf noted the “First International Congress in the House of the Rising Sun” and commented on the “wonderful tea ceremony in the gardens” and the “sophisticated dishes and drinks.”

Georges Smets, IUPAC President in 1977-1979, also signed the book during the 26th IUPAC Congress in Tokyo in September 1977, with a very hearty cheer for IUPAC (below).

We could continue to fill this issue of Chemistry International with fascinating entries from chemists at various IUPAC meetings. Given the space limitations and the fact that the entire Nozoe Autograph collection is available online along with relevant essays and perspectives [12]—and free for at least three more years—we shall consider this article an appetizer rather than as a meal.

Now, to tie up some loose ends

The IUPAC Symposia on the Chemistry of Natural Products continues to this day. The 27th International Symposium on the Chemistry of Natural Products and the 7th...
An International Union of Pure and Applied Chemistry

International Conference on Biodiversity (ISCP-27 & ICOB-7), were jointly held in Brisbane, Australia, on 10-15 July 2011. The 24th, 25th, 26th, and 27th ISCP all featured biodiversity. IUPAC continues to champion international connectivity of people and the union of science. The ISCP-28/ICOB-8 was held in Shanghai 19-24 October 2014, and the ISCP-29/ICOB-9 will be held in Turkey in 2016. The progress of chemistry continues, marked by continuous reinvention [18, 19], as old challenges become textbook classics and new opportunities—or crises—arise.

Even the Nozoe Autograph Books continue, nearly 20 years after Nozoe’s passing! While it is true that the entire Nozoe Autograph Books collection has now been published in The Chemical Record [12], Brian P. Johnson, Managing Editor of TCR, and I are organizing a ‘new volume’ of autographs. Autographs will be collected at this summer’s International Symposium on Novel Aromatic Compounds (ISNA-16, in Madrid from 5-10 July 2015), and these will be collated, bound, and presented to Tohoku University, which houses the original nine volumes. All who wish can send in their autograph along with their favorite structures, poems, or chemical pictographs. Full details are found online in our recent essay titled “The Nozoe Autograph Books: “It Ain’t Over ’Til It’s Over” [20], or by following these directions:

1. Write on a white sheet of paper using black ink. You may optionally use your personal or organization’s letterhead. Importantly, please both sign and date the entry and also clearly print your name.
2. Send your inscription in one of the following ways: (a) Scan your inscription (≥300 dpi for best reproduction) and e-mail to ChemicalRecord@wiley-vch.de as a graphics file or PDF. Please include in the subject line of your e-mail: NOZOE INSCRIPTION. (b) You may mail your inscription to Brian P. Johnson, Wiley-VCH Verlag, Boschstr. 12, 69469 Weinheim, Germany. The deadline for receipt is June 30, 2015.

Conclusions

The sound of “IUPAC” easily rolls off the tongue as a three-syllable acronym that chemists around the world recognize. Happily, IUPAC succeeds beyond being “a scientific, international, non-governmental and objective body . . . serving[ing] to advance the worldwide aspects of the chemical sciences and to contribute to the application of chemistry in the service of Humankind.” [21] The stories told in this report, and countless more, reflect the special union between people and their passions fostered by this Union. IUPAC transcends national boundaries and temporary disciplinary distinctions, for the well-being of all. 😊

Acknowledgments

The author thanks Ted Becker, Brian P. Johnson, Fabienne Meyers, and Eva E. Wille for helpful discussions.

Dr. Seeman <seeman@richmond.edu> is a visiting senior research scholar at the University of Richmond. His professional activities include research in the history and sociology of science including responsible conduct of research.

References

by @beardedchemist

D. Brynn Hibbert
President of the IUPAC
Analytical Chemistry Division

It is ironic that an article about Twitter, the quintessential social medium, should appear in a glossy print magazine for the benefit of the reading public. One might almost “lol” [1]. But all organisations are coming to grips (with more or less facility), with Facebook, Twitter, Instagram and all the paraphernalia of Web 2.0 [2]. The great movement to ‘open science’ is changing the way we communicate what we do.

On the way to this new millennium, I happened to have the idea that the 140-character messages of Twitter could help me with lectures to my first year chemistry class at the University of New South Wales, in Sydney Australia. The group numbered about 600 and the lectures were given in the largest auditorium on campus. Even with my voice, a microphone was necessary, and it quickly became apparent that no one in my audience was going to put their hand up to ask or answer a question. Hence Twitter. With hashtag #chem1011 (and later #1031) a student could anonymously post a tweet that would appear on a screen (separate from the one I was using for my PowerPoint presentation of the lecture) [3]. The first year of this experiment was 2011, and following another round of use, with a student survey before and after the lectures, we published a short paper in the Journal of Chemical Education in April 2013 [4].

What happened in the first lecture? Nothing. After fifteen minutes there were no tweets at all. I asked the class if anyone could tweet anything, not being sure the system was working. Soon a tweet “When did you grow your beard?”. After that there was a steady, but manageable flow of questions and answers. I asked what was the latest element IUPAC had named (copernicium, element 112), and received the answer “Copernicus”. When I suggested this was nearly correct, as the element had indeed been named after the 16th century astronomer but conventions of naming elements required the -ium ending, a further tweet told me that the correct name was tweeted, but ‘the spell checker changed it’.

Having a stream of tweets to augment a lecture has several advantages beyond the immediate asking and answering of a short question. I encouraged the class to tweet their own answers to the questions before I gave the official word, which allowed some measure of communal learning, and gave me an idea of what they actually knew and understood. Tweets continued after a lecture, and provided a quick way of obtaining short facts. Finally, the novelty of an old, bearded professor using the new social medium was a most strange thing. (One tweet: “Omg, we get to use Twitter.”).

The majority (55%) of tweets were about lecture content, and 1/3 were extraneous (birthday greetings, chemistry jokes, but luckily no malicious or unconscionable material). Full information is in our paper [4]. A summary of the responses from the class after using Twitter is given in Table 1. Interestingly, at the start of the course in 2012, only 23% of the class had Twitter accounts. (Does Australia lag behind the rest of the world?) There was no statistical difference in the responses from existing users of

<table>
<thead>
<tr>
<th>Perceived Value to Twitter in Lectures</th>
<th>Prior</th>
<th>New</th>
<th>Non-User</th>
<th>All</th>
</tr>
</thead>
<tbody>
<tr>
<td>Percentage “Yes” Responses</td>
<td>n=54</td>
<td>n=41</td>
<td>n=144</td>
<td>N=239</td>
</tr>
<tr>
<td>In general, did you find the tweets useful to your learning?</td>
<td>78%</td>
<td>66%</td>
<td>72%</td>
<td>72%</td>
</tr>
<tr>
<td>Did the availability of Twitter make it easier to ask questions?</td>
<td>85%</td>
<td>69%</td>
<td>75%</td>
<td>77%</td>
</tr>
<tr>
<td>Did the availability of Twitter make it easier to answer questions?</td>
<td>73%</td>
<td>62%</td>
<td>67%</td>
<td>67%</td>
</tr>
<tr>
<td>Did the tweets intrude on the flow of lecture?</td>
<td>63%</td>
<td>74%</td>
<td>63%</td>
<td>66%</td>
</tr>
<tr>
<td>Did the tweets increase your engagement with the course?</td>
<td>59%</td>
<td>54%</td>
<td>53%</td>
<td>55%</td>
</tr>
<tr>
<td>Did the tweets make the lecture feel more personal for you?</td>
<td>57%</td>
<td>59%</td>
<td>57%</td>
<td>57%</td>
</tr>
<tr>
<td>Would you recommend that Twitter be used routinely in large lectures?</td>
<td>67%</td>
<td>74%</td>
<td>70%</td>
<td>70%</td>
</tr>
</tbody>
</table>
Twitter, new users, or non-users.

Responses were generally positive, although not entirely. Across all respondents, 72% saw Twitter as useful to learning. Among the 72% who rated tweets as useful, 60% of them also found that they were intrusive. Among the 28% who did not rate tweets as useful, 78% found them to be intrusive. Across other items, 70% recommended that Twitter be used routinely in lectures, 77% agreed that it was easier to ask questions, and 67% agreed that it was easier to answer questions. Smaller majorities agreed that tweets increased their engagement in the course (55%) or the personal feel of the lectures (57%).

How useful is social media in teaching, or for communicating the ideas of a learned society such as IUPAC? Many of our colleagues at the older end of the demographic cannot see the point, while those at the other end cannot see why not. Facebook has 1.23 billion monthly active users and there are 500 million tweets sent each day. Perhaps there might be some room for chemistry and IUPAC in there. It took just over one year to approve an IUPAC project “Increasing IUPAC’s Social Media presence” (2013-055-2-024, see this issue page 22), but hopefully the team has started their work early in 2015 and will report progress at the IUPAC General Assembly in Busan. Meanwhile if you see a tweet from @beardedchemist please take note!

Notes and References

1. lol: ‘laugh out loud’ in the shorthand used in such media.
2. Web 2.0: The second stage of development of the Internet, characterized especially by the change from static web pages to dynamic or user-generated content and the growth of social media.
3. hashtag: On social media sites, the hash, or number sign, is often used to classify content. Messages on twitter ‘tagged’ with #chem1011 could be recognized as relating to the lectures.
Drug Design and Development

Part II: Reflections from an Academic-based Center

by Paul Erhardt

As a follow-up to a previous issue of Chemistry International, which conveyed a feature article about the University of Toledo’s Center for Drug Design and Development (UT’s CD3) accompanied by a conference report on its special anniversary celebration [C/ 2014, Vol 36, No 6, p. 8 and 27, respectively], I am delighted to share a few insights that I have gained while serving as the CD3’s Director during the last 20 years. Intended for IUPAC readers and the medicinal chemistry community at large, my comments may be particularly useful for the numerous academic-based drug discovery centers bursting upon the scene of today’s pharmaceutical enterprise.

I will focus upon just three topics: people, people, and people. As I have emphasized repeatedly within the CD3’s newsletters, it is our active participants who constitute the true heart-beat of our academic-based, core resource center. And I submit that it is only the enthusiasm of these active participants that can make an R&D center successful over time, regardless of a given technology’s promising utility or a parent institution’s array of physical resources and prestigious reputation.

In this regard the CD3 is extremely fortunate to have been blessed with a long list of talented people who have always been committed to selflessly working together as a team to accomplish common goals in a collaborative manner.

My first ‘people comment’ is directed to a drug discovery center’s need for a range of highly interdisciplinary scientists. A critical mass of five or more individuals is key to establishing the core expertise required to seriously undertake drug discovery and development. The range of disciplines should encompass: molecular pharmacology/biology/bioinformatics; computational chemistry/molecular modeling/docking; synthetic medicinal/process chemistry; intellectual property (IP) management and patenting; analytical/bioanalytical chemistry with competency in devising validated Good Laboratory Practice (GLP)-compliant methods; pharmacology/pharmacokinetics/toxicology; and physical pharmacy/formulation.

While the need for this breadth of expertise quickly becomes apparent to anyone reading about the overall process of drug design and development [1-3], I would like to share two subtle additional insights that may be useful in allowing a cohesive team to flourish within the distinct environment of an academic setting. First, despite frequently outstanding individual qualifications, it is generally very difficult for faculty within U.S. institutions to serve as members of a team dedicated toward providing core resources for others. These same faculty are typically obliged to operate in a tenure system that places high priority on teaching and personal scholarly activity, while service duties are finally recognized at a distant third. Despite even the highest levels of willingness and sincere collegiality, it remains difficult for faculty to devote serious time toward advancing someone else’s technology when they are obliged to develop their own scholarly works and research activities. Thus, the cadre of experts needed for a drug discovery center is better assembled as non-traditional, non-teaching faculty, i.e. as ‘research faculty’, which typically means that these people will be on non-tenure track lines. Working along this type of strategy the CD3 was able to assemble a critical interdisciplinary mass by bringing in extramural dollars at an annual rate of $1M or more in direct funds for several years. This, in turn, supported more than 20 staff members and participating graduate students at its peak. Seemingly a remarkable success, this strategy has been repeatedly acknowledged quite favorably by UT’s administrators, who also become the beneficiaries of the very hefty indirect dollars that accompany such high levels of extramural research funding. But in an insider’s closer analysis, is this really such a success? Here’s the quandary which then constitutes the second, more subtle insight to conclude my first ‘people comment’: we were so busy during this funding heyday trying to accomplish the numerous milestones associated with the aims in our own CD3 grants, sponsored research agreements, and contracts, that we had very little time to help anyone else. While ‘successful’ within the context of our own lab, we could not even begin to fulfill the CD3’s broader mission to truly assist others. On the positive side we were able to serve as a source of equipment/instrumentation, offer a wide range of considerable expert consultation, and importantly to join collaborative grant submissions on behalf of others. However, actual preliminary data is often needed for grant submissions by those that need core assistance the most, and our free time to help generate this real data in any major, hands-on capacity was extremely limited. So what is the key insight I might offer to address this dilemma? Any administration assembling a drug discovery center as a core resource should be prepared to fund the salaries of several research staff whose paid mission is to serve the organization at large. Most U.S. institutions can already do this in some ways,
such as by aligning the IP/patenting component (generally staffed by non-tenure track positions within a university’s typical technology transfer office) as a collaborative operation with the center. The suggested new positions might be funded only in part—ideally at some level just above 50% so as to allow the incumbents to be fully entitled to the organization’s standard benefits packages, providing a strong base for longevity rather than continual turnover. The remainder of these salaries could then be funded by grant or contract applications to extramural sources that the research staff would be expected to submit in collaboration with regular faculty across the campus. The staff’s partial rather than fully funded base would thereby act as further incentive for establishing these highly desirable modes of collaborative initiatives. Having finally come to appreciate this specialized arrangement myself, I will admit that, although it is quite easy to convey as advice, in practice the CD3 is still striving to adopt such an ‘ideal’ arrangement—we rely on a very mixed version at this time. As will be indicated below, the Director is a full-time tenured faculty who can buy himself out of didactic teaching with extramural funds that are then used by his academic department to hire a visiting professor to cover the teaching gap. This, however, has been working exceptionally well in our case because it also affords the Director a formal academic advisor/mentoring relationship with a constant flow of truly inspiring graduate students. In line with the recommendation, the CD3 has formed a strong collaborative relationship with UT’s technology transfer office/staff that goes even beyond just IP strategies and patenting matters. This is synergistic in our case because the Director happens to be a U.S. Patent & Trademark Office (PTO) certified Patent Agent. The CD3’s synthetic medicinal chemistry staff and students likewise remain strongly supported, but in this case largely by several collaborative, extramural grants wherein the demand for this particular component appears to be highly needed by several ‘Project Teams.’ Alternatively, the bioanalytical core is only minimally funded in a similar manner, while the computational and biology cores remain struggling during these tough financial times to gain funding from any/all sources so as to just be able to sustain their presence within the CD3’s overall structure.

My second ‘people comment’ pertains to hiring the director for a newly forming drug discovery center. A regular faculty member is again unlikely to have the time and appropriate effort priorities to accommodate this service role. However, this may be less important if the director functions more as a scientific administrator and consultant than as a hands-on, lab-based practitioner trying to directly assist others’ technologies in a manner analogous to the center’s core technical staff. In my case I was hired as a tenured Full Professor, but I am also allowed to use extramural funding to ‘buy out’ my teaching load. This has worked very well for me personally and is the only way that I can do the homework needed to become even adequately informed about the wide variety of projects in our center’s portfolio. The director must advocate appropriate strategic options and offer the best advice to progress a given technology, while optimally deploying center and network resources in conjunction with addi-
Drug Design and Development

The technology becomes debatable (as is so very often between chemist and biologist. Even when the quality relationship (SAR) details gained in a collaborative manner upon the methodical elaboration of structure–activity relationship (SAR) details gained in a collaborative manner is recommended confirmation, by the way, of the hit’s supposed expertise needed at that point (after a highly recommended confirmation, by the way, of the hit’s supposed chemical structure) will be ‘hit follow-up’ testing based upon the methodical elaboration of structure–activity relationship (SAR) details gained in a collaborative manner between chemist and biologist. Even when the quality of such initial hits as adequate leads for progression of the technology becomes debatable (as is so very often the case), this still represents a good point to embark on intelligence-driven ‘directed library’ exploration (perhaps accompanied by earlier rather than later scaffold-hopping if there is indeed skepticism about the initial hit’s quality), rather than continuing in yet another excursion across large, structurally diverse libraries using ultra-HTS that relies upon a random search to address perceived shortcomings in the hit. Alternately, there appears to be considerable value in the special knowledge uniquely gleaned from industry experience associated with the practical development of a preclinical candidate compound. Still requiring considerable research but now in more of an applied mode, the drug development process is also governed by strict analytical procedures and standard compound comparisons at every step of the way, and in the U.S., a considerable amount of protocol-driven experiments mandated by the FDA, particularly with regard to drug safety. Thus, depending upon which end of the drug design and development spectrum a given center wants to emphasize, the nature of the credentials and background needed by the director can be somewhat different. Ideally for a comprehensive center, a director should have the complete gamut of rational (efficient) ligand design / hit follow-up credentials, plus actual drug development experience. He/she must also be willing to accommodate an academician’s pay scale after having come to fully appreciate the unique attributes that an academic environment has to offer within this overall enterprise.

My third and final ‘people comment’ is simple but is perhaps the most important: cherish the academic base and be prepared to nurture the students. On behalf of the latter, encourage collaborative arrangements with third parties able to recognize the students’ inherent potential, if not their immediately applicable technical attributes, and discourage arrangements that are exclusive of your center’s academic ties via strict contract specifications. In almost all cases, clear win/win scenarios can be devised for the benefit of both the student and the center’s collaborative partners. It is from the academic arrangement that an unending flow of bright and eager new participants will flow into the center. I have learned that whatever their level, these students can often be a tremendous source of creative ideas because of the questions they seemingly cannot help but ask, as well as always being a source of unending energy generally coupled to unbridled enthusiasm. The camaraderie that can be nourished among interdisciplinary scientists when coupled across generations, rich international cultural backgrounds, and widely differing levels of professional maturity can itself lead to distinct synergisms. These apply to accomplishing serious research and educational...
initiatives, and also for simply deriving some important fun while doing so.

The accompanying three pictures provide glimpses of some of our CD3 people across the last 10 years, the first two while ‘at work’ in the lab or out in the field, and the third while taking a break to share in some ‘fun.’ The first picture also attempts to capture the pride that the CD3 takes in its educational activities. Having stepped into one of our synthesis labs, I am surrounded in this picture by several students all of who have now gone on to become accomplished medicinal chemists. The second picture is one of our ‘Soybean Harvest Teams’ gearing up for a field trip to collect infected plants as a source for a unique family of phytoalexin natural product compounds that demonstrate high potential to treat breast and prostate cancers [4]. The last and most recent picture shows the CD3 staff and students gathered to celebrate the U.S. New Year (Chinese New Year and Diwali celebrations followed) while enjoying one of the CD3’s periodic ‘Friday lunch outings’ at a local restaurant. These three pictures serve as a perfect closing to my overall remarks and again emphasize the importance of a center’s “people, people and people.”

References
PMMA, from plexiglass window to a packaging for an implantable glucose sensor

by Elke Van De Walle

The unique versatility of polymers allows them to be manufactured into both commonly used household items and specialised medical devices. ‘Plastic’ windows and contact lenses form one such example, as both are manufactured from the same material, called poly(methyl methacrylate), or PMMA.

PMMA, a thermoplastic polymer often used as a substitute for glass, was discovered in 1877 and patented in 1933. Referred to as ‘acrylic glass’ or ‘plexiglass’, PMMA has one important feature in common with inorganic glass, namely its transparency. Nevertheless, from a chemical perspective each is a completely different material. Glass mainly consists of SiO₂, rendering it an inorganic material, while PMMA is an organic material built up of carbon, hydrogen and oxygen (see structure in Figure 1). PMMA is often preferred over glass because of its higher shatter resistance, ease in processing, and low cost and weight. Conversely, this plastic is less scratch-resistant and more flammable than glass [1]. Because of its advantages, plexiglass can be found in aquariums, caravans, and in the delineation of a children’s playground, but also in police shields, car lights, etc...

Medical discovery: lucky strike or pure observation?

The first major application of PMMA took place during World War II, when it was used for aircraft windows, submarine periscopes, gun turrets for airplanes, etc. It was during this time that the biocompatibility of PMMA was discovered by the English ophthalmologist Harold Ridley. Pilots often suffered from eye injuries caused by PMMA splinters coming from the windows of their airplanes. Dr. Ridley observed that, compared to glass splinters, almost no rejection occurred in these cases. As a consequence, in 1949, Dr Ridley implanted the first intra-ocular lens in an attempt to cure cataract. Meanwhile, plastic PMMA contact lenses began to replace their glass antecedents [2-4]. (see Figure 2).
Customising polymer properties based on future application—My research = a small piece of the future puzzle

Polymer implants should of course fulfill certain requirements determined by the implantation site in the body (subcutaneous, heart, knee, bone, etc.), its surrounding environment, and the physiological role that it has to play (skin graft, bone defect filler, heart valve replacement, etc.). Subcutaneous implants, for example, require soft and flexible material to assure patient comfort.

Known for its hard and strong nature, PMMA is frequently used for load-bearing functions. In the 1950s, for example, PMMA was mainly used for head prostheses. It is still frequently used as “glue” to fixate hip and knee replacements (see Figure 2). In dentures and biochips, too, its robust nature is desirable [5-7].

Recently, PMMA has been investigated as a potential packaging material for implantable medical devices, including glucose sensors. How to create such a polymer packaging? In order to ensure sufficient flexibility, the bulk properties of hard and brittle PMMA are adjusted by introducing long side chain oligomers in the basic structure of PMMA, creating copolymers with improved flexibility and softness. An implant interacts with the human body mainly through its surface; surface properties of the packaging material therefore play an important role and must be tailored accordingly. In the case of a glucose sensor, it would be advantageous to grow blood vessels in the vicinity of the implant, as glucose needs to reach the sensor. Since blood vessels are built up of endothelial cells, these are the ideal cell types to attract towards the sensor.

Figure 1. Chemical structure of PMMA. x denotes a repetition of its building units, called monomers.

Figure 2. Applications of PMMA in the medical world include bone cement (top left), an intra-ocular lens (bottom left), and a contact lens (bottom right).
Youth Views on Sustainability

Researchers have immobilised biological compounds on the packaging outer surface through various surface modification techniques in an attempt to improve sensor sensitivity towards glucose. Such research is presently followed within the Polymer Chemistry and Biomaterials (PBM) Group at Ghent University.

The next piece of the puzzle is how to manufacture such a polymer packaging? A film casting technique is one possibility often used in industry and academia due to its straightforward approach and concomitant results. As shown in the figure below, a monomer solution is injected between two glass plates and irradiated with UV-light. Through irradiation, the initiator (present in the solution) will be activated and form radicals (i.e. reactive species). These radicals will then trigger the initiation of different monomers in the solution and, as a result, polymer chains will start to form and grow (i.e. propagation). In the end, a solid material will be obtained. The shape of the material will be determined by the shape of the central cavity (in this case rectangular). This technique differs from other processing techniques, such as bioplotting or electrospinning, in the sense that the polymer production and moulding are combined in one step. In other techniques the polymer needs to be produced prior to processing.

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References

Figure 3. Film casting technique: the central hole in the silicone spacer (blue rectangle) will determine the shape of the plastic created.
Launch event for SDGs review held at UN in New York

The International Council for Science (ICSU), in partnership with the International Social Science Council (ISSC), organized an event during the second intergovernmental negotiations session on the Post-2015 Development Agenda at the United Nations in New York on 17-20 February 2015. At the event, ICSU launched the "Review of Targets for the Sustainable Development Goals: The Science Perspective" [1], an independent scientific review of the Sustainable Development Goals targets by over 40 scientists to assist in their consolidation and support their effective implementation and monitoring. The event brought together a wide range of stakeholders, government delegates and UN staff: about 70 people in all.

Several contributing scientists were present to illustrate the role of science in defining measurable targets and robust indicators to support the ambition of the SDGs. Lucilla Spini, Head of Science Programmes at ICSU, moderated the event. Anne-Sophie Stevance, lead coordinator of the ICSU review, introduced the report, its methodology, and key findings highlighting its importance as a tool for strengthening the targets. She also discussed the broader contributions that science can play in building a robust and evidence-based Post-2015 Agenda.

Claudia Ringler from the International Food Policy Research Institute reflected on the interconnected nature of the SDGs. In particular, SDG 2 on tackling hunger, food security, nutrition, and sustainable agriculture will require contributions from the other goals and targets during its implementation and monitoring. She also highlighted the importance of identifying and managing critical synergies and trade-offs across the SDG framework, especially with goals such as climate change or water and sanitation.

Berta Martín-López illustrated how social and natural systems interconnect from the local to the global scale and discussed the need for a multi-scale approach to successfully deliver the SDGs. This is particularly important for the preservation, restoration and promotion of sustainable use and management of terrestrial and fresh-water ecosystems at local, regional and global scales.

Susan Parnell, from the African Center for Cities and University of Cape Town, emphasised the importance of cities as a key implementation scale of sustainable development where innovations and transformative actions can be nurtured.

Finally, Michelle Scobie from the University of West Indies addressed a need to embed the SDGs in national policies, with a particular focus on Small Island Developing States. Governance and institutional arrangements will be key to translate global goals into locally-relevant priorities and action. This will require facilitating processes for better governance, including through the participation of non-state actors and through capacity building and knowledge-sharing.

Discussion from the floor raised a number of questions on the engagement of the scientific community with the definition of indicators for the SDGs, and in particular work undertaken on integrated indicators that could better the interconnected nature of the SDGs.

The report was covered in several scientific and news publications [2-5].

References
2. www.sciencemag.org/content/347/6223/702.full
4. http:/ /tmsnrt.rs/1zcJfAA
5. http:/ /wef.ch/1E7ip0b

African Leaders Endorse a Science Funding Platform for Africa: the Alliance for Accelerating Excellence in Science in Africa (AESA)

In a key development for scientific and health research in Africa, the African Union (AU) Heads of State and Government Summit in Addis Ababa, Ethiopia, endorsed the establishment of the Alliance for Accelerating Excellence in Science in Africa (AESA), a platform created by the African Academy of Sciences (AAS) and the NEPAD Agency. This pan-African platform offers an opportunity for the long-term development of research leadership, scientific excellence, and innovation that will have an impact on Africa’s developmental challenges. The AESA platform will, among other things, identify challenges that hinder rapid scientific advancement in Africa, run open calls for proposals with transparent review processes, actively manage grants, and evaluate and measure the impact of such investments. AESA will promote the collaborative and coordinated implementation of the African Union’s (AU) Science, Technology and Innovation Strategy for Africa (STISA 2024) in the area of health.

H.E. Dr. Martial De-Paul Ikounga, Commissioner of Human Resources, Science and Technology (HRST) at the AU, said, “We developed STISA as a multi-purpose policy advocacy strategy for mainstreaming innovation in the priority areas of the African Union of which health and wellbeing are part. Mobilization of domestic excellence and financial resources and leveraging external support are vital for the successful implementation of STISA 2024”.

H.E. Dr. Ibrahim Assane Mayaki, CEO of NEPAD Agency remarked that the NEPAD Agency is committed to work with African institutions in applying science, technology and innovation to address Africa’s health challenges and is pleased to draw upon the capacity that resides at the African Academy of Sciences to establish AESA.

African leaders at the 24th Summit meeting from 30-31 January 2015 also called upon Member States, regional and global partners, as well as private foundations to support the Alliance in order to strengthen health research and innovation in Africa. AESA has already received the recognition and financial support of three developmental partners, the Bill and Melinda Gates Foundation, the Wellcome Trust, and the UK’s Department for International Development (DFID). In a response to a call by the Summit, these three partners issued a statement saying, “We welcome the African Union’s recent call to establish the Alliance for Accelerating Excellence in Science in Africa (AESA), to be led by the African Academy of Sciences (AAS) in collaboration with the NEPAD Agency. The announcement marks a major step toward advancing global health and development across the continent. We are funding the development of AESA and share the vision of supporting the next generation of outstanding African researchers, who will help solve some of the continent’s greatest health and development challenges.”

When announcing AESA at a recent meeting of twenty African Academies, the AAS President Prof. Aderemi Kuku referred to this development by saying “this marks a new dawn for science development on the continent.”

A formal launch of AESA is planned during the next AU summit in June 2015 in South Africa.

www.aasciences.org

The EuCheMS Award for Service - Call for Nominations

The EuCheMS Award for Service acknowledges outstanding commitment with regard to fostering chemistry and molecular sciences in Europe and the goals of EuCheMS. In addition to recognized service to EuCheMS, this may include activities in governmental, non-governmental or funding organizations, publicity-related activities, etc. Nominations must demonstrate achievements for improved competitiveness, visibility, coherence or structure of chemistry in Europe.

All EuCheMS member organisations, Divisions/Working Parties and individuals are invited to submit nominations for the Award. Self-nominations are not accepted. Decisions on making the Award are taken by the EuCheMS Executive Board, normally annually.

The nomination must demonstrate service to EuCheMS and/or to European chemistry over and above the basic voluntary contribution that would normally be expected.
Submissions for nominations for the EuCheMS Service Award 2015 can be made until the 30 June 2015.
More details at www.euchems.eu/awards/award-for-service.html

In Memoriam: Anthony R. H. Goodwin

Dr. Anthony R. H. Goodwin (Tony) left us on 13 December 2014. We have lost a good friend and a very valuable colleague. We present our heartfelt condolences to his family.

Tony was extraordinarily active in our Union. He was an associate member of Commission I.2 (Thermodynamics) from 1996-2001, a member of the Physical and Biophysical Chemistry Division (Division I) Advisory subcommittee from 2002-2009, and an associate member from 2008-2011. In 2012 he became a titular member of Division I and Commission I.1 (Physicochemical Symbols, Terminology, and Units). He was also the Division I representative on the Interdivisional Committee on Terminology, Nomenclature and Symbols (ICTNS).

Tony's prominent presence in these different bodies sometimes overshadows the notable scientific work that he achieved within the numerous projects that he was involved in: 2007-039-1-024 (Extension of ThermoML—the IUPAC standard for thermodynamic data communications), 2007-059-1-100 (Heat capacities of liquids and vapours), 2007-024-2-100 (Guidelines for reporting of phase equilibrium measurements), 2008-014-1-100 (Experimental Thermodynamics Vol. VIII: Applied Thermodynamics of Fluids), 2011-037-2-100 (Recommended Reference Materials for Phase Equilibrium Studies), 2012-041-1-100 (Future Energy Revisited), 2012-051-1-100 (International standard for viscosity at temperatures up to 473K and pressures below 200 MPa, as chair), 2013-003-3-100 (Experimental Thermodynamics Volume IX B: Nonequilibrium Thermodynamics and Applications), 2014-010-1-100 (IUPAC Recommendations for the definition, preferred symbol for all transport properties), 2014-021-1-100 (The IUPAC Green Book—Preparation of the 4th revised printing of the 3rd edition).

We will forever admire Tony’s remarkable knowledge and understanding of thermodynamics, and also remember fondly the tenacious, but always friendly, discussions when he was defending what he believed in. Goodbye, Tony.

Roberto Marquardt and Jürgen Stohner, President Division I and Chair Commission I.1, in the name of Division I and Commission I.1

In Memoriam: Peter A.S. Smith

Peter Smith (1920-2014), from the Chemistry Department of the University of Michigan, was a member of the Commission on Nomenclature of Organic Chemistry (III.1) from 1979-1991. He was an Associate Member 1979-83, a Titular Member 1983-91, and chair 1987-91. As chair of the Class Names project, he was an author of “Glossary of class names of organic compounds and reactive intermediates based on structure. Recommendations 1995”, Pure Appl. Chem., 1995, 67:1307-1375. He served as the book review editor for the Journal of the American Chemical Society and published in two volumes of Open-Chain Organic Nitrogen Compounds (1965-6).

Outside chemistry, his passion was the stamps of Egypt, on which he published a definitive work. Only a few days before his death he attended a stamp show in New York, where he won a prize for his exhibit and received a letter of appreciation from the organisers.

http://um2017.org/faculty-history/faculty/peter-s-smith

Election of IUPAC Officers and Bureau Members: Call for Nominations

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

Project Place

Increasing IUPAC’s Social Media Presence

Facebook, LinkedIn, YouTube, and Twitter are woven into the lives of billions of people around the world. It is no surprise that some of those people are IUPAC members. IUPAC is at a critical point and must engage in the lives of current and potential future members via social media to build on existing and future opportunities. Active engagement with social media will help increase the presence of IUPAC via awareness of IUPAC’s mission and goals, as well as disseminating information on awards, news and scientific articles.

The idea for this project began as a Young Observer (YO) initiative in 2013 to increase communication between current and past YOs. The first step into social media was the creation of a simple YO page on LinkedIn where current YOs could connect and network: with IUPAC committee members and past YOs to discuss experiences and advice; and with other current YOs for meet ups, travel advice, and career discussions. If you are a recent or past YO and would like access to the LinkedIn group, please email Christine Straut at cmstraut@gmail.com.

This first step worked so well with that a few of the new YOs wanted to extend the social media reach of IUPAC beyond its current state. This subsequent project explores the many avenues of social media in order to identify the best and most productive routes to increase IUPAC’s social media presence and user engagement. Our approach in the creation of new social media accounts will allow more attention to be paid to each and will promote the positive reputation that IUPAC social media pages are accurate, reliable, and up-to-date. The project outcome will be a guideline for the maintenance of IUPAC’s social presence.

To date, this project has created and updated accounts on both LinkedIn and Facebook. Both pages are at or above 200 followers and include weekly updates on IUPAC news items, articles, and general information. The newest addition to the social media posts have been scientific articles. An increase in the number of interactions with current followers (in the form of comments and clicks) was seen for these scientific articles. Based on this initial data it was decided to add unique scientific articles from around the world to our weekly posts.

Our task group is continually trying to improve, so please send any comments, suggestions, or related news and scientific articles to the project Chair, Christine Straut at cmstraut@gmail.com.

www.iupac.org/project/2013-055-2-024

Glossary of Terms Used in Neurotoxicology

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

Comments by 31 May 2015

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www.iupac.org/project/2013-001-2-700
Nomenclature and graphic representations for chemically modified polymers (IUPAC Recommendations 2014)


A new source-based nomenclature system is described which indicates that a particular polymer has been chemically modified. A connective within the name of a polymer, -mod-, is introduced for this purpose as in poly[(A)-mod-(B)]. This system is intended to be used in accordance with source-based naming of polymers but also provides for the use of structure-based names when unavoidable. It embraces: (1) the modification of one constitutional unit into another, the unique structure of which is known; and (2) a more general modification of a constitutional unit resulting in any one of a number of possible structures. In addition, a new symbol, ->, is proposed for use in graphic representations of the structure of modified polymers.

http://dx.doi.org/10.1515/pac-2014-0610

Reference correlations for the viscosity and thermal conductivity of fluids over an extended range of conditions: hexane in the vapor, liquid, and supercritical regions (IUPAC Technical Report)


This report is focused on the development of wide-range reference correlations for the thermal conductivity and viscosity of fluids that incorporate as much theoretical knowledge of these properties as possible. The thermal conductivity and viscosity correlations developed here for pure fluids are functions of temperature and density. The best available equations of state for a given fluid are used to calculate the thermodynamic properties required for these correlations, often from measured temperatures and pressures. The correlation methodology developed during this project has been applied to hexane in this report but can be applied to any pure fluid with a reliable equation of state and reliable data for the thermal conductivity and viscosity over a significant range of temperatures and densities.

This article summarizes the correlation procedures developed for IUPAC project 2012-040-1-100 [Reference correlations for the thermal conductivity and viscosity of fluids over extended range of conditions (vapor, liquid and supercritical regions)].

http://dx.doi.org/10.1515/pac-2014-0104

Definitions of terms relating to individual macromolecules, macromolecular assemblies, polymer solutions, and amorphous bulk polymers (IUPAC Recommendations 2014)


This document defines terms relating to the properties of individual macromolecules, macromolecular assemblies, polymer solutions, and amorphous bulk polymers. In the section on polymer solutions and amorphous bulk polymers, general and thermodynamic terms, dilute solutions, phase behaviour, transport properties, scattering methods, and separation methods are considered. The recommendations are a revision and expansion of the IUPAC terminology published in 1989 dealing with individual macromolecules, macromolecular assemblies, and dilute polymer solutions. New terms covering the principal theoretical and experimental developments that have occurred over the intervening years have been introduced. Polyelectrolytes are not included.

http://dx.doi.org/10.1515/pac-2013-0201

Time-resolved fluorescence methods (IUPAC Technical Report)


This report describes and compares the currently applied methods for measuring and analyzing time-resolved fluorescence traces using phase-modulation fluorometry as well as pulse fluorometry (direct emission decay mea-
measurements, single-photon timing, streak camera measurements, fluorescence upconversion, and optical Kerr gating). The paper starts with a brief description of the basic principles for time and frequency domain fluorescence spectroscopy. The fundamental equations are given, and recommendations for adequate use are emphasized. The up-to-date, commonly-employed excitation sources and photodetectors are described in detail. The analysis of time-resolved fluorescence data is discussed. Attention is paid to possible artifacts and remedies are presented on how to avoid them or to account for them. Finally, fluorescence lifetime standards for the nanosecond and picosecond timescales are collected. This report was prepared in the framework of IUPAC project 2004-021-1-300.

http://dx.doi.org/10.1515/pac-2013-0912

Guidelines for checking performance and verifying accuracy of rotational rheometers: viscosity measurements in steady and oscillatory shear (IUPAC Technical Report)


This report addresses techniques for checking the performance of rotational rheometers with cone–plate, plate–plate, or concentric cylinder geometry. The authors focus on the determination of viscosity as a function of the shear rate and of the magnitude of the complex viscosity as a function of the angular frequency. After summarizing the relevant definitions and test modes, they show examples of measurements in the linear viscoelastic range and applications of the Cox–Merz relationship. Sources of reference fluids with defined viscosities are presented and their use in tests for verification of accuracy is demonstrated. Relevant issues, predominantly for Newtonian reference liquids, are the exploration of measurement limits related either to the shear rate range or to reliably accessible viscosity levels. Viscoelastic reference samples are also discussed. Prerequisites for sample preparation and loading are addressed. In particular, recommendations based on experience from various laboratories are presented. Finally, the problem of temperature calibration is discussed, presenting techniques that allow the determination of the true sample temperature for a given set temperature of the rheometer. This paper summarizes contributions from various industrial and academic laboratories and was prepared in the framework of IUPAC project 2007-004-1-400.

http://dx.doi.org/10.1515/pac-2013-0601

The NPU format for clinical laboratory science reports regarding properties, units, and symbols


The terminology of NPU (nomenclature for properties and units) aims at describing properties examined in clinical laboratories for a patient. It was originally jointly approved in 1966 by IUPAC and by the International Federation of Clinical Chemistry (IFCC) and covers multiple disciplines in the field of clinical laboratory sciences, including clinical allergology, clinical chemistry, clinical haematology, clinical immunology and blood banking, clinical microbiology, clinical pharmacology, molecular biology and genetics, reproduction and fertility, thrombosis and haemostasis, and toxicology. The NPU terminology adheres to international standards of metrology and of terminology, in particular the International System of Quantities (ISQ) and International System of Units (SI), the International Vocabulary of Metrology (VIM), and also to ‘An outline for a vocabulary of nominal properties and examinations – basic and general concepts and associated terms,’ recently prepared on behalf of the IFCC-IUPAC Committee-Subcommittee on Nomenclature for Properties and Units.

The present document recalls the definitions of the concepts used to express a property of a patient, regarded as a system. The aim is to promote by this comprehensive summary the proper NPU terminology for reliable exchange of patient examination data. The use of this syntax and of SI units enables the translation of these descriptions into other languages without loss of meaning or accuracy. The NPU format is also well adapted for comparative and epidemiological studies.

More information will be found in the upcoming 2nd edition of the Compendium of Terminology and Nomenclature of Properties in Clinical Laboratory Sciences, the IUPAC and IFCC ‘Silver Book’, and in the recently published ‘Properties and units in the clinical

http://dx.doi.org/10.1515/pac-2013-0920

**Spectroscopy of Water**

reviewed by Jonathan Tennyson and Attila G. Császár

Scientific questions demand scientific explanations. Our understanding of the greenhouse effect on earth and of the radiation balance on planets raises a number of complex scientific questions. These questions and the answers are often discussed in the public media as if the background knowledge was complete, while this is not the case. Most significantly, many of the questions lead to unexplored or at least underexplored territories of high-resolution molecular spectroscopy. In order to move beyond the state-of-the-art in our understanding of the greenhouse effect and the radiative balance of atmospheres of planets, the way the water molecule absorbs and emits light must be understood all the way from the microwave to the visible and ultraviolet regions. This important challenge led the IUPAC Physical and Biophysical Chemistry Division to sponsor the activities of two task groups: first, “A database of water transitions from experiment and theory,” (project 2004-035-1-100) and then, “Intensities and line shapes in high-resolution spectra of water isotopologues from experiment and theory,” (project 2011-022-2-100). The two task groups have recently completed their work and reported their results and recommendations [1,2], some of which are reviewed briefly below.

Water vapor is both the major absorber of incoming sunlight in a clear sky and also the dominant greenhouse gas in our atmosphere. As a result, a trace species, isotopically-substituted water, H$_2^{18}$O, is already the fifth biggest absorber of sunlight in the Earth’s atmosphere.

From the theoretical point of view, water is also an interesting molecule. It is a rather non-rigid system meaning that its vibrational modes can absorb light and be excited by multiple quanta. It is also a light, asymmetric rotor which means that the vibrational bands have a very open structure. The result of this is that strong absorption by water bands is found throughout the infrared and, increasingly weakly, throughout the visible region of the electromagnetic spectrum. Indeed, recent atmospheric studies are focusing on vibration-rotation absorption in the near-ultraviolet which means transitions involving the jumps of 8 or 9 vibrational quanta.

The first task group used a methodology co-developed by the two co-authors to create an information system of refined empirical rotation-vibration energy levels, and hence transition frequencies, for altogether nine water isotopologues. The MARVEL (measured active rotation-vibration energy levels) procedure for doing this was refined significantly during the course of the IUPAC-sponsored research efforts. The resulting MARVEL procedure is both robust and computationally efficient; it is now being applied to a number of other molecules of scientific and practical interest.

The energy levels and the comprehensive sets of transition frequencies generated by the TG for the water isotopologues are being used for a variety of applications. For example, a complete set of lines has been generated for H$_2^{18}$O and H$_2^{17}$O by combining MARVEL-based transition frequencies with transition probabilities computed using high-accuracy, first-principles quantum chemistry. These results are incorporated in the latest edition of the canonical HITRAN database, which is extensively used for atmospheric modeling. The energy levels are also being used to update the so-called steam tables, which tabulate the temperature-dependent thermochemical properties of water.

The second task group was formed to answer the question of how to represent the precise shape of a spectroscopic line observed under high resolution, a property which depends considerably on the environment in which the system is being observed. The so-called Voigt profile, a convolution of the Doppler profile, to represent thermal motions, and a Lorentzian, to model collisional effects, has been widely used. But the Voigt profile is known to be inadequate for precise modeling work, leading, for example, to W-shaped systematic residues in atmospheric water spectra. Going beyond the Voigt profile requires the inclusion of a variety of rather subtle collisional effects. Consideration of these effects has led to the proposal of a whole zoo of different possible models and functional forms to represent the line shape. It was clear that databases and modelers require a clear recommendation of a single beyond-Voigt line profile. The TG-recommended profile, which we named the Hartmann-Tran Profile (HTP), has the advantage that it captures the complex physics involved in collisional line-broadening with a functional form that can easily, and rapidly, be evaluated. Furthermore, the HTP profile reduces to other, simpler profiles including Voigt in the absence of a full parameter set.
The HTP profile is suitable for modeling the line profiles of a range of molecules and is beginning to be used for this purpose. It is expected that the HTP profile will also be useful for a number of other molecules and chemical environments.

References


The Chemistry of Vision

The postal authorities of several countries, including Israel, Italy, the Vatican, Bosnia and Herzegovina, Liechtenstein, and Moldova, have recently issued postage stamps to commemorate the International Year of Light and Light-based Technologies (IYL 2015). The colorful stamp released by Israel Post on 27 January, the centerpiece of this note, is not only chock full of symbolism but has particularly strong connections to chemistry.

The top right portion of the stamp features the molecular structure of rhodopsin, a light-sensitive receptor protein that consists of a bundle of seven transmembrane alpha-helices connected by peptide links and a central pocket that binds the chromophore retinal (shown in gray), the photoisomerization of which triggers the process of vision. An open eye, the visible spectrum with the colors of the rainbow, and Schrödinger’s equation – every chemist’s introduction to quantum mechanics – appear on the stamp to the left of the rhodopsin molecule. The bottom portion of the stamp displays the IYL 2015 logo and a schematic representation of the two common photoreceptor cells found in the retina: rods (shown in yellow), which enable vision under low-light conditions, and cones (shown in blue, green, and red), which allow color vision.

Significantly, the stamp also honors Martin Karplus (Harvard University and Université de Strasbourg), Michael Levitt (Stanford University), and Arieh Warshel (University of Southern California), the recipients of the 2013 Nobel Prize in Chemistry “for the development of multiscale models for complex chemical systems”. These pioneers of computational biology devised ingenious methods that combined quantum and classical mechanics and allowed the study of a variety of inherently complex processes, including enzymatic and electron transfer reactions, ion transport, and the chemistry of vision. Interestingly, the three scientists closely interacted at various times of their careers and conducted critical aspects of their research at the Weizmann Institute of Technology in Israel. (For biographical sketches of the 2013 Chemistry Nobel laureates, see: J.-M. André, Chem. Int. 2014, 36(2), 2-7).

Written by Daniel Rabinovich <drabinov@uncc.edu>
In this monograph the reader will find 22 contributions dealing with volume properties and related thermodynamic properties of liquid systems and gases/vapours, both pure and mixed. The topics are approached from different angles, representing the varying research background of the respective authors. This book has its origin in committee meetings of the International Association of Chemical Thermodynamics (IACT), an associate organization of IUPAC. The IACT developed from the IUPAC Commission on Thermodynamics and has continued to play an active role in the definition and maintenance of standards in all aspects of thermodynamics, in the development of the subject, and in the encouragement of young scientist to take up research careers in chemical thermodynamics (further information can be found at www.IACTweb.org).


In true IUPAC spirit, the authors represent some of the most important names in their respective fields and come from many countries around the world, including Australia, Austria, Canada, Belarus, Czech Republic, France, Germany, Israel, Japan, Poland, Russia, South Africa, Spain, United Kingdom and the United States of America.

One of the objectives of the book is to bring together research from disparate disciplines which have a bearing on volume properties of fluids. Cross-links between these chapters, we believe, will lead to new ways of looking at volume property-related issues, and thus to new ways of solving associated problems in physics, chemistry and engineering. Underlying this philosophy is our inherent belief that a book is still an important vehicle for the dissemination of knowledge.

Two features are of paramount importance in monographs like this one: the timeliness of the topic and the coverage and critical evaluation of the pertinent publications. Important features of this book include the underlying theory; some of the most important experimental techniques, modelling and computer simulation; as well as significant and new results related to volume properties. The authors have endeavoured to cover the relevant literature up to 2013. This book is meant for researchers in chemical thermodynamics, either from academia or from chemical industry, and provides an overview of the progress recently achieved. Its success ultimately rests with the 32 authors and we, the editors, would like to thank them all for their cooperation and for their enthusiastic contributions, which are highly valued. We would also like to thank Professor Ron Weir who, on behalf of the IUPAC Interdivisional Committee on Terminology, Nomenclature and Symbols (ICTNS), checked each chapter for the correct usage of thermodynamic quantities, units and symbols, always exercising the liberal spirit invoked in the Green Book of IUPAC.
Macromolecular Symposia

Recent Volumes of *Macromolecular Symposia* include contributions from recent IUPAC-sponsored conferences.

See MS online at http://onlinelibrary.wiley.com/journal/10.1002/(ISSN)1521-3900

Polymer-Solvent Complexes and Intercalates POLYSOLVAT–9 Part I & Part II


The international conference on Polymer-Solvent Complexes and Intercalates (POLYSOLVAT-9) took place from 11-14 September 2012 at the Taras Shevchenko National University of Kiev. The meeting was jointly organized by the Faculty of Chemistry and the Faculty of Physics of the university.

Since the first conference held in 1996, this one-of-a-kind series of conferences has been sponsored by IUPAC. In 2012, formation mechanisms, morphology, molecular structure, and the properties of compounds involving solvents and/or synthetic polymers, biopolymers, proteins, supramolecular polymers, and systems formed at surfaces/interfaces were discussed. The 21 papers selected for the *Macromolecular Symposia* volumes provide an overview of the topics discussed during this conference.

http://dx.doi.org/10.1002/masy.201470001
http://dx.doi.org/10.1002/masy.201470005

Polymers and Materials


The 12th Annual UNESCO/IUPAC Workshop and Conference on Macromolecules & Materials which took place 2013 in Stellenbosch, South Africa, focused on the synthesis, advanced characterization and properties of biopolymers, polyolefins, medical applications of polymers and novel materials. Abridged versions of a number of important papers are compiled to create the present volume of *Macromolecular Symposia*.  
http://dx.doi.org/10.1002/masy.201470008

Polymer Spectroscopy


The 19th European Symposium on Polymer Spectroscopy (ESOPS19), organized simultaneously as the 77th Prague Meeting on Macromolecules (PMM), took place in Prague on 7-11 July 2013. The symposium was organized by the Institute of Macromolecular Chemistry, Academy of Sciences of the Czech Republic as an IUPAC-sponsored meeting. Both the ESOPS and PMM series have more than 40 years of tradition behind them. The aim of the ESOPS meetings is to bring together scientists specializing in different spectroscopic techniques to review the latest research, as well as developments in the spectroscopic characterization of polymer systems. 100 active participants from 23 countries took part in ESOPS19.

The scientific program consisted of 9 invited lectures, 28 oral communications, and 60 poster presentations. The symposium highlighted all fields of spectroscopy (infrared, Raman, UV-vis, fluorescence, NMR, EPR, mass, X-ray, dielectric and mechanical spectroscopy), from theoretical and fundamental aspects to recent advances and novel developments in the characterization and analysis of polymers. The invited lectures, each presented by outstanding specialists in the given field, along with oral communications, offered participants a survey of the most up-to-date problems and well-founded new findings and views. Many interesting results were presented in two poster sessions.

The full texts of selected, peer-reviewed contributions are published herein and provide an overview of the topics discussed during the meeting.

http://dx.doi.org/10.1002/masy.201470016
Molecular Order and Mobility in Polymer Systems

*Macromolecular Symposia* Vol 348, February 2015, edited by Tatiana Birshtein

The 8th International Symposium “Molecular Order and Mobility in Polymer Systems” (MOMPS-14) was held in Saint-Petersburg, Russia, 2–6 June 2014. This was a continuation of the series of St. Petersburg Symposia titled, in alternating meetings, “Molecular Mobility and Order in Polymer Systems (I - 1994, III - 1999, V - 2005, VII - 2011), and “Molecular Order and Mobility in Polymer Systems” (II - 1996, IV - 2002, VI - 2008).

The main organizer of the Symposium was again the Institute of Macromolecular Compounds of the Russian Academy of Sciences (RAS), with the Department of Chemistry and Material Science of RAS as co-organizer. This time the St. Petersburg National Research University of Information Technologies, Mechanics and Optics also performed as co-organizer of the Symposium. The Symposium was supported and sponsored by IUPAC, the Russian Foundation for Basic Research (RFBR), Saint-Petersburg Research Center of RAS, and L’Oreal.

The scope of the Symposium was highly relevant to both fundamental science and technological applications. The plenary lectures were given by outstanding scientists from different countries actively working in this domain of polymer science and making major contribution to its development. The subjects of plenary lectures and the Symposium as a whole characterized the fundamental trends in contemporary physics and chemistry of polymers, showing that the interest of investigators has moved from polymer structure and properties in solutions to the structure and properties of polymer materials. Considerable progress made in investigations of the structure and properties of polymer materials, polymer nanocomposites, polymer membranes is connected with the development of multiscale modeling methods using the power of modern supercomputers. This multiscale approach combines classical simulation techniques with quantum-mechanical ones and uses a hierarchy of molecular and coarse-grained models. Polymer networks (gels) represent another class of actively studied polymer systems. Previous success in investigating and analyzing complex macromolecules with different interactions in solutions has stimulated the creation and study of polymer networks with unique properties. Polymer nanostructures in solutions remain a focus of modern polymer science.

This issue contains only seven papers, but it provides a good picture of the Symposium topics. The content reflects the progress of researchers’ interests towards more complicated systems with nanoscale organization.

http://dx.doi.org/10.1002/masy.201570005
Human Errors and Quality of Chemical Analytical Results

by Ilya Kuselman

An International Workshop on Human Errors and Quality of Chemical Analytical Results was held 13 January 2015, in Kfar Maccabiah, Israel, as a milestone of IUPAC project 2014-027-1-500. An earlier workshop on human error was held in Israel in 2013 to discuss experiences classifying and modeling human error accumulated in aviation, medicine and other fields, which could be helpful in analytical chemistry, as well [1]. The idea of the current workshop arose from the quality management system approach. Applied for routine chemical analytical (testing) laboratories, this approach provides continual improvement of a laboratory quality system. One of the improvement targets is the prevention of human error. However, human activity is never free from error: they are the root cause of the majority of incidents and accidents. In analytical chemistry, human error may lead to atypical test results of questionable reliability [2]. There are, for example, test results that fall outside the established specifications in the pharmaceutical industry, or that do not comply with regulatory, legislative or specification limits in other industries and fields, such as environmental and food analysis. When an atypical test result is identified, it is important to determine the root cause of the event and to avoid recurrence of such results. Where no limits have yet been established (e.g., for an environmental object or a new material), human error may lead to an incorrect evaluation of the tested property. Thus, a study of human error is necessary in any field of analytical chemistry. A laboratory demonstrating competence in analytical chemistry and conformity assessment should also be able to develop relevant, human error-related corrective and preventive actions [3].

The workshop was organized by the Israel Analytical Chemistry Society (IACS) with the participation of the Israel Laboratory Accreditation Authority (ISRAC), in cooperation with the International Union of Pure and Applied Chemistry (IUPAC), Cooperation on International Traceability in Analytical Chemistry (CITAC), and A Focus for Analytical Chemistry in Europe (Eurachem). The event was sponsored by Sigma-Aldrich Corporation and arranged by Bioforum Ltd.

Opening remarks were given by Dr. Ilya Kuselman, Modiin, Israel, Chair of the Workshop Organizing Committee, and Prof. Wolfhard Wegscheider, the University of Leoben, Austria, Chair of Eurachem. Prof. Wegscheider then delivered the keynote lecture “The measurement cycle: principles of quality of analytical results and decisions which can be made on their base”. The lecture described a logically structured approach consisting of a closer examination of the customers’ needs by mapping them onto the performance characteristics of the anticipated analytical procedure. This approach may be regarded as a “measurement cycle” if it is followed up to the actual usage of measurement results in the decision process of the customer. More reliable decisions are reached by reducing the size of the guard band around a specification limit where no decisions can realistically be made, i.e. reducing the measurement uncertainty. An optimization of the analytical procedure may be necessary, even resorting to an alternative measurement principle based on the quality-by-design methodology.

Another keynote lecture “Metrology and quality of test results: documents of the Joint Committee for Guides in Metrology (JCGM)” was delivered by Dr. Walter Bich, Istituto Nazionale di Ricerca Metrologica (INRIM), Italy. Dr. Bich discussed the publications of JCGM, in particular the guides for measurement uncertainty evaluation. The scope of the new revision of the guide to the expression of uncertainty in measurement (JCGM 100) and a separate collection of examples (JCGM 110) attracted the attention of the workshop participants. It was important to hear that methods for the evaluation of measurement uncertainty will be agreed upon and adopted world-wide. This implies that the methods will be universal, in the sense that they can be useful in any application, including analytical chemistry.

Dr. Raphael Bar, BR Consulting, Israel, provoked a discussion by his lecture “Should the pharmaceutical laboratory report test results with uncertainty?” Dr. Bar said that the current regulatory requirement in a pharmaceutical laboratory is only the validation of analytical methods. Yet, a typical certificate of analysis of a drug substance or product shows no uncertainty of the test results. The new USP-suggested approach for validating analytical methods will discuss measurement uncertainty evaluation in the validation process.

Dr. Kuselman’s lecture reported on the progress of IUPAC projects 2012-021-1-500 and 2014-027-1-500, as well as quantification of human error in an analytical laboratory based on expert judgments. Examples were provided using earlier published sets of expert judgments on human error in pH measurement of groundwater [3], multi-residue analysis of pesticides in fruits and vegetables [4], and elemental analysis of geological samples by inductively coupled plasma mass spectrometry [5]. Evaluation of the residual risk of human error remaining after the error reduction by the laboratory quality system and the risk influence on the quality of the analytical
results and associated measurement uncertainty were discussed [6].

Monte Carlo simulation of expert behaviour in quantification of human error was the subject of the lecture by Dr. Francesca Pennecchi, INRIM, Italy. Any expert is a human being whose judgments are influenced by interpersonal conflicts and other factors. Therefore, an evaluation of the robustness of the error quantification scores to the doubts of an expert is required. To that aim, a Monte Carlo simulation of expert judgments on human error was used for determining the distributions of the error quantification scores. An expert judgment, represented by a choice on the scale (0, 1, 3, 9), is a discrete quantity characterized by a probability mass function (pmf). Appropriate pmfs were considered in order to model confident, reasonably doubting, or irresolute expert behavior, respectively. An R code was developed for the random generation of expert judgments as discrete values and the propagation of the considered pmfs according to the Monte Carlo approach [5].

After these lectures Dr. Michela Sega, INRIM, Italy, moderated the round-table discussion “Can human error be taken into account as a component of measurement uncertainty?” First, she proposed that the participants ask questions to the lecturers. The question posed to Dr. Bich was “how can one explain the difference between Type A and Type B evaluations of measurement uncertainty, as well as the benefit of this classification?” The problem is that Type A evaluation is defined as the method of evaluation by statistical analysis. However, Type B evaluation is also based on rectangular, triangular or another distribution of observations, in spite of the definition in JCGM 100 and JCGM 200 as evaluation by means other than statistical analysis. Dr. Bich explained the historical reasons for that problem, and noted that such a classification of methods for uncertainty evaluation will not be used in the new JCGM 100 issue under development. Dr. Kuselman briefly presented the position of the task group of the IUPAC projects on the possibility of taking human error into account as a component of measurement uncertainty. While gross errors are easily identifiable and corresponding results can be separated from the data set, small human errors are in principle not distinguishable from other components of measurement uncertainty. Therefore, an uncertainty budget is not complete when consequences of possible human error are not evaluated as a contribution to the budget. Quantifying residual risks of human error allows such evaluations to be made.

The second half of the workshop day began with the lecture by Dr. Kuselman “Knowledge is Power (Francis Bacon 1597): comparability concept and global metrology system”. The lecture was dedicated to knowledge-based mistakes, which are more frequent than other kinds of human error and have significant severity in different scenarios. On the other hand, these mistakes are

A group of the lecturers. From left to right: Prof. Wolfhard Wegscheider, Dr. Walter Bich, Dr. Ilya Kuselman, Dr. Michela Sega, and Dr. Francesca Pennecchi.
the simplest to prevent. The lecturer directed the attention of the participants to the global metrology system and publications in this system containing knowledge important for chemical analytical laboratories. There are guidelines, recommendations and documents of the International Bureau of Weights and Measures (BIPM), the International Organization of Legal Metrology (OIML), the International Organization for Standardization (ISO), the International Laboratory Accreditation Cooperation (ILAC), the National Conference of Standard Laboratories – International (NCSLI), IUPAC, CITAC, Eurachem and others.

Ms. Erica Pinco, ISRAC, Israel, reported on the improvement of error management in accredited medical laboratories in the country. The identification and control of nonconformities of test results are a part of the quality management system, based on ISO 15189. Those results that are not in line with specifications may indicate a medical condition, when in fact they result from human error. When the management identifies that the irregularities of the results are due to human error, a set of activities including corrective actions should be taken in order to reduce the error probability.

Dr. Shula Levin, Waters (TC) Ltd, Israel, impressed the workshop participants with the lecture “Distinguishing between human error and instrumental malfunction in HPLC”. HPLC instrumentation and software have advanced significantly in recent years and have become technologically sophisticated. Therefore, the task of distinguishing between human error and system malfunction has become more and more challenging, and requires collaboration between service engineers and analytical chemists. Dr. Levin presented examples of investigations during which there were real instrument malfunction vs. human error; recommendations for minimal details of the HPLC method which must be specified in a standard operation procedure; and some useful Chromatographic Data Systems’ modules and reference chemical kits, which can reduce human error.

“Can human error be reduced in a pharmaceutical laboratory?” asked Dr. Orna Dreazen of Nextar Chempharma Solutions Ltd, Israel, in her lecture. Human error, said Dr. Dreazen, is the main source of unnecessary activities in a laboratory, wasting energy and resources. In the worst case, human error may cause an adverse effect and the recall of pharmaceutical products. GMP, GLP and ISO 13485 contain requirements designed to reduce human error. The lecturer analyzed examples from a pharmaceutical laboratory and discussed corrective and preventive actions for error reduction.

Finally, a round-table discussion “Is a laboratory quality assurance system effective against human errors?” moderated by Prof. Emil Bashkansky, ORT Braude College, Israel, again allowed participants to receive answers to their questions to the lecturers. Dr. Kuselman presented the scores for evaluation of the quality system effectiveness developed by the task group of the IUPAC projects. Prof. Bashkansky reported about his matrix approach to human error problems in engineering. The opinions on the effectiveness of a laboratory quality system against human error were diverse, but the majority of the participants agreed with the optimistic position of the IUPAC project task group.

It was a very fruitful, interesting, and pleasurable meeting. Some participants expressed their wish to continue the traditional biannual workshop, and supported further development of the topic of human error and quality in an analytical chemical laboratory.

The next two days, 14-15 January, the workshop lecturers and participants took part in the Isranalytica 2015 Conference and Exhibition. A summary of these events is available at http://bioforumconf.com/isonanalytica15.

References

Dr. Ilya Kuselman <ilya.kuselman@gmail.com> worked at the National Physical Laboratory of Israel and is a member of the IUPAC Interdivisional Working Party on Harmonization of Quality Assurance.

www.iupac.org/project/2014-027-1-500
Macromolecules & Materials
7-10 September 2015, Port Elizabeth, South Africa

On behalf of the organizing committee of Conference 2015, it is my great pleasure to invite you to participate in the 13th Annual UNESCO/IUPAC Workshop & Conference on Macromolecules & Materials to be held in Port Elizabeth, South Africa in September 2015. The workshop will be held 7 September 2015 and 8-10 September 2015 at The Boardwalk International Convention Centre (ICC).

This event is a continuation of a very successful series of conferences that were held over the last ten years, mainly in South Africa. It is a unique opportunity for (mainly) Southern African researchers and students to present and discuss their research in polymer science. Over the years the conferences has had specific themes, ranging from polyolefins over composites to materials with biological and medical applications. In 2015, the focus of the conference will be on biologically active polymer systems and polymer characterization.

The following topics will be covered:

- Biologically active polymer systems (synthesis, properties and application)
- Polymer characterization (special focus on characterization of biopolymers, biologically active polymers and systems)
- Directed session on polyolefin research
- Directed session on rubber technology, chemistry, recycling and devulcanization
- General topics

Port Elizabeth, located in the Eastern Cape of South Africa, is the fourth largest city in South Africa and has a modern airport situated fifteen minutes from the Boardwalk International Convention Centre. The famous Addo Elephant National Park is just over an hour’s drive from Port Elizabeth. Come enjoy the wildlife of South Africa, some top lectures on polymer science, and the South African way of life. We look forward to welcoming you to Port Elizabeth in September of 2015!

For more information, contact Albert van Reenen, Chair of the organizing committee, Stellenbosch University or the Conference Secretary: Aneli Fourie <aef2@sun.ac.za>

http://academic.sun.ac.za/unesco/

CHEMRAWN XX – Herbal Medicine for Health Care in the 21st Century
6-9 November 2015, Dhaka, Bangladesh

The 20th IUPAC Conference on Chemical Research Applied to World Needs will be held in Dhaka, Bangladesh in early November 2015 and will focus on herbal medicine.

The main objective of the conference is to provide a global perspective on the future development of the many chemical, biological, botanical, and legal facets of herbal (traditional) medicine as they relate to the accessibility of a safe, efficacious and consistent supply of herbal medicines for the improvement of healthcare globally. Analytical and natural product chemistry, including metabolomics, will be significantly represented, along with chemical and biological information system development, new technologies, efficacy-focused clinical trials, agroeconomics and sustainable development, intellectual property rights and patents, production, marketing, and synergistic integration with evolving government regulations.

Researchers from relevant disciplines; herbal product manufacturers from abroad and Bangladesh; herbal practitioners from several regional countries; government regulators from Europe, Bangladesh, India, USA, China, and Australia; a representative from the World Intellectual Property Organization (WIPO); a representative from the World Health organization (WHO) Office for Traditional Medicine; pharmaceutical manufacturers who also produce herbal medicine products; scientists (chemists, botanists, biologists, and clinicians) involved with quality control of herbal medicines; and herbal medical academicians are expected to attend the meeting.

Participants interested to present their original works are invited to submit abstracts by 31 July 2015.

See website for more details or contact <chemrawnxx@buhs-edu.org> www.chemrawnxx.net.bd
Research in Chemical Education
22-27 November 2015, University of Venda, Thohoyandou, South Africa

ACRICE 2, the 2nd African Conference on Research in Chemical Education, will be held at the University of Venda in Thohoyandou, South Africa, 22-27 November 2015. The conference, under the auspices of FASC, the Federation of African Societies of Chemistry, wishes to emphasise the role of chemical education for development and, in particular, for sustainable development in Africa, by offering an ideal opportunity for sharing experiences among specialists across the African continent and with specialists from other continents. All areas and levels of chemical education will be considered, with known major challenges given specific attention. Explorations of novel approaches and of novel collaborations will be actively encouraged. The main themes will include:

- Chemical education at the primary, secondary, and university level
- Communicating across the educational levels
- Communication and language in chemical education
- Context-oriented chemistry
- Green chemistry education and the requirements of sustainable development
- Microscale chemistry
- Responsible research and innovation
- Teacher training

A couple of round tables will also be organized on chemical education at the post-graduate level (mentoring as a chemical education endeavour) and on globalisation and attention to local characteristics in chemical education.

The University of Venda (UNIVEN) is located in an area rich in natural beauties and cultural heritage, offering excellent opportunities for combining an exciting high-quality scientific experience with a delightful immersion in the warmth of Africa. The Conference Chair, Liliana Mammino, is eager to welcome you in Thohoyandou.

For more information, email <acrice2015.mail@gmail.com>

https://sites.google.com/site/acrice2015

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Program at a Glance:

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See also www.iupac.org/home/conferences.html for links to specific event websites

2015 (After May 1)

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

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

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

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

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

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

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

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

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

12-16 July 2015 • Organic Chemistry • Lisbon, Portugal
ESOCXIX - The 19th European Symposium of Organic Chemistry
Dr. Nuno M. Xavier (Scientific Secretary) nmxavier@fc.ul.pt, SPQ - Sociedade Portuguesa de Química, Av. da República, 45, P-1050 - 187 Lisboa, Portugal, E-mail: eventos@spq.pt, http://esocxix.eventos.chemistry.pt

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

30 August–1 September 2015 • CONvINCE • Como, Italy
2nd ICSU/IUPAC Workshop on Crystal Engineering - “CONcepts and terminology in Crystal Engineering”
Scientific Secretariat: Johanna Syvanen, Telephone: +390223993049, E-mail: Johanna.syvanen@polimi.it
http://conviceproject.eu

30 August–2 September 2015 • Chitin and Chitosan • Münster, Germany
Prof. Bruno M. Moerschbacher, University of Münster, Institute of Plant Biology and Biotechnology (IBBP), Schloßpark 8, D-48143 Münster, Germany, E-mail: bruno.moerschbacher@uni-muenster.de, www.chitin2015.eu

30 August–4 September 2015 • Solution Chemistry • Prague, Czech Republic
34th International Conference of Solution Chemistry (ISCS)
Professor Ivo Nezbeda, Conference Chair, Faculty of Science, J. E. Purkinje University, Ceske mladeze 8, 40096 Usti nad Labem, Czech Republic, E-mail: ivonez@icpf.cas.cz, CONFIS agency, E-mail: org@icsc.cz, www.icsc.cz

7-10 September 2015 • Macromolecules and Materials • Port Elizabeth, South Africa
13th Annual UNESCO/IUPAC Workshop and Conference on Macromolecules and Materials
Prof. A.J. van Reenen (Conference Chair), University of Stellenbosch, Department of Chemistry & Polymer Science, Private Bag X1, Matieland 7602, South Africa, E-mail: ajvr@sun.ac.za, http://academic.sun.ac.za/unesco

3-8 October 2015 • Physical Organic Chemistry • Sydney, Australia
23rd International Conference on Physical Organic Chemistry (ICPOC-23)
Prof. Jason Harper, School of Chemistry, University of New South Wales, Sydney, NSW 2052, Australia, E-mail: j.harper@unsw.edu.au, www.icpoc23.unsw.edu.au

6-10 June 2016 • Mycotoxins • Winnipeg, Canada
9th World Mycotoxin Forum & XIVth International Symposium on Mycotoxins
Prof. Rudolf Kréka (Program co-chair), University of Natural Resources & Life Sciences, Tullin, Austria, E-mail: rudolf.krksa@boku.ac.at and Prof. Hans P. van Egmond, Institute of Food Safety, Wageningen, Netherlands, E-mail: hans.vanegmond@wur.nl, Ms. Helena B. Bastiaanse (coordinator), Bastiaanse Communication, E-mail: wmf@bastiaanse-communication.com, www.WMFmeetsIUPAC.org

6-9 November 2015 • ChemRAWN XX • Dhaka, Bangladesh
ChemRAWN XX - Herbal Medicine for Health Care in the 21st Century
Prof Dr Mohammed Mosihuzzaman, International Centre for Natural Product Research (ICNPR), Bangladesh University of Health Sciences (BUHS), 125/1 Darus Salam, Mirpur, Dhaka-1216, E-mail: mmosihuzzaman@yahoo.com or chemrawnxx@buhs-edu.org, www.chemrawnxx.net.bd

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Bangladesh Chemical Society (Bangladesh)
The Royal Academies for the Sciences and Arts of Belgium (Belgium)
Brazilian Chemical Society (Brazil)
Bulgarian Academy of Sciences (Bulgaria)
National Research Council of Canada (Canada)
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Chinese Chemical Society (China)
Chemical Society located in Taipei (China)
Croatian Chemical Society (Croatia)
Sociedad Cubana de Química (Cuba)
Pancyprian Union of Chemists (Cyprus)
Czech National Committee for Chemistry (Czech Republic)
Det Kongelige Danske Videnskabernes Selskab (Denmark)
National Committee for IUPAC (Egypt)
Chemical Society of Ethiopia (Ethiopia)
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Comité National Français de la Chimie (France)
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Academy of Sciences of Mozambique (Mozambique)
Nepal Polymer Institute (Nepal)
Koninklijke Nederlandse Chemische Vereniging (Netherlands)
Royal Society of New Zealand (New Zealand)
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