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## Chemistry—A Core Science with a Political Dimension

by Leiv K. Sydnes



**C**hemistry plays a key role everywhere in the world, irrespective of a particular country's level of development. Whether the issue is nutrition, crop production, water quality, pollution cleanup, pest control, drug development, fuel efficiency, or biofuels, chemistry is a central discipline for solving many of the crucial problems facing us today.

For our science, such a position is quite prestigious. However, since issues such as those listed above are also hot items on the political agenda, it is inevitable that chemistry, clearly or indirectly, becomes entangled in political processes and at times even ends up playing a major role in events that chemists cannot control. It is therefore no exaggeration to state that there is a significant political dimension associated with chemistry. Surprisingly enough, many chemists are astonished to discover this fact and they typically react by declining to interact with the public and refusing to become involved in any political process.

However, such a remote and isolated relationship with the public is not in accordance with the principles to which IUPAC adheres. This is clearly reflected in the Union's vision statement, "IUPAC advances the worldwide role of chemistry *for the benefit of Mankind*," and its mission statement, which includes the passage "IUPAC effectively contributes to the worldwide understanding and application of the chemical sciences, *to the betterment of the human condition*." To realize this goal, the Union is bound to interact with society and to address global issues of political importance.

If we browse through the list of IUPAC activities, we see that IUPAC is indeed supporting a lot of projects of political relevance. Of significant importance in this respect are the CHEMRAWN conferences, past and

present work related to the chemical weapons convention, and initiatives to contribute to capacity building in Africa. There are also a number of divisional projects, dealing with, for instance, green chemistry, water issues, endocrine disruptors, and a range of environmental problems, in the same category.

All IUPAC projects and activities, including those with a political dimension, have a firm scientific foundation, consisting of established IUPAC terminology, evaluated data, and standardized methods, which are applied in accordance with the norms, values, and ethics of science. However, the more practical the world need that is being addressed, the more likely individual participants will have opinions on the topic. Even though these opinions are not always supported by scientific proof, participants' decisions should always be based upon a thorough knowledge of chemistry applied with the best ethical standards. Therefore, when IUPAC projects apply chemistry in the service of Mankind, it is inevitable that political attitudes and personal taste will have to be acknowledged and taken into proper consideration.

For the Union, this nonscientific, but human influence is a challenge, which calls for adequate caution. However, in the long run it makes no sense whatsoever to avoid issues that are, or have the potential of becoming, politically controversial. When one takes a global perspective, it becomes obvious that a large number of international agreements, conventions, and treaties regulating international cooperation

*... there is a significant political dimension associated with chemistry.*

on, for instance, trade, pollution control, and industrial production, in fact are useless and cannot be implemented if the chemistry and the chemists involved are below standard, are unavailable, or have to work under unsatisfactory conditions from a scientific point of view. It is therefore extremely important that IUPAC, to the best of its ability, is visible when political issues involving the chemical sciences are on the agenda. If IUPAC is not engaged up front in issues of chemical importance, it is quite likely that no other organization will take an objective stand on behalf of the chemical sciences and the chemical enterprise and argue with authority and a global perspective.

Any organization that aspires to become an efficient, reliable, and objective nongovernmental organization (NGO) that takes on politically sensitive

international issues has to meet at least three requirements. First of all, the reputation has to be irreproachable. It gives me great satisfaction to repeat that IUPAC fulfils this requirement. However, we have to work hard to maintain our standing as an impartial and trustworthy NGO by 1) supporting and developing relevant activities of high scientific quality year after year, and 2) disseminating the results of our activities effectively, especially in emerging and developing countries.

Second, the organization has to be active and visible in international circles where science policy is discussed and worked out, and has to cooperate with other organizations in the implementation of the policies when approved. Here IUPAC has to improve, but significant improvements have been made in recent years. The cooperation between IUPAC and UNESCO in the field of chemistry education is well established, and the memorandum of understanding between the two organizations, signed in December 2005, has paved the way for collaboration in other areas as well. Furthermore, our cooperation with the Organization for the Prohibition of Chemical Weapons (OPCW) continues to grow and has enabled IUPAC to contribute to world peace. A more recent development is IUPAC's stronger involvement in the International Council for Science (ICSU), which was established in 1931 "to promote international scientific activity in the different branches of science and their applications for the benefit of humanity." At the ICSU general assembly in September 2005, our president, Bryan Henry, was appointed as chair of the Committee on Finance.


Finally, the organization has to maintain a productive relationship with the media. Here IUPAC has a major problem to tackle because the chemical enter-

prise suffers from a dubious public image: Chemicals are so often associated with bad things happening to people and in the environment that the presence of chemicals in products and processes is frequently denied, and the positive, daily contributions from chemistry and chemical engineering are barely communicated. How to turn this negative trend around is far from obvious, but work in progress, particularly within the Committee on Chemistry Education (CCE), will hopefully contribute to a change. That is one of the reasons why I am participating with keen anticipation in the 19th International Conference on Chemical Education in Seoul, Korea, where CCE has put together a two-day symposium/workshop on "Public Understanding of Chemistry."


From the preceding paragraphs it can be concluded that IUPAC will not be out of work in the future; on the contrary, it will be facing significant challenges that are both scientific and political in nature. However, the Union will be meeting these challenges on behalf of all of us, not first and foremost for our science, but for our common future and the benefit of Mankind. That is why the old plea is still valid: Find a niche that interests you and contribute to the application of chemistry for a better world, nationally, regionally, or globally! 🌍

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*... the organization has to maintain a productive relationship with the media.*



**Learn more about recent IUPAC activities.**

 [www.iupac.org/news/archives/2006/report.html](http://www.iupac.org/news/archives/2006/report.html)

# Chairing Scientific Symposia

by Roger Fenwick  
and Leiv K. Sydnes

**T**he chairperson constitutes an essential component of any major scientific symposium. It is important that those selected for such a task understand that the role of the chairperson is to facilitate the execution of the symposium and function as a connection between the speaker and the audience. Surprisingly, this role is frequently misunderstood. In fact, most scientists can testify that they have attended scientific sessions that were adversely affected by a chair belonging to one of the following groups:

- The *Oscar Winner*, who has spoken at conferences and chaired sessions for decades; speakers have to fit in with his/her performance, and *it is* a performance, developed and honed over many years.
- The *Know it All*, who is always ready to impose his/her stamp on any presentation and demonstrate brilliance by hogging question time.
- The *Unconstrained*, who is oblivious to the clock and is frequently ready to stimulate irrelevant discussion, which frustrates speakers—especially the next one—and audiences alike.
- The *Nervous*, who starts twitching five minutes into the lecture, shifts papers to be ready for the next presentation, and is capable of putting anyone off.
- The *Technophile*, who is looking forward to any breakdown in the presentation technology so that he/she can leap up to assist.
- The *Busy Professional*, who arrives a minute before the session starts, is completely unaware of the session order as well as the gender and the presence of speakers.

A collection of such experiences acquired over many years has inspired us to write this piece. Its purpose is to encourage chairs and conference organizers to strive to achieve fluent and effective programming by identifying the key features of effective chairing. In addition, we offer practical suggestions for organizers and prospective chairs; although targeted especially at new chairs, it will—hopefully—also be of interest to more experienced colleagues.



## Tips for Organizers

It is a fact that *not all* experts make good lecturers; it is also true that good lecturers and brilliant scientists *do not necessarily* make good chairs. One reason is that some presenters may feel inhibited by a chair who has the personality and verbal display to carry a lecture, but when directing a section of a conference can end up hogging the spotlight.

Very often, members of a conference's scientific committee are selected as session chairs. This may be appropriate, but *not* if there are linguistic or other limitations. This is especially true of opening sessions, where the audience's interest needs to be ensured. In order to reduce the probability that sessions turn out poorly, organizing committees should:

- *Identify session chairs early*—Their role is as important as the role of speakers.
- *Provide clear guidance about what level of activity is required by the chair*—For example, will the chair be required to give a brief introduction to the session or provide a short summary of the presentations at the end.
- *Provide the chair with complete details of the sessions*—Conference programs may change at the last minute, since speakers drop out or are replaced, but do not wait until the last moment to inform the chair of this (usually *via* a scribbled and often illegible note). Confusion in statements from the chair can readily undo months of planning.
- *Ensure that water/soft drinks are available*. Do not forget bottle openers, if necessary; 90 minutes gazing at an unopened bottle can be torture in an airless room.

## Tips for Chairs

The chairs are in control, but the best chairs exercise the velvet glove rather than the iron fist. Pomposity and bluster are not qualities to display before an international audience, and certainly should not be passed on to younger colleagues. The activities of a successful chair may be divided into five sections.

### Before the session

Ensure that the organizers have provided correct details of the session: its timing, the program, and the speakers. Check that audio-visual aids and microphones are available and working. If a plenary or keynote lecture is included, make sure that brief biographical details of the speaker are provided, or seek the speaker out before the session to obtain these. If you do not know the speaker, ask one of the organizers to point him/her out. This can save hours of squinting at name badges of people that you imagine look like the speaker.

### At the beginning of the session

Greet the speakers and seek last minute information. Inform them about the importance of keeping to the schedule and make it abundantly clear how you will inform them that time is coming to an end and how you are going to terminate the presentation before the next speaker is introduced. Calm any last minute nerves and try not to pass on yours to them, especially when

less-experienced speakers are involved. Furthermore, make it clear that problems with the audiovisual equipment and the microphones are the responsibility of the organizers, not the speaker.

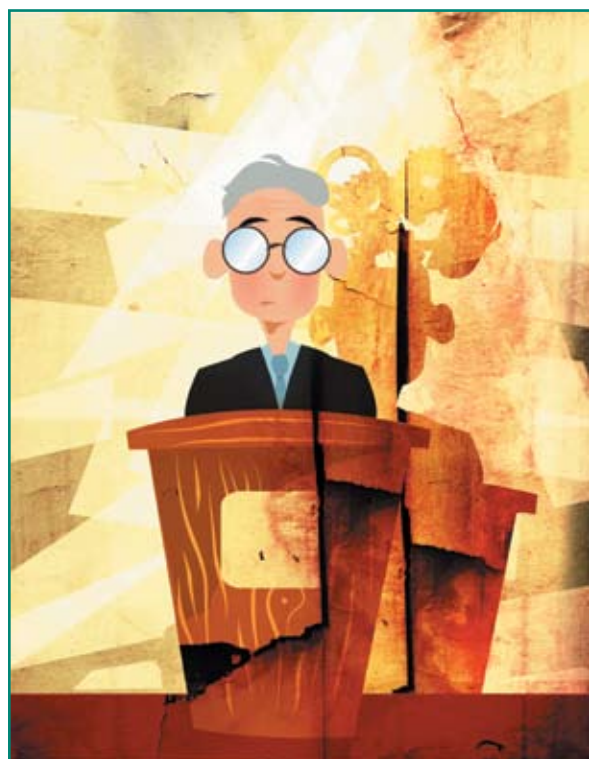
Ask the speakers to pronounce their names and, if necessary, make a note of these phonetically. It is not funny to mispronounce “foreign” names or organizations; it is, quite simply, *rude*. Remember, too, that the chair has precedence over the speaker, even if he or she is your old professor or your present boss.

Ensure that the session begins on time. Five minutes before the stated start, invite people to take their seats. Good organizers will already have been ushering people through the doors (a bell may be a useful accessory here). Check that all speakers are in the room. Do not rely on the fact that you saw the first speaker 15 minutes ago. He/she may have retired to the washroom, or returned to his/her room. Ideally, arrange for all speakers to be in the front row.

Allow yourself 30 seconds to read through the names of the authors and the titles of presentations. Then start by speaking slowly and clearly. Welcome your audience. If you feel it appropriate, welcome the audience in the language of the venue (it is always much appreciated). If you do this, ask a local colleague to repeat the words slowly and write them down phonetically. Briefly introduce yourself (and your co-chair if necessary). Make sure that the name on the table is in agreement! Do not give the audience the option of deciding whether you are Dr. Rimsky or Prof. Korsakov. Remember to remind members of the audience to switch off all mobile telephones (and ensure that yours is switched off).

Introduce the session briefly and move to the first presentation. A typical introduction to a plenary/keynote paper should be no more than one minute, and could include details of graduation, positions held, recent research interests, activities, and awards—all to demonstrate the suitability of the speaker for the presentation to come. Conclude with something like *“It therefore gives me great pleasure to invite Dr. Knoblauch to present this plenary/keynote lecture on [title].”*

For invited oral presentations, check that you have the right author identified and run through the pronunciations of the authors and their affiliations. A typical introduction could be *“The next paper is entitled [title] by Schwarz, Noir, and Black from the Institute of Chemistry of the University of Innsbruck. This will be delivered by Dr. Anni Schwarz.”*



## Chairing Scientific Symposia

### During the presentation

Be aware of any restlessness in the audience. Has the microphone gone dead? Maybe the lighting needs adjusting.

The greatest challenge—and fear—of any chair is the *over-running speaker*. Sometimes he/she is apparent from the beginning (for example, when the introductory slide is still showing after 10 minutes). In other cases the presentation dribbles or gushes on and on. The watchword in such cases is politeness. It is possible to curb such speakers, but strangulation is really not an option. Some large conferences, often running parallel sessions, still adopt a green, orange (two minutes to go), and red (stop) light system, but this is not common, and in any case may be ignored by those claiming to be color blind.

The chair must have a watch or stopwatch and should note the exact time of commencement. Prior to the session, the chair should have decided where to sit during the presentations since this can effect his/her actions. Make it clear what signal you will send to the speaker (for example, moving from front row to dais when five minutes remain). Alternatively, a hand signal may be used. Some presenters have, like some waiters, been known to lose their sight at such vital times, and so the signal should be significant. If a further indication is needed, then a firm *“Two minutes, please”* through the microphone is very effective.

Incidentally, do remember to switch off the microphone between comments, since you are not likely to gain the speakers friendship if a comment such as *“Isn't this ghastly...Where did they find this cretin?”* passes through the hall. If all else fails, then a walk to the podium and a stance next to the speaker will provide a final signal. *Again, be polite*. Indicate that it is indeed an interesting topic, but there is a tight schedule, other speakers are waiting and further discussion and exchange of views can take place later/during the coffee break.

It is the unlikely prospect of the latter scenario that causes the most stress amongst chairpersons simply because one is not totally in control. However, the audience is on your side. The only thing to remember is to work through the signals in turn and stick to the conviction that the *conference is greater than the individual speaker*.

It is good to remember the names of speakers that do not comply with the time allotted; after all you will probably organize conferences yourself at some time

and so you can avoid these people. In any case you certainly do not want to experience a re-run the next time you take the chair.

### After each lecture

Questions should only be allowed if the program is running according to or ahead of schedule. On the other hand, questions are an essential part of the scientific process and all lecturers, therefore, deserve at least one question. Thus, during the lecture it is an important task for the chair is to generate a couple of questions that can be asked if nobody else has one. (If the topic is not in your area of expertise, a question can sometimes be prepared from the available abstract). This is especially important at the beginning of a conference when potential questioners may be rather shy or doubt their ability in English. Questions from the chair, therefore, provide a little more time for the audience and give the speaker a chance to move into less formal “answer mode.” If no further questions are forthcoming, thank the speaker and perhaps comment that further discussion will be possible after the session/over lunch.

Usually there are questions, sometimes too many. Ensure that the speakers have access to a traveling microphone, or ask them to speak up so that the whole audience can understand. Often questions addressed to the speaker are inaudible to those sitting behind the questioner so, if necessary, repeat the question (this also gives the speaker a few more seconds to prepare an answer).

Show that you have seen potential questioners so that they do not wave furiously. If there are a number of questioners, politely discourage the person who has *“three questions and a comment”* by inviting him to ask one question to give others a chance. Do not be tempted to let questions continue to the detriment of the overall timing; it is far better to cut a discussion short and invite its continuation at coffee or during lunch.

Remember that every speaker deserves his/her allotted time. If the session is running over, do not put pressure on later speakers to speed up their presentations. It is not their fault. If necessary, ensure that a message is sent to the caterers alerting them that teas/coffees or lunches will be 10 or so minutes late. Remember that they are working to a schedule too. One memorable conference session managed to “lose” 90 minutes over a three-hour period.

## At the end of the session

If there is a link to the next session refer to it briefly, such as *"In this session we have heard about the methods developed to measure vitamin deficiency. After coffee/lunch we will see how these have been used in a clinical situation."* Thank all the speakers, the translators (if appropriate), and the lecture theatre staff, and ask the audience to express this *"in the usual way."* Announce the time at which the next session will begin.

Make a special point to informally thank the speakers in your session after the session has come to an end, especially those at the beginning of their careers. If you have constructive criticism to put forward, make it after some positive comments. A few words of support and encouragement at such a time will do wonders for their confidence.

Before leaving, look over the facilities and make sure you leave them as you would wish to find them. Hand the meeting over to your successor efficiently and on time, and make sure that your name plate has been removed.

## Parallel Sessions

Concerns about sessions running smoothly and attention to timing are particularly important when there are parallel sessions. Even if time for moving out/settling in seems to have been included in the program, most participants will probably still experience a time crunch when switching from one session to another, particularly if deviations from the lecture schedule are combined with complex logistics. Organizers can assist by briefing all chairs on the importance of timing (it just takes one laggard to cause chaos) and to ensure that the various lecture rooms are in reasonably close proximity.

## Chairing the Last Session

*The last session of the conference was coming to an end; the speaker and chair looked out across an audience of one. The speaker drew to a close and thanked the chairman, who thanked the speaker and congratulated the audience member for his perseverance and willingness to remain to the end. In reply the audience member informed the chair that he was, in fact, the last speaker.*

There is really no denying that the last session is equivalent to the speakers' "graveyard" of the after-

lunch plenary. Some of the audience will have left, some will be leaving during the session, and those who remain will wish to get the earliest taxi or train to the airport. This is not to say that departures should not be quiet—the person who wanders around kissing friends *au revoir* is not doing a service to the speaker, nor is the person sitting in the middle of a row who decides to move. No manner of wit or wisdom will delay those desperately wanting to avoid the traffic jams to the airport. The basic rule, therefore, remains the same: Stick to the timetable and do not prolong the session!



*Often, the last session of a conference can be the speakers' "graveyard."*

## Selecting Young Co-Chairs

In order to support and encourage the next generation of scientists to become involved in conferences, it is a good idea to have younger (this being up to the organizers to define) and more-experienced (a euphemism for "older") colleagues co-chair certain sessions. We believe this will improve conference chairing in the long run and certainly increase the quality and knowledge transfer of conferences. It also gives other young people in the audience the feeling that, in time, they could do the same. However, potential young chairs should be selected with care—not sleeping the night before and facing the audience rigid with fear is not what this experience is all about. In such circumstances, the responsibility is with the senior person to "look after" their more junior colleague. This is not, after all, a Ph.D. viva.

# Chairing Scientific Symposia

## Concluding Remarks

It should be emphasized that it is not our intention to outline *The Only Way* of chairing scientific symposia. On the contrary, each individual chair, like each presenter, should be encouraged to build on his/her own personality and develop his/her own style. However, there is no doubt that the overall quality of scientific

symposia can be improved significantly by good and constructive chairing, characterized by clear leadership and the ability to catalyze scientific discussions during the sessions.

Good chairs will learn from their experiences and should not, knowingly, turn in a poor performance since this will reflect badly on themselves and on the organizers. So before you accept that next invitation to Honolulu or Crete, ask yourselves what you can bring to the conference and prepare yourself.

Good luck! 🍀

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### Remember

- The chair is the servant of the meeting and the speaker, not the other way around.
- Read through the program in advance.
- Identify speakers and check names.
- Explain how you will chair (timing, etc.).
- Speak clearly (and, if a native English speaker, do not speak too fast).
- Keep to time.
- Let questions flow.
- Thank everyone (and head for the bar).
- Note the performance of other chairs, draw up a list of personal dos and don'ts.
- Adapt good rules to your personality, don't try to change your personality.
- Above all, enjoy the experience.

## Make Your List

### Dos

- \_\_\_\_\_
- \_\_\_\_\_
- \_\_\_\_\_
- \_\_\_\_\_
- \_\_\_\_\_

### Don'ts

- \_\_\_\_\_
- \_\_\_\_\_
- \_\_\_\_\_
- \_\_\_\_\_
- \_\_\_\_\_





# Beyond Classical Chemistry: Subfields and Metafields of the Molecular Sciences

by Jesper Sjöström



**T**he boundaries between both basic research and engineering and between the classical sciences are becoming increasingly blurred. This is partially a consequence of the increased interaction between science and society. For chemistry, the blurring of boundaries and an increased emphasis on

applications have led to the emergence of two “super-sciences,” material sciences and biomolecular sciences, respectively. In these, chemistry is only a part, although an important one. The increased interaction between chemistry and society has also resulted in the emergence and development of metadisciplines such as green chemistry, chemistry education, and the philosophy of chemistry. This article discusses—based on “knowledge maps” of chemistry—ongoing trends in the molecular sciences (MS). As a consequence of the more application-oriented research—mainly to do with medicines, new materials, and the environment—the position of chemistry as an independent discipline has become indistinct.

## From Academic to Post-Academic

The research practice of chemistry has changed tremendously during the last few decades, not only in the laboratory—due to advances in instrumentation—but also in the organization of research. Especially since WWII, chemistry has been influenced by physics on the one hand, and biology and medicine on the other hand. Physics has influenced both theories and experimental methods of chemistry, and is the basis for the revolution in instrumentation. From the 1950s one can talk about a “physicification” of chemistry. Similarly, one can talk about a “biofication” of chemistry from the 1970s. Biology and medicine have had a huge effect on the choice of research questions in chemistry. Furthermore, the development of gene and computer technologies have had big influences on the research practice of chemistry.

The identity, rhetoric, and organization of chemistry have shifted from an “academic” mode to a more application-oriented mode (“post-academic chemis-

### Classical Chemistry

“academic chemistry”

- Classical subdisciplines: organic chemistry, inorganic chemistry, analytical chemistry, physical chemistry, biochemistry
- Chemistry has a disciplinary self-value (in addition to its usefulness)
- Research organizations subdivided according to the classical subdisciplines

### Molecular Sciences

“post-academic chemistry”

- Interdisciplinary fields: material sciences and biomolecular sciences (chemistry as a service discipline)
- Application focus: blurring boundary between science and technology
- Interdisciplinary research centers and industry-sponsored research programs

Table 1. Comparison between Academic and Post-Academic Chemistry.

try”), which is driven as much by the surrounding society as by the chemistry community itself (see Table 1). The dichotomy of *academic* and *post-academic* is borrowed from Ziman.<sup>1</sup> Chemistry after WWII has been different in three ways: (1) research has become increasingly more specialized in parallel with the blurring of the boundaries with other disciplines,<sup>2</sup> (2) the revolution in instrumentation has had a big influence on the research practice,<sup>3</sup> and (3) new patterns of collaboration between academia and industry have developed. These trends are both a consequence of and a reason for the “physicification” and “biofication” of chemistry.

1. Ziman, J. (1994) *Prometheus Bound—Science in a Dynamic Steady State*. Cambridge: Cambridge University Press; Ziman, J. (2000) *Real Science—What It Is, and What It Means*. Cambridge: Cambridge University Press.

2. Reinhardt, C. (ed.) (2001) *Chemical Sciences in the 20th Century—Bridging Boundaries*. Wiley-VCH

3. Morris, P.J.T. (ed.) (2002) *From Classical to Modern Chemistry—The Instrumental Revolution*. RSC, Science museum och CHF.

## Beyond Classical Chemistry

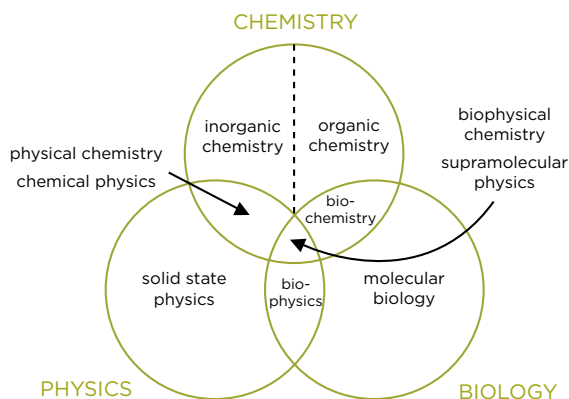


Figure 1: A “knowledge map” for chemistry.

### Knowledge Maps of Chemistry

Traditionally “pure” chemistry is seen as situated in-between physics and biology. In Figure 1 a somewhat more complex “knowledge map” is shown. In the boundaries have evolved subdisciplines such as physical chemistry and biochemistry. These two—together with organic chemistry, inorganic chemistry, and analytical chemistry—are often seen as the five classical subdisciplines of chemistry. As a result of the “physicification” and “biofication” of chemistry, new fundamental subdisciplines such as theoretical chemistry and macromolecular chemistry have complemented the classical five.

Chemistry as a discipline has changed a lot during recent decades. The U.S. National Research Council’s (NRC) 2003 report on the future of the field noted that “Chemistry and chemical engineering have changed very significantly [...] They have broadened their scope—into biology, nanotechnology, materials science, computation, and advanced methods of process systems engineering and control—such that much of what is done and taught in chemistry and chemical engineering departments is now quite different from the classical subjects.”<sup>4</sup> Today it is application-oriented fields, such as nanotechnology, polymer technology, biotechnology, and biomedicine, that are regarded as hot. All of these fields are problem-oriented and interdisciplinary. Therefore, they are crossing the border between science and technology. Baird and Schummer

4. NRC (2003) *Beyond the Molecular Frontier: Challenges for Chemistry and Chemical Engineering*. Committee on Challenges for the Chemical Sciences in the 21st Century, National Research Council. Washington: The National Academies Press, p. 11.

write: “[T]he nanotechnology movement spreads across the disciplines and ignores classical boundaries [...]and] the boundary between science and technologies increasingly blurs.”<sup>5</sup>

Figure 2 shows a more modern knowledge map. In the boundary between applied chemistry and physics one finds materials science. Similarly, biotechnology is situated in the intersection between applied chemistry and biology. More generally, it is the two supersciences, material sciences and biomolecular sciences, that we find in the intersections. In the intersection between the two supersciences has evolved the field of bionanotechnology. This is for the moment a hot area, which can be illustrated by the fact that Elsevier launched the journal *Nanotechnology, Biology, and Medicine* in the beginning of 2005. In addition to bionanotechnology, a large part of surface and colloid technology also is situated in the boundary between the two supersciences. Other examples are biosensors and artificial photosynthesis. It is interesting to note that for several years chemical research at Uppsala University in Sweden has been subdivided according to the supersciences; bioresearch and material-oriented research are performed in two distinct interdisciplinary research centers.

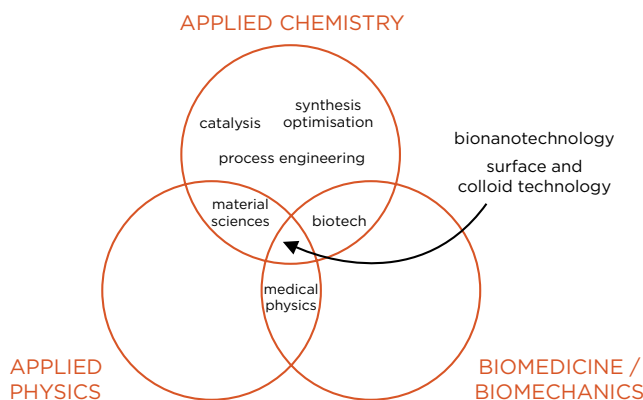


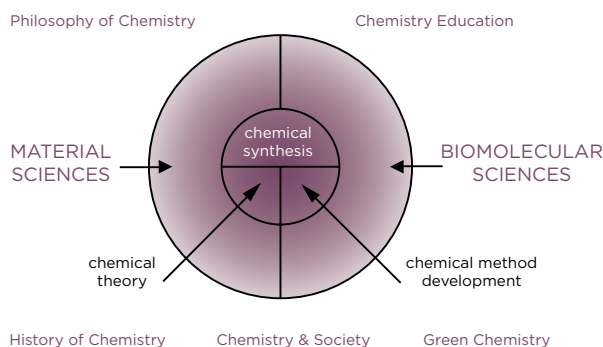
Figure 2: A revised—more modern—“knowledge map” for chemistry.

During the last decade, several authors and policy documents have stated that synthesis (and catalysis), biotechnology (and biomedicine), materials sci-

5. Baird, D.; Schummer, J. (2004) “Editorial: *Nanotech Challenges, Part I*” *HYLE—Int. J. Phil. Chem.* 10(2):63-64.

# Beyond Classical Chemistry

ences, and environmental technology will be important research areas in chemistry in the future.<sup>6</sup> With this as a basis, Figure 3 shows a model over the molecular sciences. In the middle one finds *the core* of chemical knowledge (i.e., chemical synthesis, chemical theory, and chemical method development). The latter should be understood broadly to encompass instruments, computational chemistry, and process technology. In *the boundaries* one finds the supersciences of material sciences and biomolecular sciences, respectively. The diffuse borders between chemistry and other knowledge fields in these supersciences are symbolized with the purple circle, covering the knowledge area of classical chemistry.



**Figure 3:** A knowledge map for molecular sciences and metadisciplines.

New medicines and the environment are recurring themes in much of modern chemical research. Much synthetic chemistry is today oriented towards medicinal chemistry, with some research aimed at developing “green chemicals.” Similarly, within material sciences, research is directed toward new drug delivery systems and “green materials.” For the biomolecular sciences, most research is aimed at finding new drugs. However, during recent years, scientists in this field have been exploring using biotechnology for environmental remediation and protection.

6. ACS; ACC; AIChE; CCR; SOCMA (1996) *Technology Vision 2020: The U.S. Chemical Industry*. Washington, D. C. (Executive Summary: <[www.ccrhg.org/vision/](http://www.ccrhg.org/vision/)>); AllChemE (1996) *Chemistry—Europe & the future* <[www.cefic.be/allcheme](http://www.cefic.be/allcheme)>; vide supra, reference 4; SusChem (2005) *A European Technology Platform for SUSTAINABLE CHEMISTRY—The vision for 2025 and beyond*. Final Draft, endorsed at a stakeholder event in Barcelona, 4 March 2005.

## Metachemistry

In addition to the real molecular science subdisciplines, the model in Figure 3 also indicates the presence of several metadisciplines, of which some have developed a lot during the last decade. Together, I call these metadisciplines *metachemistry*, which can be understood as the meeting of knowledge between chemistry and different subareas of the humanities. The five chemical meta-areas are the philosophy of chemistry, chemistry education, history of chemistry, chemistry and society, and green chemistry. Below I describe these areas in more detail.

The five metachemical knowledge fields and the chemists within them, which aim at contextualizing and analyzing chemical practice, have so far been relatively separated from each other. However, these fields must become a natural part of chemistry curricula, and become integrated in chemists’ and chemistry teachers’ reflectivity and practice. Clearly, there is a need for more coverage of metachemical disciplines in chemistry courses as a result of the increased interaction between science and society.



**Philosophy of Chemistry** is a metadiscipline on the border between chemistry and philosophy of science. It mainly deals with the nature of chemistry and its disciplinary boundaries (epistemological, methodological, and metaphysical reasoning), but also to some extent the culture of chemistry, its aims, and its disciplinary identity. Furthermore, questions about chemical ethics<sup>7</sup> and aesthetics are discussed. Although chemistry is a large science that has had a big influence on all other experimental sciences, the philosophy of chemistry in a modern sense is a very new area; it was formed as a research field in the mid 1990s.<sup>8</sup> In 1997 the International Society for the Philosophy of Chemistry was founded, and at about the same time two journals were launched: *HYLE—International Journal for Philosophy of Chemistry* and *Foundations of Chemistry*. To quote Schummer, “ironically, philosophy of chemistry emerged at a time when scientific activities increasingly transcended disciplinary boundaries towards problem-oriented research.”

7. See especially: Special Issues on ‘Ethics of Chemistry’ in *HYLE—Int. J. Phil. Chem.* (2001/2002) vol. 7(2) and 8(1).

8. Schummer, J. (2003) “The philosophy of chemistry” *Endeavour* 27(1):37-41.

## Beyond Classical Chemistry



**Chemistry Education** is a metadiscipline on the border between chemistry and the educational sciences.<sup>9</sup> It has a long history, but has to some extent changed its character during recent decades. Chemistry education deals with questions such as why and how to teach chemistry. Furthermore, it deals with the question of appropriate curricula. Three different types of knowledge can be regarded as important to the teaching of chemistry: (1) “ontological” (i.e., real chemistry), (2) “epistemological” (i.e., philosophical and cultural perspectives on the chemical enterprise), and (3) “ethical” (i.e., problematization of the role of chemistry in society).<sup>10</sup> Historically, ontological knowledge has been the main focus of this field. The traditional focus of this field has been on unproblematizing learning, but recently there has been increasing emphasis on more contextualized chemistry teaching,<sup>11</sup> ethical perspectives,<sup>12</sup> philosophical perspectives,<sup>13</sup> and the connection to environmental education.<sup>14</sup> Johnstone’s triangle, which contains symbolic, molecular, and macroscopic levels, has been complemented by Mahaffy with a humanistic dimension, emphasizing both real-life problems in the interface between science and society and the importance of putting the student in the center.<sup>15</sup> Important journals in this field include the *Journal of Chemical Education* and *Chemistry Education: Research and Practice*. Furthermore, many articles in the field are published in more general science education journals.



**History of Chemistry** is a metadiscipline on the border between chemistry and the history of science. It has a long history, but has—similarly to chemistry education—changed its

character during recent decades. It is possible to identify four different subtypes within the history of chemistry field: (1) history of the science, (2) history of chemistry teaching, (3) history of the industry, and (4) history of the environment. In September 2005 in Portugal, the section for History of Chemistry within the European Association for Chemical and Molecular Sciences held the 5<sup>th</sup> International Conference on the History of Chemistry on the theme “Chemistry, Technology, and Society.” In other words, modern history of chemistry tries to place the science in technological and social contexts. However, the journals *AMBIX: The Journal of the Society for the History of Alchemy and Chemistry*, *Chemical Heritage*, and *Bulletin for the History of Chemistry* mainly deal with old chemistry.



**Chemistry and Society** is the knowledge area on the border between chemistry and society. This field has two areas of focus: (1) “chemistry-as-society” (i.e., the chemical communities), and (2) “chemistry-in-society” (i.e., the use and effects of chemistry in society). It is an area where the values and perspectives of the authors have a big influence on the positions presented. There tend to be three general perspectives in the debate over chemistry and society: (1) persons from academia arguing for more and better basic chemical research, (2) politicians and persons from industry arguing for more focus on chemical innovations, and (3) persons with an analytical perspective<sup>16</sup> influenced by the research area STS (Science and Technology Studies). It is often the latter perspective that is the basis for university courses in chemistry and society.<sup>17</sup> This article can also be regarded as an example of the latter perspective. An example of the second perspective is a section about chemistry and society that appeared in a European report that argued that chemical research and chemists are important for future economic growth.<sup>18</sup> News magazines that cover this field include

9. Tsaparlis, G. (2003) “Globalisation in Chemistry Education Research and Practice” *Chemistry Education: Research and Practice* 4(1):3-10.
10. Krageskov Eriksen, K. (2002) “The Future of Tertiary Chemical Education—A Building Focus” *HYLE—Int. J. Phil. Chem.* 8(1):35-48.
11. Zoller, U. (2000) “Interdisciplinary systemic HOCS development—The key for meaningful STES oriented chemical education” *Chemistry Education: Research and Practice in Europe* 1(2):189-200.
12. Kovac, J. (1996) “Scientific Ethics in Chemical Education” *J. Chem. Education* 73(19):926-928.; Kovac, J. (1999) “Professional Ethics in the Collage and University Science Curriculum” *Science and Education* 8:309-319.; Coppola, B. P. (2000) “Targeting Entry Points for Ethics in Chemistry Teaching and Learning” *J. Chem. Education* 77(11):1506-1511.
13. Erduran, S. (2001) “Philosophy of Chemistry: An Emerging Field with Implications for Chemistry Education” *Science & Education* 10:581-593.
14. Zoller, U. (2004) “Chemistry and Environmental Education” *Chemistry Education: Research and Practice* 5(2):95-97

15. Mahaffy, P. (2004) “Tetrahedral Chemistry Education: Shaping What is to Come” *Chemistry International* November-December, p. 14-15; Mahaffy, P. (2004) “The Future Shape of Chemistry Education” *Chemistry Education: Research and Practice* 5(3):229-245.
16. Vide supra, reference 11.
17. Schwartz, A.T.; Bunce, D.M.; Silberman, R.G.; Stanitski, C.L.; Stratton, W.J.; Zipp, A.P. (1994) *Chemistry in Context: Applying Chemistry to Society*. Brown: Dubuque.; Andersson, S.; Sonesson, A.; Vannerberg, N.G. (1999) *Kemin i samhället*. Liber: Stockholm (in Swedish).
18. AllChemE (1996) *Chemistry—Europe & the Future* <[www.cefic.be/allcheme](http://www.cefic.be/allcheme)>.

*Chemistry International, Chemistry World, Chemical Week, and Chemical Market Reporter.*



**Green Chemistry** is a metadiscipline on the border between chemistry and industrial ecology.<sup>19</sup> It is based on 12 widely spread principles<sup>20</sup> that cover most of chemistry and chemical engineering.<sup>21</sup> The main principle is prevention. The other principles can be summarized in the following way: (1) renewables as chemical feedstocks, (2) substitution of hazardous chemicals, and (3) reduced consumption of chemicals and energy. More generally, green chemistry is about creating a more environmentally friendly chemistry practice, from the laboratories to chemical production to chemicals in society.<sup>22</sup> The green chemistry movement started in the USA in the early 1990s and has since spread all over the world.<sup>23</sup> The number of scientific publications with the key word “green chemistry” has increased substantially during the last five years. The main journal for the metadiscipline is *Green Chemistry*, which was launched in 1999. However, several journals have had special issues about the area during the last five years. It is interesting to note that green chemistry is the metafield that is most closely related to real chemistry. Most of its practitioners are also active as chemists. The relationship to real chemistry is indicated by the fact that green chemistry is the only metadiscipline that was discussed in the NRC report mentioned previously,<sup>24</sup> although the importance of good science education also was emphasized.

## Future of Chemistry

After considering the different metafields in modern chemistry, it is interesting to again look at real chemistry research and try to say something about the future of the discipline. Today there are signs that “chemist” as a professional identity is losing its former strength. The reason is that chemistry has become more special-

ized, has mixed with other sciences, and has become more oriented towards applications. As a result of this transformation of chemistry, Nye’s definition of disciplinary identity is no longer applicable to chemistry. She writes, “Scientific disciplines identify new problems and solve them. This happens within well-established disciplines and within areas of investigation that become new specialties or disciplines. It is the shared problem-solving activity [...] that [...] prolongs the disciplinary identity.”<sup>25</sup> Modern chemistry is working with a complex mix of different problems. Therefore, today the different subdisciplinary identities are more important than a common “chemist” identity.

“Chemistry” as a term does not encompass as many research fields as it did in the 1960s. As a result of first the physicification and then the biofication of the field, “chemistry” as a discipline is both very broad (including both biochemistry and physical chemistry in a broad sense) and rather limited (mainly the core of chemistry, synthetic chemistry with its molecule makers) at the same time. There are signs that chemistry in the future mainly will be a service discipline to the life sciences and other interdisciplinary fields. To cover the broader area, where classical chemistry is the core, but not the whole knowledge base (remember Figure 3), there are a number of examples where “chemistry” is being exchanged with—or at least complemented with—the broader “molecular sciences” as the name for the field. For example, it has been suggested that the American Chemical Society change its name to the “Society for Molecular Sciences and Engineering.”<sup>26</sup> The Federation of European Chemical Societies changed its name in 2004 to the European Association for Chemical and Molecular Sciences. The broader name molecular sciences (MS) covers a larger part of the two supersciences—biomolecular sciences and material sciences—than chemistry does on its own.

Some chemists, such as the editor of *Chemical Innovation*, are worried about the future of chemistry as a discipline: “Chemistry as a subject is facing difficult times, and we chemists are the only people who can do anything about it. [...] If we don’t do anything,

*continued on page 15*

19. Graedel, T. (1999) “Green Chemistry in an Industrial Ecology Context” *Green Chemistry* 1:G126-G128.

20. Anastas, P.T.; Warner, J. (1998) *Green Chemistry: Theory and Practice*. Oxford: Oxford University Press.

21. Mestres, R. (2004) “A Brief Structured View of Green Chemistry Issues” *Green Chemistry* 6:G10-G12. 22. Sjöström, J. (2006) “Green Chemistry in Perspective—Models of GC Activities and GC Policy and Knowledge Areas” *Green Chemistry*, 8(2):130-137.

23. Anastas, P. T.; Kirchoff, M. M. (2002) “Origins, Current Status, and Future Challenges of Green Chemistry” *Accounts of Chemical Research* 35(9):686-694.

24. vide supra, reference 4, p. 152.

25. Nye, M. J. (1993) *From Chemical Philosophy to Theoretical Chemistry—Dynamics of Matter and Dynamics of Disciplines, 1800–1950*. Berkeley: University of California Press, p. 30.

26. Baum, R.M. (2004) “A Radical Notion” *Chemical & Engineering News* 82(45):5; Ritter, S.K. (2004) “Redefining Chemistry” *Chemical & Engineering News* 82(48):31.

# Tools of the Trade

The following review introduces a new series of articles on "Tools of the Trade," which will provide a forum for views and discussion on one of the Union's goals: "IUPAC will facilitate the advancement of research in the chemical sciences through the tools that it provides for international standardization and scientific discussion."

The series, which will run through 2006–2007, was initiated by Kip Powell, past president of the IUPAC Analytical Chemistry Division (Division V). It will allow for a presentation of key outputs from IUPAC projects and will cover all fields of chemistry. As well as informing readers, it is hoped that the series will renew awareness of the valuable contributions IUPAC continues to make in facilitating the advancement of research in the chemical sciences. If you wish to contribute to this series, please contact <kip.powell@canterbury.ac.nz>.

## The IUPAC Stability Constants Database

by Leslie D. Pettit

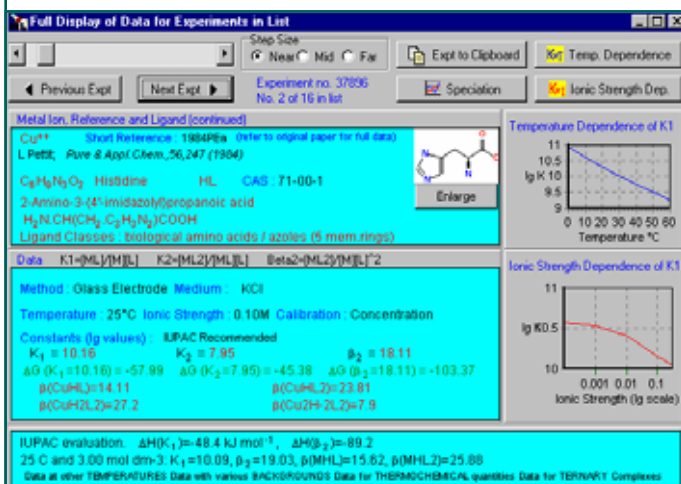
**M**etal-ligand stability constants (SC) are of vast importance to all scientists (not just chemists) working quantitatively in solution. IUPAC has been actively involved in the compilation of literature values of such constants for over half a century. The project was first considered in 1951 and the first compilation was published in 1957 under the auspices of IUPAC. This was followed by further volumes in 1964, 1971, and 1983. The editors of these volumes, which included data to about 1973, included most of the major pioneers in the field: G. Schwarzenbach (Switzerland), L.G. Sillen (Sweden), G. Anderegg (Switzerland), J. Bjerrum (Denmark), A. Martell (USA), H. Irving (UK), E. Högfeldt (Sweden), and D. Perrin (Australia).

## Background to SC-Database

A mainframe computer-based system was proposed in 1979 and trialled in Stockholm. A PC-based system was proposed in 1989 and a FORTRAN-based version was first demonstrated by Academic Software in 1991. Data from the book-based compilations were added over the following years using specially prepared software. Software was subsequently rewritten for 16-bit Windows operating systems, followed by fully object-orientated versions for 32-bit Windows using fast, indexed searching techniques. The graphical interface was further improved by including structures for ligands in mol-file format and routines for substructure searching—essential for distinguishing similar ligands. Routines for comparing the stabilities of complexes with specified metals and for faster journal and reference searching were also added. Interactive graphical speciation software was included.

## Overview of SC-Database

The SC-Database is a compilation of all significant metal-ligand complex stability constants published in the scientific literature. The database, which is regularly updated and maintained, currently includes data from 1887 to 2004/5 on over 9200 ligands from over 22500 references in 108000 records. It holds all data previously published in the book volumes (about 35 percent of the total) and completely supersedes them. Data held includes ligand details (full and short name, empirical formula, CAS-registry number, and structure) metal ion details, full literature reference, many experimental details (method used, temperature, and ionic background), published values of stability constants and protonation constants) and other data as available (e.g., solubility product,  $\Delta H_f^\circ$  values). On entry, the constants are not critically evaluated, but where they have been evaluated in parallel projects by the Analytical Chemistry Division (V), the IUPAC-rec-

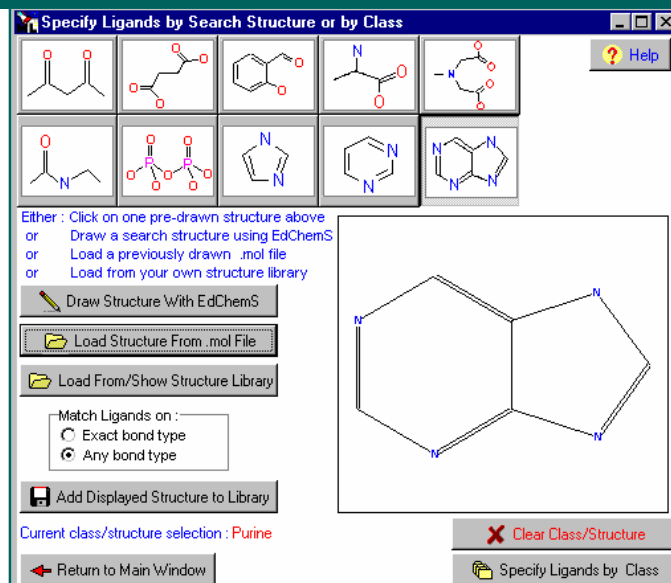


ommended values are also included.

Searching is designed to be fast and flexible. The database may be searched on any fragment of a ligand name (not necessarily the start), author, or journal, on experimental conditions, for a range of temperatures, range of numerical values of a constant, or any fragment of a descriptive comment. It is also possible to enter a ligand substructure fragment (in mol-file format) and to search the entire ligand database for ligands containing this fragment. The structure fragment may be prepared by any major structure-drawing program, or by the program EdChemS which is provided with SC-Database.

## Peripheral Programs

The speciation program is a powerful attribute. It has many applications, such as calculation of species distribution curves, calculation of pM or pL values as a function of solution pH and stoichiometry, and the determination of solution stoichiometry required for metal ion buffers. It can handle a mixture of up to 11 reactants and 30 constants (including solubility products). Data may also be used in programs for ionic strength and temperature corrections prepared as part of the IUPAC project on ionic strength corrections. These are supplied with SC-Database and are also available separately from [www.iupac.org/projects/2000/2000-003-1-500.html](http://www.iupac.org/projects/2000/2000-003-1-500.html) or from [www.acadsoft.co.uk/aq\\_solutions.htm](http://www.acadsoft.co.uk/aq_solutions.htm). Output (text and graphical) can be directed to disk, to printer, or to the clipboard in a selection of formats.



## Database Maintenance and Availability

The SC-Database suite of programs has been developed and is maintained by Academic Software. Data collection and compilation is in close collaboration with the IUPAC Analytical Chemistry Division. SC-Database is currently managed and distributed by Academic Software (Leslie and Gwyn Pettit) for IUPAC. An order form, a demonstration database, and additional details can be accessed via [www.acadsoft.co.uk](http://www.acadsoft.co.uk) or [www.iupac.org/publications/scdb](http://www.iupac.org/publications/scdb).

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we'll be extinct in a generation."<sup>27</sup> However, other chemists instead emphasize the need for classical chemical knowledge in the broader and even more heterogeneous field of MS: "As the borders between scientific disciplines blur (a process that will only continue), fundamental chemistry skills such as synthesis and analysis will be crucial for the interdisciplinary subjects that emerge."<sup>28</sup>

With increasing interaction between the classical sciences and also between science and society, the meta-molecular fields discussed in this article are needed to give perspective and guidance to and about the practitioners and teachers of the molecular sciences. It is time to redefine ourselves as (meta) molecularists.

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 [www.fpi.lu.se/en/sjoestroem](http://www.fpi.lu.se/en/sjoestroem)

27. Birkett, D. (2001) "Yuletide, Chemical Warfare, and Essential Micronutrients" *Chemical Innovation* 31(12):IBC.

28. Editorial (2001) "A Discipline Buried by Success" *Nature* 411:399.

## Emerging Issues in Developing Countries

*This series seeks to inform readers, explore new ideas, and promote discussion on themes related to developing countries and emerging analytical communities. To contribute to this series, contact Series Coordinator Jan-Åke Jönsson <jan\_ake.jonsson@analykem.lu.se>. Articles in this series are available from <www.iupac.org/publications/ci/indexes/emerging-issues.html>.*

### Maintenance of Scientific and Technical Equipment—Challenges Faced by African Institutions

*by Dzenzo Mzengeza*

Scientific equipment is essential for performing research, education, and quality assurance services, as well as for allowing sustainable development and output to take place. Equipment should be functional and well maintained, and users should be trained on how to operate and care for it.

A survey\* carried out by the International Foundation for Science in 2002 revealed that a major constraint on the output of research in Africa has to do with equipment problems. This paper analyzes the present situation and suggests some strategies that can be adopted to improve it.

#### Situation Analysis

Problems related to equipment are varied and may include procurement and purchasing procedures, installation, servicing and repair, spare parts, new technology, training, users, researchers, administra-

tors, donated equipment, suppliers, agents, custom duties, and institutional policies.

- **Procurement and purchasing procedures**

Procurement and purchasing of equipment in many institutions is not properly coordinated, often resulting in equipment being bought that cannot be used because of a lack of space or incorrect specifications. In addition, individuals with appropriate expertise are not always available to use, support, or service the equipment. The situation is further compounded by difficult bureaucratic procedures that often hamper efficient procurement.

- **Researchers**

Some researchers lack basic information concerning the best type of equipment to use—but often don't want to admit their ignorance. Catalogs may be unavailable or outdated, and “prestige pieces” are sometimes chosen rather than those that are most appropriate to an institution's scientific and educational needs.

- **Technical personnel**

Many institutions have technical personnel who are responsible for the operation and maintenance of scientific equipment and who support the academics and researchers. Technicians tend to be less qualified today than they were in the past, resulting in substandard performance. To make matters worse, after joining an institution, new technicians often receive little organized training and, perhaps as a result, often seem poorly motivated.

- **Administrators**

Institution administrators have the prime responsibility for decision making. They approve budgets, allocate funds for new equipment, and are responsible for paying for it. However, equipment problems seem to fall low on the priority list, as seen by a lack of institutional policies guiding the procurement and

*... a major constraint on the output of research in Africa has to do with equipment problems.*

\* Gaillard, J., M. Hassan, and R. Waast in collaboration with D. Schaffer. “Africa: Status of Science.” In *UNESCO Science Report 2005*, UNESCO, Paris, France, 2005, pp. 182-194.



use of equipment, an absence of staff training on the equipment, and an absence of any systems for replacing, retiring, or donating obsolete equipment. There is need for institutional planning related to the allocation of equipment resources that can take into account the short- and long-term needs of the institution.

- **Donors and donated equipment**

The majority of the equipment in educational and research institutions in the developing world has been donated. Unfortunately, a lack of coordination at the institutional level regarding donated equipment means that some equipment is underutilized—even though a need for it exists. In many instances, donors do not even involve local staff in selecting the specifications for equipment, instead giving the responsibility to overseas procurement agencies.

- **Equipment manufacturers, suppliers, and agents**

Local suppliers and agents usually charge more than overseas suppliers do, but yet may not be adequately equipped to give good back-up service. Some local agents act as agents for different equipment and therefore tend to neglect the equipment from which they are getting the least income. In addition, many local suppliers are inadequately staffed and cannot meet all of their customers' demands, prioritizing the needs of their regular customers and ignoring the rest.

Overseas suppliers often neglect the market in developing countries because it is considered to be very small. Accordingly, they rarely design equipment suited to the hot and humid conditions typical of developing countries. What's more, overseas suppliers rarely give local suppliers the training that would allow them to adequately maintain equipment. As a result, local agents and suppliers struggle to find and retain skilled maintenance and service employees.

## Conclusion and Recommendations

There is an urgent need to address equipment problems if we are to see improvement in research and education in developing countries. There are no easy solutions; some of the problems discussed here are



deeply rooted in the cultures of people and organizations, and many organizations seem to have priorities that don't include equipment problems. Nonetheless, here are some recommendations for improvement.

- **Acknowledge the problem**

These problems must be recognized, and those in power—including donors, institutions, and government representatives—must be willing to address them.

- **Develop and implement equipment policies**

Policies should be put in place to facilitate the efficient, effective procurement and use of equipment.

- **Encourage and support thematic networks and centers of excellence**

Doing so will encourage the sharing of ideas and strategies for solving common problems.

- **Encourage and support training programs**

Educational and research institution should learn from industry and invest in regular training programs for their laboratory staff related to lab management and the use, maintenance, and repair of equipment.

Dzengo Mzengeza <mzengeza@nusesa.org> is secretary general for the Network of Users of Scientific Equipment in Eastern and Southern Africa (NUSESA), P.O. Box 255, Kasselsvlei 7533, Cape Town, South Africa. Tel: +27 21 959 3327; fax: (27) 21 959 3311

## Malcolm F.G. Stevens is Awarded the First IUPAC-Richter Prize

**T**he newly established IUPAC-Richter Prize in Medicinal Chemistry has been awarded in 2006 for the first time. The recipient is Prof. Malcolm F.G. Stevens, Ph.D., D.Sc., OBE, of Nottingham University, U.K.

Dr. Stevens received this award in recognition of his leadership and contributions to the discovery of anti-cancer drugs. His work has resulted in the discovery of six novel small molecule agents that have progressed

into clinical trials. Two of these are now registered drugs. Among them is Temozolomide (Temodal™), used to treat glioblastoma multiforme (a deadly brain cancer), which is licensed to the Schering-Plough Corporation and has been marketed worldwide since 1999. Another product, Phortress, is in early-stage clinical trial against breast tumors; other products from his current research, exploiting other mechanisms for anticancer agents, are also expected to enter development.

The IUPAC-Richter Prize—a plaque and a check for USD 10 000—will be presented on 29 August 2006 at the XIXth

International Symposium of Medicinal Chemistry in Istanbul, Turkey. The plaque is signed by Prof. Bryan Henry, president of IUPAC, and Erik Bogtsch, chief executive officer of Gedeon Richter Limited.

Dr. Stevens studied pharmacy at the University of Nottingham, England, and obtained his Ph.D. in 1963, also at Nottingham. He was subsequently awarded a D.Sc. in 1979 for his published research on the novel synthesis of heterocyclic compounds. He pursued an academic career, spending seven years as a lecturer in medicinal chemistry at Heriot-Watt University in Edinburgh, Scotland, and then as a reader (i.e., an associate professor) in medicinal chemistry at Aston University in Birmingham, England. He was appointed professor of experimental cancer chemotherapy at Aston in 1979, and starting in 1983, spent six years as head of the Department of Pharmaceutical Sciences. In 1992 he returned to Nottingham University as

Cancer Research UK professor of experimental cancer chemotherapy and director of the Centre for Biomolecular Sciences, the position that he holds today. In addition, he is also chief scientific officer of Pharminox, a spin-off of Oxford University focused on the discovery and development of novel small molecule drugs for the treatment of cancer.

Dr. Stevens has received other forms of recognition from learned societies during his career: the UK Royal Society of Chemistry (RSC) Interdisciplinary Award (1991), the Royal Pharmaceutical Society of Great Britain Harrison Memorial Medal (1994), the RSC George and Christine Sosnovsky Award for chemical contributions to cancer research (2002), and the American Association for Cancer Research Bruce F. Cain Memorial Award (2003) for translational cancer research.



[www.iupac.org/news/archives/2006/Richter\\_prize.html](http://www.iupac.org/news/archives/2006/Richter_prize.html)



Malcolm F.G. Stevens, winner of the first IUPAC-Richter Prize in Medicinal Chemistry

## Capacity Building in Science

**T**he Committee on Scientific Planning and Review (CSPR) of the International Council for Science (ICSU) recently appointed a panel to conduct a priority area assessment (PAA) of capacity building in science. This is ICSU's third PAA; the other two dealt with "Environment and its Relation to Sustainable Development" and "Scientific Data and Information." These assessments have been carried out as part of ICSU's defining a strategy for 2006-2011.

In its report, *Priority Area Assessment of Capacity Building in Science*, the ICSU panel calls attention to three crucial challenges to building scientific capacity.

The first challenge, a development problem, is the widening gap between advances in scientific knowledge and technology and society's ability to capture and use them. This is not just a question of the digital divide, although the use of knowledge does lag behind in developing countries; it is more the fact that having information does not necessarily translate into having knowledge. In addition, introducing science and technology to a world with diverse experiences presents a significant barrier. Finding ways to better communicate information about science to the public can help transcend this barrier and begin a constructive dialogue about scientific discoveries and new technologies. Developing national strategies for science and

## Priority Area Assessment on Capacity Building in Science



technology development and “national innovation systems” linked to policy development can also help close knowledge gaps, as can strengthening international cooperation and information exchange related to science.

The second challenge is the apparent declining interest in the study of science and engineering around the world. To turn this trend around, educators and scientists must find better ways to teach science and mathematics at all levels, in ways that “turn students on” to science early and often. Over the past decade, the international scientific community has increasingly focused on science education at all levels and has identified enhancing science education as one of the critical paths to strengthening the scientific workforce. The issues involved include improving the quality of science education, teacher training, and science curricula; expanding the number of educators and the links between formal and informal education; encouraging more women to enter careers in science; creating effective forums for sharing experiences in science education and educational reform movements; and instituting more uniform methods of testing, evaluating, and assessing which reforms work and which do not. The bottom line is that attracting, developing, and retaining talent in science and technology should be a priority for the entire scientific community.

The third challenge, an institutional problem, is the need to turn knowledge *consumers* into knowledge *creators*. Better institutions are needed to move knowledge to where it is needed, especially in devel-

oping countries. Education and science ministries, international organizations (including aid agencies), and the international scientific community must help build local capacities in science and technology to produce useable knowledge. They must also help connect local universities and research institutions with national innovation systems for economic development.

The recommendations included in the *Priority Area Assessment* report are put forward for consideration by ICSU itself, as well as its international scientific unions, national members, interdisciplinary bodies, and joint initiatives. Capacity building is a challenge that should affect the entire ICSU family. By working jointly in implementing the recommendations, the ICSU family should be able to increase scientific capacity building through its research programs, conferences and symposia, and other dedicated efforts world wide.

*ICSU Report of the CSPR Assessment Panel on Capacity Building in Science*, 2006 [ISBN 0-930357-64-7]

 [www.icsu.org/2\\_resourcecentre/Resource.php4?rub=10&id=33](http://www.icsu.org/2_resourcecentre/Resource.php4?rub=10&id=33)

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## Four Awards, One Passion: Chemistry

**T**he sun of Philadelphia beamed through the large reception room of the Chemical Heritage Foundation (CHF) on May 18, and excitement stirred the 200 people seated in the room. This was Heritage Day 2006, CHF's annual awards ceremony recognizing individuals who embody the advancement of the chemical world.

The celebration opened with the award of the Othmer Gold Medal to Ronald Breslow, professor at Columbia University since 1956. Breslow has worked to synthesize new molecules and study their properties, and he discovered the phenomenon of anti-aromaticity and the mechanism of the thiamine (vitamin B1) in the biochemical field. Recently, his work has focused on the mimicry of enzymatic molecules, which he hopes will help in the fight against cancer.

Breslow's award was introduced by an old friend and former student: Robert Grubbs, 2005 Nobel Prize winner in chemistry. Then, with classical piano music playing in the background—recorded by Breslow himself—Arnold Thackray, president of CHF, placed the

medal around Breslow's neck. From Breslow's speech: "People understand science as exploring the world. They don't necessarily yet understand science as extending the world. But that's one of the major things that chemistry does, and it's one of the things that has made it always so exciting to me."

Next, the new CHF Award for Supporting Industry was presented to Richard Bolte Sr., founder and chairman of BDP International. Richard Bolte Jr., president and CEO of the company, accepted the award on his father's behalf and thanked CHF. BDP International, created in 1966, is a leader in global logistic and transportation solutions, and more than 60 percent of BDP's logistic business is in serving the chemical industry. "BDP is very much a family business and has a strong family spirit," Bolte said. "We contributed early on to my father's success. One of his first offices was in the Lafayette Building . . . on Saturdays and Sundays he'd bring us in to the office. While he was looking at files, we were looking for entertainment."

The AIC Gold Medal was next presented to Roald Hoffmann. A Nobel laureate in chemistry in 1981, Hoffman is a professor at Cornell University and also a poet and playwright. Hoffmann's began his acceptance speech by displaying a Donald Duck comic book featuring Donald as a mad chemist; he then moved on



*Benjamin Franklin is a regular visitor at Heritage Day.*

to more serious topics, such as the necessity of theory: "There is a special connection of theory with teaching," he confided. "I think that the person who tries to explain thermodynamics to a first-year class must be learning something about how to explain something to other people . . . That's the lesson that I learned from teaching first-year classes: how to explain things. The pedagogical imperative is deeply rooted, and I'm proud to be a teacher to this day."

Finally, the Chemist's Club offered its Winthrop-Sears Award to Sol Barer, founder and CEO of Celgene. This biopharmaceutical company works on the development of molecules for cancer

and immunological disease. Barer told the up-and-down history of Celgene, which is linked with the infamous drug Thalidomide, found to cause deformities in babies whose mothers had used it during their pregnancy. Barer explained thusly: "In 1965, Dr. Jacob Sheskin at Hadassah Hospital at Hebrew University in Jerusalem provided a drug to a patient suffering from an inflammatory condition called ENL, associated with leprosy. It's a very painful condition, the patient couldn't sleep, and Dr. Sheskin gave [thalidomide] as a sleeping pill to this patient. The patient improved. He gave it to six other patients who had ENL. Within a few days they got better and within weeks all of the symptoms resolved. Skin lesions resolved, rheumatologic symptoms resolved, and the patients returned to normalcy. Nothing else had ever done that. So, from that point onward, Thalidomide became the standard of care for the treatment of ENL around the world."

Then he related: "In a very courageous, much-publicized, and not uneventful decision, the FDA granted approval to Celgene for Thalidomide for the treatment of ENL on July 16, 1998." Barer concluded, "There was no precedent in building a major pharmaceutical company from such a base, but we did."

 [www.chemheritage.org/events/heritage06/index.html](http://www.chemheritage.org/events/heritage06/index.html)

Report by Laure Joumel <laurejoumel@gmail.com>, freelance writer.



*Heritage Day 2006 awardees (from left) Sol Barer, Roald Hoffmann, and Ronald Breslow. Photo credit: Douglas A. Lockard.*

## In Memoriam—Allan Ure

IUPAC lost a valued and honored friend when Allan Ure died on 18 December 2005, after a period of illness. Allan was a world-renowned analytical chemist and spectroscopist who made many seminal contributions to environmental analysis, fractionation methods, and speciation. He will be remembered for his enthusiasm and energy as well as his good humor and quick smile. We who knew him had our lives enriched by his presence and are deeply saddened by the news of his death.

The *Journal of Soils and Sediments* (JSS) has published an extensive and thoughtful tribute to Allan [JSS 6(1), 62 (2006); doi:10.1065/jss2006.02.003] and is organizing a memorial section in an upcoming issue (to contribute, contact Philippe Quevauviller <philippe.quevauviller@cec.eu.int>). Here, we pay tribute to Allan's many contributions to IUPAC.

Allan began his IUPAC work in 1981 as an associate member of the Commission on Spectrochemical and Other Optical Procedures for Analysis (V.4). At the time, he was head of the Department of Spectrochemistry of the Macaulay Institute for Soil Research in Aberdeen,



## Safety Training Program



## Call for Host Companies



The IUPAC Committee on Chemistry and Industry (COCI) is seeking Host Companies for the IUPAC-UNESCO-UNIDO Safety Training Program (STP). The STP enables experts from developing countries to learn about safety and environmental protective measures by visiting and working with IUPAC Company Associates in industrialized countries. The STP brings IUPAC together with the United Nations Educational, Scientific, and Cultural Organization (UNESCO) and the United Nations International Development Organization (UNIDO) to promote interactions between developed countries and the developing world by disseminating state-of-the-art knowledge on safety and environmental protection in chemical production.

Seven trainees are currently awaiting placement at Host Companies. All are professional scientists and engineers who are supervisors or managers in chemical companies, government institutions, or academic laboratories. They have all been chosen for their experience and for their ability to influence leaders and staff in their workplaces and within their home countries. IUPAC and UNESCO provide funding for trainee travel to the Host Company, and the Host Company provides for local expenses during training.

STP Trainees visit the research and manufacturing facilities of IUPAC CA Host Companies for a two- to three-week period, during which the trainees shadow health, safety, and environmental professionals to gain first-hand experience in state-of-the-art practices. Trainees then apply their new knowledge at home in their workplaces, communities, and governments. Nine trainees, from Turkey, China, Egypt, Nigeria, Kenya, and Uruguay have participated in the STP at six Host Companies in the USA, UK, Japan, and South Africa since 2000.

There are many benefits to Host Companies. Besides the favorable publicity that all Host Companies gain, productive long-term relationships can build with the trainees and their home countries that can benefit the company and the trainee long after training is concluded. Dialogs between Host Company staff and trainees can lead to suggestions for improvements and new initiatives.

COCI is ready to assist Host Companies with trainee selection and scheduling and planning of site visits. Contact Mark Cesa <mark.cesa@innovene.com>, COCI chairman and STP coordinator, for more information and to volunteer!

 [www.iupac.org/standing/coci/safety-program.html](http://www.iupac.org/standing/coci/safety-program.html)



Scotland. During his tenure as associate member, two parts of the V.4 series on *Nomenclature, Symbols, Units and their Usage in Spectrochemical Analysis* were published: *Part V: Radiation Sources* (PAC 1985, 57:1453-1490) and *Part VI: Molecular Luminescence Spectroscopy* (PAC 1984, 56:231-245).

Allan was elected to be a titular member of Commission V.4 in 1985, a position he held until 1989 when he was elected to serve as secretary of the commission from 1989 to 1993. During those years, several more parts of the V.4 series were published, including *Part VII: Molecular Absorption Spectroscopy, Ultraviolet and Visible (UV/Vis)* (PAC 1988, 60:1449-1460) and *Part VIII: Nomenclature System for X-Ray Spectroscopy* (PAC 1991, 63:735-746).

Allan was the principal author of three V.4 recommendations—*Part X: Preparation of Materials for Analytical Atomic Spectroscopy and Other Related Techniques* (PAC 1988, 60:1461-1472), *Part XII: Terms Related to Electrothermal Atomization* (PAC 1992, 64:253-259) and *Part XIII: Terms Related to Chemical Vapor Generation* (PAC 1992, 64:261-264)—utilizing his expertise in standardized extraction procedures for soil analysis (now widely used in laboratories throughout the world) and his numerous international contacts to harmonize the terminology used worldwide in his field of expertise.

Even after completing his term as secretary, Allan continued to contribute his vision to V.4 recommendations. In 1993, IUPAC's Analytical Chemistry Division Committee conscripted Allan to cochair the working party assembled to produce the third edition of the

*IUPAC Compendium of Analytical Nomenclature* (the so-called Orange Book). The incredible task of assembling and integrating the large number of IUPAC analytical chemistry recommendations published from 1984 to 1997 into the second edition occupied 4 years (and undoubtedly produced many gray hairs) and resulted in an extremely accurate, well-used volume. Later on, the working party produced electronic versions of most of the chapters, allowing the *Compendium* to be presented on the IUPAC website <[www.iupac.org/publications/analytical\\_compendium](http://www.iupac.org/publications/analytical_compendium)> and enhancing its utilization and influence.

Through all of his IUPAC work, Allan was always enthusiastic and engaged, and his extensive knowledge of etymology and languages was extremely useful. We find it a wonder that he could juggle so many duties and tasks, considering his close involvement with the Royal Society of Chemistry Analytical Division, several journal editorial boards, a University of Strathclyde lectureship (in his retirement, no less), his IUPAC work, and his varied travels. We will be forever grateful for the body of work that Allan left behind and for the trails that he blazed, and we will remember him both as an extremely accomplished and able colleague and a good friend. We send our deepest sympathies to Allan's wife, Dorothy; his daughters, Jenny and Helen; his son, Allan; and his four grandchildren.

David S. Moore and Janos Inczédy wrote this tribute on behalf of the entire IUPAC organization.










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## Solubility and Thermodynamic Properties Related to Environmental Issues

Solubility is a basic phenomenon that determines the extent of most pollution problems, both environmental and industrial. However, no book is currently available on the importance of solubility and thermodynamic properties to environmental issues.

The objective of this project is to publish a 25-chapter book on recent developments in solubility and in thermodynamics that have a bearing on environmental issues. This, we the project leaders believe, could lead to new ways of thinking about and solving environmental problems. In true IUPAC style, the authors of this book have been drawn from 17 countries.

The chapters focus on such areas as predicting and modeling of environmental pollutants from basic thermodynamics considerations; designing remediation and cleaner industrial processes; predicting and measuring the uptake of pollutants and new industrial chemicals in humans and in animals; and environmental issues related to health science, mining, pesticides, soil chemistry, supercritical and phase equilibria separation processes, gasoline additives, ionic liquids in industry, corrosion control, surfactants, green synthesis, surface adsorption, and biodegradable plastic films.

The book is scheduled to be published in 2007. Another book on Developments and Applications in Solubility is the subject of a separate project and is scheduled to be published later in 2006.

For more information and comments, contact the Task Group Chairman Trevor Letcher <[trevor@letcher.eclipse.co.uk](mailto:trevor@letcher.eclipse.co.uk)>.

 [www.iupac.org/projects/2005/2005-048-2-100.html](http://www.iupac.org/projects/2005/2005-048-2-100.html)

## Terminology for Self-Assembly and Aggregation of Polymers

With nanoscience and nanotechnology enabling many of the key developments in modern functional materials, aggregation and self-assembly in polymers is of growing importance. The physical and chemical properties of aggregated polymers and polymer molecules that spontaneously assemble into ordered structures are more often determined by these macroscopic structures than by the individual polymer molecules from which they are built. Many of the terms used to

describe the different aggregated structures and self-assemblies, their methods of formation, their characterization, and any related terminology might be totally unfamiliar to scientists whose background is not in this discipline.

This project, therefore, will develop a list of terms and definitions for chemists and materials scientists within academia and industry. The definitions will be harmonized for acceptance by the chemistry, polymer, and materials communities. To assist in achieving this assent, members of the learned societies of different countries will be consulted to ensure that the definitions are accepted worldwide.

For more information, contact Task Group Chairmen Christopher Ober <[cober@ccmr.cornell.edu](mailto:cober@ccmr.cornell.edu)> or Richard Jones <[dick@rgjones.freereserve.co.uk](mailto:dick@rgjones.freereserve.co.uk)>.

 [www.iupac.org/projects/2005/2005-043-2-400.html](http://www.iupac.org/projects/2005/2005-043-2-400.html)

## Nomenclature of Phosphorus-Containing Compounds of Biochemical Importance

The objective of this project is to update and clarify recommendations for naming phosphorus-containing compounds. Many of these compounds are extremely important in biochemistry and hence in nearly all branches of biology and medicine. Most biochemically important compounds are esters and/or anhydrides of various phosphorus-containing acids with complex organic alcohols and organic acids.

Existing recommendations, available at <[www.chem.qmul.ac.uk/iupac/misc/phospho.html](http://www.chem.qmul.ac.uk/iupac/misc/phospho.html)>, have not been revised since 1976; since that time, much more has become known about many classes of phosphorus-containing compounds (e.g., inositol phosphates). The Chemical Nomenclature and Structure Representation Division (VIII) and the IUBMB-IUPAC Joint Commission on Biochemical Nomenclature are supporting this project in recognition of the need to redraft the recommendations more clearly, define the symbols used, and use as examples compounds that feature widely in biochemistry.

For more information, contact Task Group Chairman Hal Dixon <[h.b.f.dixon@bioc.cam.ac.uk](mailto:h.b.f.dixon@bioc.cam.ac.uk)>.

 [www.iupac.org/projects/2006/2006-019-1-800.html](http://www.iupac.org/projects/2006/2006-019-1-800.html)

## The Project Place

### Determination of Selenomethionine in Selenized Yeast Supplements

Production and consumption of Se supplements have increased dramatically in recent years as yeast-based supplements have emerged as an acknowledged means of alleviating selenium nutrient deficiencies for both animals and humans. However, it is evident from earlier studies that these supplements are often inconsistent in their makeup relative to label indications.

Significant efforts have been made in the development of analytical methods for the speciation of Se in yeast in recent years [selenomethionine (SeMet) is the dominant Se species in yeast-based Se supplements]. Extraction procedures used are of paramount importance for the accurate determination of SeMet in yeast

or other solid samples, and numerous ones have been developed. However, there remains a lack of consensus regarding whether there are forms of selenium other than SeMet in yeast. Consequently, the four major industrial companies producing selenized yeast boast their SeMet content as a proof of the quality of their yeast without a consensus existing on the methodology used and the validity of the measurements supplied.

The purpose of this project is to examine existing methodologies

published in peer-reviewed journals and issue recommendations on the determination of this extremely important nutritional supplement. The task group is composed of five scientists with considerable experience in the field, and the work will be carried out in close collaboration with the potential stakeholders.

For more information, contact Task Group Chairman Zoltan Mester <zoltan.mester@nrc.ca>, Canadian national representative to the IUPAC Analytical Chemistry Division, Institute for National Measurement Standards National Research Council, Ottawa, ON, K1A 0R6, Canada.



[www.iupac.org/projects/2005/2005-041-2-500.html](http://www.iupac.org/projects/2005/2005-041-2-500.html)

### Selection and Use of Proficiency Testing Schemes for Limited Number of Participants (Chemical Analytical Laboratories)

The IUPAC Interdivisional Working Party on Harmonization of Quality Assurance has recently revised the international harmonized protocol for the proficiency testing (PT) of (chemical) analytical laboratories. The IUPAC Technical Report was published in *PAC* 78(1), 145-196, 2006.

However, PT schemes described in the protocol were developed mostly for a relatively large number of laboratories-participants (more than 20 to 30). These laboratories form a representative statistical sample from the corresponding theoretical population of an infinite number of participants. Even if analytical results of the laboratories-participants are distributed arbitrarily, the sample mean distribution is close to the normal one. Therefore, the assigned/certified value of the PT test material can be calculated from the PT participant results as a consensus value [i.e., as the mean (or the median) of the results]. The performance of these participants is assessed based on the difference between their results and the assigned value.

The problem is that even for 30 participants, their (statistical) sample mean and standard deviation differ significantly from the corresponding population characteristics. For fewer than 30 participants, the difference between the sample and the population values is increasing with decreasing the number of participants, especially dramatically when it is less than 20.

Moreover, if the size of the population of laboratories is not infinite, and the size of the statistical sample is more than 5 to 10 percent of the population size, the ratio between the sample and the population sizes should be taken into account. In addition, not only are the sample mean or median of laboratory results biased in general from assigned/certified value (to be traceable to SI units), the population mean and median can be biased as well.

Thus, selection and use of a PT scheme for a limited number of participants (less than 20 to 30) are not routine tasks. Such schemes are quite often required for analysis of materials and/or for environmental analysis specific for a local region, for an industry under development, for analysis of unstable analytes, for a local laboratory accreditation body to control the performance of numerous unaccredited laboratories,



*Illustration depicts a 3D model of the yeast enolase protein, showing three areas of selenomethionine incorporation (red dots). Image reproduced by permission of Zoltan Mester and The Royal Society of Chemistry from *The Analyst*, 2005, 130, (1), cover page © Crown Copyright of Canada.*



## The Project Place

and so forth. Therefore, the aim of the project is to develop guidelines that could be helpful for PT providers and accreditation bodies in solving this task.

For more information, contact Task Group Chairman Ales Fajgelj <A.Fajgelj@iaea.org>.

 [www.iupac.org/projects/2005/2005-019-2-500.html](http://www.iupac.org/projects/2005/2005-019-2-500.html)

### Young Ambassadors for Chemistry in Korea

As Korea celebrates 2006 as the Year of Chemistry, the Korean Chemical Society hosted a Young Ambassadors for Chemistry (YAC) workshop in Gwangju in the southern part of South Korea. The event took place from 20–24 February 2006 at the Chonnam National University in Gwangju.

YACs is a project of the Committee on Chemistry Education (CCE) and the Science Across the World program; its aim is to increase the public's understanding of chemistry using young people to mediate between chemistry and the general public. The students (age 10–18) perform chemistry-related activities at public locations and explain what they are doing to the passers-by, who are usually unable to keep away from the interesting



*The line of cosmetics developed by the students.*

hubbub they witness taking place among the group of children. The event in Gwangju was the fourth YAC event, following on the heels of others held over the past two years in Taipei, Taiwan; Buenos Aires, Argentina; and Krasnoyarsk, Russia.

#### Train the Trainers

Prof. Choon Do, the Korean representative to CCE, organized and hosted the event and translated all event materials into Korean (the materials are downloadable from the Science Across the World Website <[www.scienceacross.org](http://www.scienceacross.org)> for all Korean teachers).

The event included a four-day training program for

middle-school science teachers, high-school chemistry teachers, and English teachers from around the region, as well as guests from Taiwan and Japan. The English teachers played an invaluable role at the event, stepping in to help interpret when we couldn't make ourselves understood and helping create a truly collaborative, multilingual experience.



*Production of the cosmetics.*

On Monday, teachers carried out activities from the Science Across the World topics “Chemistry in our Lives” and “Talking about Genetics around the World”—including counting the number of taste buds on each others' tongues and surveying variation in their own group in the classroom.

On Tuesday, we carried out a “Post-It” debate on the issue of genetic science. At the same time, the teachers discussed the chemical “products” that students would produce and the advertisements for them they would prepare.

Colleagues were invited to subscribe to the Science Across the World program and join more than 5 000 teachers in some 120 countries in exchanging cultural

*Students perform television commercials for the cosmetics.*



## The Project Place

and scientific information. The teachers coped extremely well with the English-language website; although the site is available in many languages, Korean is not yet one of them.

On Wednesday, teachers built a model of DNA from local sweets, successfully managing the challenge of melting marshmallows, and produced their own cosmetics. Thursday featured planning and preparation for Friday, when the teachers would help their learners

perform these same chemistry-related activities in a public place.

The day ended with an evaluation of the week and a discussion of the future. The participants reported that they liked the hands-on activities that helped to enhance motivation and relate chemistry to everyday life. They appreciated the chance to improve their presentation skills, particularly in English. They also expressed an interest in organizing additional YAC events and in having the chance to learn more and further their international collaboration. In particular, they expressed an interest in topics related to drinking water, conservation and recycling, renewable energy, diet and food, keeping healthy, fieldwork, dyes and coloring, and science games.

### YAC Day

The YAC Public Understanding Event got started at the Gwangju bus terminal around 10:00 a.m. The teachers and about 70 students gathered to conduct science activities aimed at enhancing public interest in chemistry.

The candy DNA the students built grew longer and longer, advertising campaigns were prepared, groups delivered their product presentations, the final length of DNA was put together, and prizes and gifts were handed out to the participants.



All told, 3 600 visitors viewed the event, the press covered it (see <[www.ikbc.net](http://www.ikbc.net)>), the teachers and students worked together confidently, the weather was glorious, and everybody had a great time with chemistry—the whole point of the event.

All of the teachers who participated in the event worked hard and were very patient—particularly with our

interpretation challenges. Prof. Choon Do, who was the host and organizer, discussed the event at the 19th ICCE conference held in Seoul in August 2006.

The following partners also helped make this event a success:

- Korean Chemical Society <[www.kcsnet.or.kr](http://www.kcsnet.or.kr)>
- National Chonnam Normal University, Prof. Wang Keun Lee
- National Science Council
- British Council, Seoul <[www.britishcouncil.org/korea.htm](http://www.britishcouncil.org/korea.htm)>, and Director Gavin Anderson
- GlaxoSmithKline <[www.gsk.com](http://www.gsk.com)>, who is the main sponsor of the Science Across the World program and who sent goody bags for all participating teachers and students

In addition, Cognis Korea <[www.ko.cognis.com/korea/kocognis.html](http://www.ko.cognis.com/korea/kocognis.html)> donated the main ingredient used in preparing the shampoo and BioRad <[www.biorad.com](http://www.biorad.com)>, Life Science Education, donated the “Genes-in-a-Bottle Kit” that enabled students to extract their own DNA.

This report was prepared by Lida Schoen, science education consultant, and Keith Kelly, language education consultant. Schoen is a titular member of IUPAC CCE, team member of Science Across the World, and task group chairman for the initial YAC project. Kelly is FACTWorld coordinator <[www.factworld.info](http://www.factworld.info)> and NILE associate trainer <[www.nile-elt.com](http://www.nile-elt.com)>.

For more information, contact Lida Schoen <[amschoen@xs4all.nl](mailto:amschoen@xs4all.nl)>.

 [www.iupac.org/projects/2003/2003-055-1-050.html](http://www.iupac.org/projects/2003/2003-055-1-050.html)

### Moderators of the “Post-It” Debate.



## The Project Place

### Adjustment, Estimation, and Uses of Equilibrium Reaction Constants in Aqueous Solution

IUPAC project #2000-003-1-500 has produced a suite of programs to study quantitatively the influence of ionic strength changes on equilibrium constants, with particular emphasis on using specific interaction theory (SIT). This new project is intended to extend this previous work in the following ways:

- apply Pitzer parameters in a more general way to equilibria of environmental and industrial importance, with particular importance given to seawater and mixed fluids
- extend and improve a database of published SIT- and Pitzer-related parameters that can be accessed by all relevant programs in the suite and may be edited by the user
- extend the package to cover other environmentally important gases such as air, H<sub>2</sub>, N<sub>2</sub>, rare gases, N<sub>2</sub>O, CH<sub>4</sub>, and other paraffins (currently the package allows calculations on the effects of dissolved O<sub>2</sub>)
- explore and test ways of displaying graphically the relationship between ionic strength and temperature with activity coefficients  $\lg K^0$  and  $\lg K$
- explore and test ways of displaying graphically the effects of errors on the relationships studied above
- calculate and demonstrate graphically the effect of errors on species distribution curves
- provide the outline of a database of reliable literature values of the dependence of stability constants on temperature

The current version of the suite of programs (Aq\_solutions.zip, about 7 MB) is available from project #2000-003-1-500.

For more information, contact Task Group Chairman Igor Sukhno <sukhno@chem.kubsu.ru>.



[www.iupac.org/projects/2006/2006-010-1-500.html](http://www.iupac.org/projects/2006/2006-010-1-500.html)

### Design of Polymer Education Material for French-Speaking Countries

The need for a standard in polymer education has been recognized by French-speaking academics in both emerging and developed countries. The aim of this project is to set up a basic course at the undergraduate level for French-speaking countries that takes into account their local contexts. This course will be illustrated with attractive materials (e.g., a database, teaching documents, videos) provided by partners of the project and will be made available free of charge to the education community.



*Task group participants (from left): P. Degee (Belgium), D. Jhurry (Mauritius), H. Kaddami (Morocco), A. Soldera (Canada), M. Popa (Romania), and G. Froyer (France).*

The first meeting of the project was held at the Institut des Matériaux Jean Rouxel in Nantes, France, on 9-10 June 2006, under the sponsorship of the Université de Nantes. At this workshop, participants further improved the standard program that has been proposed via e-mail exchanges during the previous year. Attendees worked on existing available materials such as CDs and videos, rating their quality, appearance, and scientific consistency. This exercise gave them a better picture of how the polymer course should be mounted and how to make it as attractive as possible for the undergraduate students.

The group decided to share the task of mounting the polymer course among five subgroups, each one having responsibility for designing a specific part of the agreed-upon standard course. A follow-up meeting is planned for mid-2007 to validate the work done by the different subgroups.

For more information, contact Task Group Chairman Gerard Froyer <gerard.froyer@cnsr-immn.fr>.



[www.iupac.org/projects/2004/2004-037-1-400.html](http://www.iupac.org/projects/2004/2004-037-1-400.html)

## Provisional Recommendations

### IUPAC Seeks Your Comments

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



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

### Glossary of Terms Used in Toxicology—Expanded and Revised from “Glossary for Chemists of Terms Used in Toxicology” (IUPAC Recommendations 1993)

This glossary is a revision of the IUPAC *Glossary for Chemists of Terms Used in Toxicology*,<sup>1</sup> which incorporates new and redefined terms from the Glossary of Terms Used in Toxicokinetics.<sup>2</sup> It contains definitions and explanatory notes, if needed, for terms frequently used in the multidisciplinary field of toxicology. The glossary is compiled primarily for those scientists and others who now find themselves working in toxicology or who require knowledge of the subject, especially for hazard and risk assessment. Many medical terms are included because of their frequent occurrence in the toxicological literature. There are three annexes, one containing a list of abbreviations and acronyms used in toxicology, one containing a list of abbreviations and acronyms used by international bodies and by legislation relevant to toxicology and chemical safety, and one describing the classification of carcinogenicity according to the weight of evidence available.

1. *Pure Appl. Chem.* **65**(9), 2003–2122, 1993

2. *Pure Appl. Chem.* **76**(5), 1033–1082, 2004

#### Comments by 30 September 2006

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[www.iupac.org/reports/provisional/abstract06/duffus\\_300906.html](http://www.iupac.org/reports/provisional/abstract06/duffus_300906.html)

### Guidelines for Potentiometric Measurements in Suspensions—Practical pH Measurements in Soil Suspension

The measured cell potentials for suspension potentiometric cells have been interpreted and explained by a detailed analysis of the schemes for these cells (Part A). Some former disagreements amongst investigations have been clarified in this document. A new unambiguous operational definition of the Suspension Effect is presented. It is defined as the difference in cell potential for two suspension potentiometric cells, one with both electrodes in the separated equilibrium solution and the other with both electrodes in the sediment or suspension. This potential difference is the sum of the change in the indicator electrode potential and the change in the liquid junction potential of the reference electrode, when the electrodes are used for measurement, once in the sediment of the suspension and then in its equilibrium solution.

#### Comments by 30 September 2006

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[www.iupac.org/reports/provisional/abstract06/oman\\_300906.html](http://www.iupac.org/reports/provisional/abstract06/oman_300906.html)

# Internet Connection

*The following review is the second in a series of articles surveying free online resources of potential interest to chemists. The first article appeared in the July-Aug 2006 CI, p. 26.*

## Free Information Resources for Chemists, Part 2

by Leslie Glasser

### Chemical Informatics

Structure representation is an important support to chemical understanding. A long history and wide applicability make RasMol and the related MDL Chime plugin two of the most important chemical display programs available (RasMol is now known as "Protein Explorer" <[www.umass.edu/microbio/rasmol](http://www.umass.edu/microbio/rasmol)>, although it can be used for much more than protein structures; MDL Chime can be downloaded at <[www.mdli.com](http://www.mdli.com)> or <[www.umass.edu/microbio/chime](http://www.umass.edu/microbio/chime)>, where further information on molecular visualization is provided). In addition, the World Index of Molecular Visualisation Resources <[molvis.sdsc.edu/visres](http://molvis.sdsc.edu/visres)> provides a comprehensive listing of programs, tutorials, and examples for molecular visualizations.

Structure drawing, naming, and query programs are also available for free downloading for noncommercial uses. KnowItAll ChemWindow Edition <[www.knowitall.com/academic/welcome.html](http://www.knowitall.com/academic/welcome.html)> from Bio-Rad provides access to spectroscopic information, Elsevier offers a number of free-to-academics programs <[www.mdli.com/solutions/solutions\\_for/academics](http://www.mdli.com/solutions/solutions_for/academics)>, including its MDL ISIS/Draw program, and ACD/Labs offers ChemSketch <[www.acdlabs.com/download/#free](http://www.acdlabs.com/download/#free)>. ChemAxon provides a wide range of Java-based chemical toolkits that can be accessed through at <[www.chemaxon.com/forum/ftopic193.html](http://www.chemaxon.com/forum/ftopic193.html)> based on its Marvin program for viewing chemical reactions and queries. The toolkits available provide facilities for the prediction of structure-based properties; structure and reaction searching and database handling; structure canonization, transformations, and library enumerations; pharmacophore and structure-based screening, clustering, and diversity analysis; and (promised for the near future) drug design.

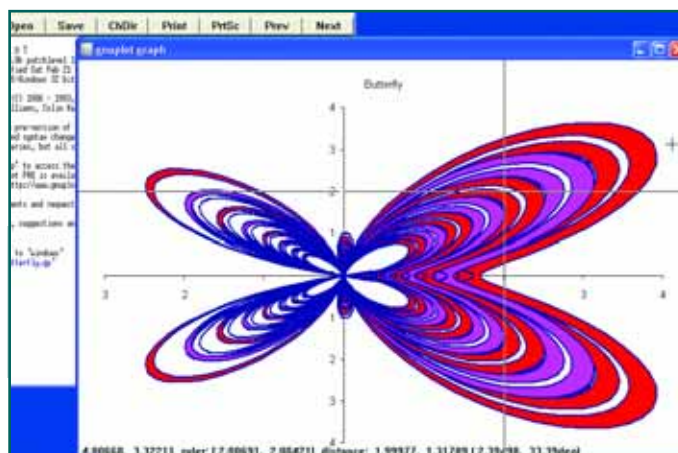
The important ORTEP program, used for crystal-structure drawing (and adaptable to single molecules), can be found in version ORTEP-III at <[www.ornl.gov/sci/ortep/ortep.html](http://www.ornl.gov/sci/ortep/ortep.html)>.

INFOTHERM <[www.infotherm.de](http://www.infotherm.de)> is a database of thermophysical properties maintained by Berlin's FIZ-Chemie, where search on the Internet is available free of charge for pure substances and by subscription for mixtures. INFOTHERM is updated monthly.

### Mathematical Applications

Having access to data fitting and symbolic mathematics is important. An enormous range of mathematical software, much of which is free, is available through the Department of Mathematics at the University of Haifa <<http://math.haifa.ac.il/msoftware.html>>. Drawing simple graphs can generally be accomplished by using the facilities available in the spreadsheet program; however, for greater versatility, the free GNU Project graph-drawing program Gnuplot (version 4.0 at <[www.gnuplot.info](http://www.gnuplot.info)>) is enormously powerful and will perform most tasks rapidly and more than satisfactorily. New users will face an initial steep learning curve, but once it is overcome, the effort expended will generally be found to have been well worthwhile.

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Sample output from Gnuplot, copied from <[www.gnuplot.info](http://www.gnuplot.info)>.

## The International System of Units (SI), 8th edition

Bureau International des Poids et Mesures, 2006  
ISBN 92-822-2213-6

The Bureau International des Poids et Mesures has released its eighth edition of the *Système International d'Unités* (*the International System of Units*), commonly called the SI Brochure. The brochure is published in hard copy and is also available in electronic form at [www.bipm.org/en/si/si\\_brochure/](http://www.bipm.org/en/si/si_brochure/).

The brochure defines and promotes the SI, which has been used around the world as the preferred language of science and technology since its adoption in 1948 through a resolution of the 9th Conférence Générale des Poids et Mesures (CGPM), known in English as the General Conference on Weights and Measures. The SI is a living system that evolves over time and reflects current best measurement practices; accordingly, this eighth edition contains a number of changes since the previous edition. As before, it defines all the base units and includes all the resolutions and recommendations of the CGPM and the Comité International des Poids et Mesures (CIPM), known in English as the International Committee for Weights and Measures, relating to the SI.

Formal reference to CGPM and CIPM decisions can be found in the successive volumes of the Comptes Rendus of the CGPM and the Procès-Verbaux of the CIPM; many of these are also listed in *Metrologia*. To simplify practical use of the system, the text explains these decisions, and the first chapter provides an

introduction to the concept of establishing a system of units in general and the SI in particular. The definitions and practical realizations of all the units are also considered in the context of general relativity. A brief discussion of units associated with biological quantities has been introduced for the first time. Appendix 1 reproduces, in chronological order, all the decisions (resolutions, recommendations, and declarations) promulgated since 1889 by the CGPM and the CIPM on units of

measurement and the SI. Appendix 2 exists only in the electronic version and can be downloaded at

[www.bipm.org/en/si/si\\_brochure/appendix2/](http://www.bipm.org/en/si/si_brochure/appendix2/). It outlines the practical realization of some important units, consistent with the definitions given in the principal text, that metrological laboratories can make to realize physical units and to calibrate material standards and measuring instruments of the highest quality. This appendix will be updated regularly to reflect improvements in the experimental techniques for realizing the units. Appendix 3 presents units for photochemical and photobiological quantities.

The eighth edition is available on the BIPM Web site in PDF and HTML format, along with a four-page summary of the brochure and a handy pocket version. In addition, an English version is available (although the official record is always that of the French text, and it must be used when an authoritative reference is required or when there is doubt about the interpretation of the text). Translations, complete or partial, of this brochure (or of its earlier editions) have been published in various languages, notably in Bulgarian, Chinese, Czech, English, German, Japanese, Korean, Portuguese, Romanian, and Spanish.

The SI brochure is prefaced by Ernst Göbel, president of CIPM; Ian Mills, president of CCU; and Andrew Wallard, director of BIPM.

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

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## Obsessive Genius: The Inner World of Marie Curie

by Barbara Goldsmith  
*Great Discoveries Series*  
W.W. Norton & Co., New York, London, 2004  
ISBN 0-393-32748-5

*reviewed by Stanislaw Penczek*

Barbara Goldsmith, a well-known historian and writer, was given access to Marie Curie's original diaries and letters and has used these documents to create a profound portrait of a brilliant scientist and a courageous woman. I believe that every chemist, and perhaps every scientist, should read this book.

Goldsmith tracks Curie's life from a childhood in Warsaw through instruction at the Sorbonne to her marriage to the young physicist Pierre Curie. She describes how the Curies built on A.H. Becquerel's discovery of radioactivity to explain its source as an



atomic property and to subsequently discover the first two radioactive elements, which they termed *polonium* and *radium*—opening the way to the exploration of the inner structure of atoms. In 1903, the Curies and collaborator Becquerel were awarded the Nobel Prize in physics in recognition for their discovery of radioactivity.

Goldsmith relates in detail, and with great sympathy, how triumph and tragedy ruled Curie's life in turn. Following the 1903 Nobel award, in 1906, Pierre Curie died in a roadside accident. In 1911, Marie Curie was awarded a second Nobel Prize, this time in chemistry—but the moment was clouded by the French Society's condemnation of Curie for her affair with married physicist Paul Langevin, a former student of Pierre Curie, and the Nobel Committee's attempt to rescind the award when news of the affair surfaced.



*The young Marya Skłodowska, who became Madame Curie, is shown standing at left, behind her father, Wladyslaw, with her sisters Bronya and Helena at right. Courtesy of the Curie and Joliot Association/Curie and Joliot-Curie Fund.*

Goldsmith quotes a letter from Curie regarding the scandal: "I cannot accept the idea that the appreciation of the value of the scientific work should be influenced by libel and slander."

During World War I, Curie commandeered the automobiles of well-to-do French women and organized a fleet of mobile X-ray units (that became known as "Les Petites Curies") to assist the doctors working on the

front lines of battle. In later years, she established two research institutes, one in Paris and one in Warsaw, dedicated to the study of radioactivity.

In 1934, the year of her death, Curie had a final triumph: her daughter and son-in-law's receipt of the Nobel Prize for their discovery of artificial radiation. Frederic Joliot-Curie, Curie's son-in-law, wrote of their discovery that "I will never forget the expression of intense joy which came over her [Marie] when Irene

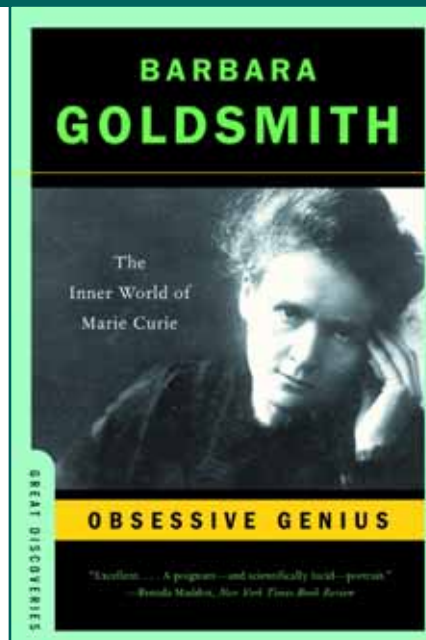
and I showed her the first artificially radioactive element in the glass tube."

Goldsmith is a long-time admirer of Curie; she writes that as a teenager, "Madame Curie was my idol. Under the picture [I tacked up] I had placed two of Madame Curie's quotations: 'Nothing in life is to be feared. It is only to be understood,' and 'You cannot hope to build a better world without improving the individuals.'" Goldsmith's accomplishment in this volume is in capturing the unparalleled joy that accompanied Curie's scientific discoveries and in revealing her dedication to scientific pursuit not as a sacrifice, but rather as the result of a fierce, internal drive—one that led her to refer to radium as "her child."

Albert Einstein has referred to Marie Curie as being "as cold as a herring," but the source material that Goldsmith mines (and reprints in this book, for the first time) paints a different picture. In a letter to her sister, the young Curie wrote, "Sometimes I laugh all by myself and contemplate my state of total stupidity with genuine satisfaction."

Einstein was correct on one count: he repeatedly stated that character, persistence, and courage were the most important qualities for a scientist. Madame Curie had all three. On 20 April 1995, more than 50 years after her death, Curie was recognized for these attributes and for her scientific brilliance. Under the chairmanship of the presidents of France and of Poland, the ashes of Marie and Pierre Curie were moved to rest under the famous dome of the Panthéon in Paris. Curie was the first woman to be buried there in recognition of her own accomplishments.

Stanislaw Penczek <spenczek@bilbo.cbmm.lodz.pl> is a professor at the Centre of Molecular and Macromolecular Studies in Lodz, Poland. He is a member of Polish Academy of Sciences and is also Dr h.c. at the Université Pierre et Marie Curie, Paris.



### Volume G: Definition and Exchange of Crystallographic Data

Sydney Hall and Brian McMahon (editors)  
*International Tables for Crystallography*  
Published for the International Union of  
Crystallography by Springer, 2005, 594 + xii pp.  
ISBN 1-4020-3138-6

The clear, efficient communication of data and results has always been fundamental to scientific work. This is especially true for data generated and used by computer software in the current era of high-throughput experimentation and e-science, particularly because

data gathered in one scientific field increasingly inform other areas of research. The ability to link different information resources together seamlessly is a major goal of the semantic Web; data need to be accompanied by rich metadata to define their meaning and context. In a field as diverse as chemistry, many data exchange standards emerge and many flourish, but only for a

time. Those that endure and have the greatest impact are flexible, extensible, and well documented—and therefore have the highest potential for interoperability.

The International Union of Crystallography (IUCr) has invested a great deal of effort in developing and promoting standards for the description of crystal and molecular structure data. Its Crystallographic Information Framework (CIF) has grown from a file format published in 1990 for the description of small-unit-cell structures to a collection of standards covering powder diffraction studies, biological macromolecular structures, area-detector and other image data, and other areas of structural science. Many of these standards are important components of large-scale database systems, such as the macromolecular (mmCIF) software ontology used by the Protein Data Bank. The crucial component of CIF is its rich semantic content, expressed not only in a large vocabulary of clearly defined tags, but also in machine-readable expressions of relationships between individual data items.

CIF has always been well documented on the Web, but now, as a mature standard, it is comprehensively described in the recent publication of *Volume G*, the latest in IUCr's flagship reference series *International Tables for Crystallography*.

The book, subtitled *Definition and Exchange of Crystallographic Data*, is edited by Syd Hall, the primary developer of CIF, and Brian McMahon of IUCr, who described CIF in the July-Aug 2002 *CI*, p. 4. *Volume G* brings together in a single location a full technical specification of CIF, with accounts of its historical background and philosophy, its use in publishing crystal structure reports, its synergistic relationship with other more general information exchange standards such as XML, and guidance on developing and using CIF-aware software.

The bulk of the volume concerns machine-readable dictionaries of individual data names that catalogue the items recorded in a structure determination experiment and the analysis of its results. The dictionaries are printed in full, and machine-readable versions are supplied on an accompanying CD-ROM (they can also be downloaded from the Web). Extensive commentary chapters have been commissioned to describe best practice in the use of the dictionaries. This level of detail is essential for software developers, but it also provides much useful information for the general scientist interested in the details of the data describing a crystallographic experiment and the resulting structure.

The volume also describes the Molecular Information File (MIF), a related standard for two-dimensional chemical structure representations, and provides food for thought on how to integrate the description of three-dimensional crystal structures with the conventional chemical description of their component molecules.

The book touches on other standards, such as Chemical Markup Language (CML), but as an authoritative reference for CIF, it provides the essential information needed to build interoperability between crystallographic information and the wide range of related chemical information systems.

In addition to the machine-readable dictionaries, the CD-ROM that accompanies the volume contains a large collection of software libraries and applications for use both by software developers and end users. The printed volume contains an up-to-date compendium on chemical informatics as of late 2005; in the rapidly changing world of software development, it will be particularly useful to have the entire contents of the volume available online, and revised on a rolling basis, as will be the case when IUCr launches its Web version of the entire *International Tables for Crystallography* series later in 2006.





### Philosophy of Chemistry: Synthesis of a New Discipline

Davis Baird, Eric Scerri, and Lee McIntyre (editors)  
*Boston Studies in the Philosophy of Science*, Vol. 242  
Dordrecht: Springer, 2006  
ISBN 1-4020-3256-0

reviewed by Stephen Weininger

Before the late 1980s the phrase “philosophy of chemistry” would have undoubtedly elicited a “huh?” from most readers. Chemists would have deemed it irrelevant; philosophers, an oxymoron. But today there are two journals devoted to the field, *Hyle* and *Foundations of Chemistry*, a rising tide of presentations, journal articles, and monographs on the topic; and an International Society for the Philosophy of Chemistry, which has held annual meetings since 1997. The volume under review, in which 20 authors representing varied disciplines address a wide range of topics, is part of a distinguished series on the philosophy of science. Clearly, the philosophy of chemistry has found its place in the sun, albeit not without considerable struggle.

In the past, philosophers have given chemistry a mixed reception. For some of the greatest—Hegel, Comte, Engels, and Whitehead—it provided a source of fundamental insights into physical reality. In contrast, Kant asserted in 1786 that chemistry, unlike physics, was not and might never become a “proper science”—a judgment that, until fairly recently, prevailed among philosophers and scientists. Why was that so?

As the book’s editors point out in their introduction, philosophers of science have traditionally preferred “grand, unifying theoretical visions instead of complicated local sights.” Since chemistry abandoned such “unifying visions” after the demise of alchemy, it seemed hardly to merit consideration by philosophers. That conclusion was reinforced by a number of physicists, especially Dirac, who asserted in 1929 that chemistry was nothing more than applied quantum mechanics. Moreover, there was the inescapable fact that chemistry was both ubiquitous and complex. Since many philosophers of science focused on dictating how science *ought* to operate, they would likely have found a welter of messy specifics more distracting than helpful. As philosopher Joachim Schummer tartly observes in his informative history of the field, “the smaller the discipline, the more philosophers write about it.”

Fortunately, the philosophy of chemistry gathered strength without the participation of philosophers. Because many of its concerns are directly relevant to chemical practice and pedagogy, chemists, chemical engineers, and historians have for some time been practicing philosophy of chemistry *avant la lettre*. Some of the major issues, insights, and conclusions in this essential work are summarized below. Note that the editors of this volume have not attempted to define “philosophy of chemistry”—rather, they have allowed the range of topics and diversity of authors to suggest the scope of the topic.

#### The Alleged Reduction of Chemistry to Physics (Hendry, Vemulapalli)

It is not hard to see why the reduction of chemistry to physics was one of the first issues to receive widespread attention in the current philosophy of chemistry, since it bears directly on the autonomy of chemistry. Not too long ago, most philosophers and scientists, including many chemists, thought that chemistry had indeed been reduced to physics and that any chemical phenomenon could be deduced “in principle” from the Schrödinger equation. A process of re-examination begun 25 years ago cast severe doubt on that supposition, and the present authors have carried that project forward very effectively.

Physical laws set limits on what can happen in nature. However, those laws have little to say about which of the myriad allowable possibilities *actually come to pass*. Quantum mechanical calculations from “first principles” can’t even account for isomerism, one of the central phenomena in chemistry. In fact, the application of quantum mechanics to problems of molecular structure *requires us* to have some prior chemical knowledge if the output is to be remotely useful. It’s clear that the autonomy of chemistry is assured, in principle as well as in practice.

#### The Dynamic Dimension in Chemistry (Benfey, Earley, Nordmann)

Chemists’ conspicuous success in unraveling chemical structures has led many to fear that we are slighting our discipline’s dynamic dimension. To paraphrase the message of these authors, it’s time to think of time as more than an axis on a graph. After all, we recognize chemical substances as such only if they persist in time, on a scale defined by our measuring instruments. Furthermore, if we endow the temporal dimension with as much complexity as we do the spatial one, we

## Bookworm

encounter some very important phenomena. For instance, the concept of symmetry has been indispensable to our understanding of structure; applied to networks of coupled reactions, it yields equally potent results. Such networks, which are central in biological organisms, can achieve sufficient stability to qualify as substances if they have the proper symmetry.

### What is the Subject Matter of Chemistry? (Needham, Weisberg)

The usual way of explaining chemical phenomena is to base the explanation on the structures and properties of molecules. Is this always the best way to proceed, and does it mean that chemistry is essentially the science of molecules? Many chemists and philosophers, including the present authors, have argued for a return to the concept of chemistry as the science of *substances*. From the molecular point of view, water, steam, and ice are pretty much the same thing, but from the thermodynamic standpoint, they are not. There are properties of the whole that are not inherent in the components, as recognized long ago by Aristotle.

### Models in Chemistry (Scerri, Hunger, Woodyard)

Chemists never deal directly with nature, but rather with *models* of nature; chemistry has a wide variety, several of which are examined closely in these three chapters. Because models are never true or false, only more or less effective for a given task, we are free to use them all at different times, even if they are in con-

flict with one another or with the underlying theory—or both. Chemists rely heavily on these models to explain various experimental observations, even though the explanatory procedures usually don't satisfy philosophical criteria for proper "explanations." No worry—this is just another example of the inadequacies of one-size-fits-all philosophical pronouncements.

### The Languages of Chemistry (Hefferlin, Johnson, Vollmer, Rothbart, and Schreifels)

Getting a true feel for chemistry requires appreciating its rich repertoire of representations. Ordinary language, specialized nomenclatures, molecular formulas, stereochemical drawings, spectrometer and microscope outputs, mathematical equations, computer simulations, physical models—all are used in various combinations to capture, describe, and assess experimental data and to plan future experiments. At one extreme, simple two-dimensional drawings can evoke a three-dimensional microworld. At the other extreme, highly sophisticated machines that are themselves reifications of complex theories allow us to "see" this microworld. Moreover, these tools are anything but passive—they interact dynamically with the science.

### Chemistry and Society (Kovac, Bhushan)

The phrase "natural kind" denotes a group of objects that share a theoretically significant characteristic or property. Philosophers have long used chemical elements and compounds as examples of natural kinds. Here, Nalini Bhushan casts severe doubt on this appropriation. Chemists constantly regroup their materials depending on the properties that are relevant at the time. Furthermore, synthetic chemists can produce artificial compounds indistinguishable from natural ones and create new compounds that have never existed before, fatally weakening the distinction between natural and artificial. These achievements remind us that chemistry's impact on society goes far beyond the material. The ability of alchemists and chemists to synthesize natural materials in unnatural ways has been a central fact in the centuries-long religious and philosophical discussion of the boundaries between the natural and the artificial—and it makes a chapter on professional ethics most fitting.

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## Recent Release

*HYLE: International Journal for Philosophy of Chemistry*, Vol. 12, No. 1, 2006

### Special Issue: The Public Image of Chemistry, Part 1

J. Schummer, B. Bensaude-Vincent, and B. Van Tiggelen (editors)

<[www.hyle.org/journal/issues/12-1](http://www.hyle.org/journal/issues/12-1)>

# Conference Call

## Chemistry for Agriculture

by Adam Pawelczyk

The XXXI International Conference on "Chemistry for Agriculture" was held 6–9 December 2005 at the famous health resort called Priessnitz, located in Jeseník, Czech Republic. Since 1999, the conference has been held in this scenic spot in the Sudetan Mountains that straddle the Polish-Czech border.

The conference was attended by 197 participants from who presented 141 posters and gave a number of lectures. Attendees included chemists, fertilizer specialists, environmental protection specialists, and representatives of scientific institutions, industry, veterinary medicine, agriculture, and local government.

The main topics of oral and poster presentations were as follows:

- technology of mineral fertilizers, feed phosphates, and other additives
- agricultural chemistry—how fertilizer nutrients and pesticides change in the environment, nutrient availability
- phosphorus and nitrogen problems in the environment
- ecotoxicology
- development in the production of chemical agents for agriculture
- new methods for applying agricultural chemicals
- impact of chemical products on plant and animal production
- harmful substances in agriculture and the environment

The conference was inaugurated by Zbigniew Dobrzanski from Wroclaw University of Agriculture who

recalled the long history of meetings of specialists of various disciplines and discussed the current state of science and agriculture in Poland. The scientific program of the introductory session included the following lectures:

- Henryk Górecki, "New Chances for Financing Scientific Research from Public Means"
- Pawel Kafarski, "On the Borderline of Biology and Chemistry—Four Stories with a Moral"
- Hennie van de Coevering, Barbara Kozłowska, "Life Cycle Analysis (LCA), a Sustainable Perspective from Cradle to Grave. An Example from Agriculture: Maize Corn Production"
- Adam Pawelczyk, "Organic Waste—EU Legislative Constraints and Future Prospects"

In his lecture, Górecki discussed new opportunities and prospects for government funding of scientific research. He encouraged scientists to put more effort into gaining grants from state entities and preparing new applications for financial support.

Kafarski presented a very interesting lecture on the frontiers of biology and chemistry in which he used four examples based on old myths and legends: He connected Santa Claus with Amanita mushrooms, showed why druids from Galia were considered dangerous by Romans, rationalized vampires from a chemical point of view, and showed how it is possible to create zombies.

Van de Coevering and Kozłowska delivered a joint lecture about life cycle analysis of products and their impact on the environment. The analysis/assessment includes the entire life cycle of the product, process, or activity, encompassing extraction and processing of raw materials, manufacturing, transportation, distribution, use, maintenance, recycling, and final disposal.

Pawelczyk focused his lecture on the recycling of nutrients from organic waste for use in agriculture. He pointed out the legislative and economical ways of promoting organic waste recycling that have been developed and implemented in Europe during the last 30 years.

For the past two years, "Chemistry for Agriculture" has been sponsored by IUPAC. In 2005, the conference



*The XXXIst Conference was inaugurated by Prof. Z. Dobrzanski (Poland).*



*A discussion during a poster session.*

## Conference Call



*Prof. Hennie van de Coevering (Netherlands) addresses the audience.*

was organized by the AGROPHOS Scientific Research Center of Chemistry, Agrochemistry, and Environment Protection, Wrocław, Poland, and the Czech-Pol-Trade Company, Jeseník, Czech Republic, on behalf of Wrocław University of Technology; Institute of Mineral Fertilizers, Pulawy, Poland; Institute of Inorganic Chemistry, Gliwice, Poland; and the University of Agriculture, Wrocław, Poland.

Evening social events, such as dances and a gala dinner, provided opportunities for attendees to talk about scientific issues with

new acquaintances. On one evening, participants were enchanted by the recital of the famous opera singer Anna Bernacka.

The next XXXII conference will be held at Priessnitz in December 2006.

Adam Pawelczyk <adam.pawelczyk@pwr.wroc.pl> has been the chairman of the organizing committee since 1998. He is an academic teacher at the Wrocław University of Technology.

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## Photodynamics

*by Jesus Rubayo Soneira*

The **Fourth International Meeting on Photodynamics** was held in Havana from 6–10 February 2006. Approximately 100 scientists from 19 countries met to discuss a range of experimental and theoretical viewpoints on the physical and chemical processes related to environmental and biological systems.

The conference was sponsored by the Cuban Ministry of Science and Technology, the Cuban Physical Society, IUPAC,\* and the Abdus Salam International Center for Theoretical Physics.

The international scientific committee consisted of Vincenzo Aquilanti (Italy), Majed Chergui (Switzerland), Gerardo Delgado-Barrio (Spain), Antonio Varandas (Portugal), Julian Echave (Argentina), Annick Suzor-

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Editor's note: this event also benefited from IUPAC's financial support via the program for Conferences in Scientifically Emerging Regions. For more information, see <[www.iupac.org/symposia/support.html](http://www.iupac.org/symposia/support.html)>.

Weiner (France), and Jesús Rubayo-Soneira (Cuba, chairman).

Prior to the conference, a seminar was held from 1–4 February 2006 that focused on a new generation of young researchers from Cuba and Latin American countries, as well as the rest of the world. Fifty students attended the following short courses, which were given by professors with excellence in both teaching and research:

- “Some Elements on Theoretical and Statistical Approaches of Elementary Reactions” (Jean Claude Rayez)
- “Van der Waals Clusters” (Gerardo Delgado Barrio)
- “Wavepacket Dynamics, Photochemistry, and Coherent Control” (David J. Tannor)
- “Molecular Science at the Nanoscale” (Vincenzo Aquilanti)
- “Lepton Chemistry: Molecular Processes and Reactions Induced by Low-Energy Electrons and Positrons” (Franco A. Gianturco)

The meeting, which featured 30 plenary lectures, 12 oral communications, and 43 poster presentations, covered the following topics: structure and energetics of molecular systems, dynamics and reactivity of isolated molecular species, dynamics of molecular species embedded in small and large clusters, dynamics of molecules in the condensed phase (liquid, solid) and at surfaces, control of chemical reactions, and collisions with surfaces.

The purpose of the meeting was to stimulate discussion about the structure and dynamics of molecular systems among scientists working in the chemical-physics. Keynote lectures were given by Peter Hering (Düsseldorf, Germany), Gustav Gerber (Wuerzburg, Germany), Osman Atabek (Paris, France), Reinhard Nesper (Zurich, Switzerland), and William Jackson (California, USA), among others.

In particular the conference provided a timely opportunity for scientific exchange among outstanding scientists and young researchers from all over the world. Based on the scientific success and interest in the Havana meeting, the participants agreed that this kind of meeting should be held again in the near future.

The seminar and meeting took place at the National Capitol, the main building of the Cuban Academy of Sciences, which is located in the heart of Old Havana.

Jesus Rubayo Soneira <[jrs@fctn.isctn.edu.cu](mailto:jrs@fctn.isctn.edu.cu)> served as the conference organizer and is currently a professor at the Instituto Superior de Tecnologías y Ciencias Aplicadas in Havana, Cuba.

### Green/Sustainable Chemistry

by M. Kidwai

The IUPAC-sponsored **Second International Symposium on Green/Sustainable Chemistry**, held in Delhi, India, from 10–13 January 2006, was a showcase for green chemistry innovations from all over the world. Green chemistry can be challenging, but it is fundamental to the future of chemical production, especially in the pharmaceutical and agricultural fields. The conference's 550 attendees from 22 countries took stock of recent advances in environmentally friendlier chemistry.

The organizing committee made a strong effort to help participants from economically less developed countries attend the event. The Third World Academy of Sciences gave USD 2000 to fellows from countries such as Ghana and Bangladesh so they could attend the conference.

The conference, which offered 8 plenary lectures, 31 main lectures, and 44 invited lectures featuring eminent scientists, focused on the vital role played by chemists in designing green methods of chemistry and how to widen the use of green technology.

A number of prominent speakers shared the results of their cutting-edge research. In his plenary lecture, E.J. Thomas from the University of Manchester, UK, discussed alternatives to allyl stannanes for remote stereo chemical control and encouraged the use of fictionalized ionic liquids. Pietro Tundo, from Ca' Foscari University, Italy, lectured about the tunable reactivity and selectivity towards C and N methylation in dimethyl carbonate chemistry using basic and acidic catalysts. Arthur C. Watterson from the University of Massachusetts, USA, discussed the chemo-enzymatic green synthesis of polymeric materials, which is an environmentally benign technique for medical, imaging, and other applications. John C. Warner, from the same university, discussed using entropic control in materials design.

In addition, there were 33 oral presentations by upcoming postdoctoral and Ph.D. fellows who shared their experiences with green chemistry. The poster presentations showcased the most up-to-date research in the areas of synthesis of bioactive compounds, green, use of biomaterials, nanotechnology, biomimetic processes, microwave technology, ionic liquids, and the edges of physical chemistry, including computational methods. Five awards were presented for best poster presentations.

Among the attendees were representatives of 28 chemical and pharmaceutical industries, a number of whom were inspired by green industrial methods described in lectures. Industries represented included Matrix Laboratories Ltd., Pfizer Global Research & Development, Emcure Pharma Ltd., Merck Research Laboratories, and Bristol-Myers Squibb Company.

M. Kidwai <kidwai\_chemistry@yahoo.co.uk> is a professor at the University of Delhi and was chairman of the organizing committee for the symposium.

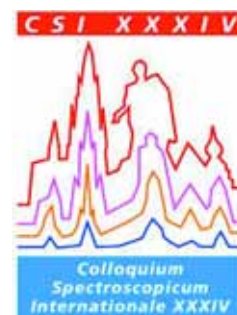
### Analytical Spectroscopy

by René Van Grieken

The **34th Colloquium Spectroscopicum Internationale (CSI-XXXIV)**, held in Antwerp, Belgium, from 4–9 September 2005, was hosted by the University of Antwerp. Since the first CSI conference, organized in Paris, France, in 1949, this prestigious series of biannual conferences has established itself as the premier forum for presentation and discussion of new developments in all branches of analytical spectroscopy. While many conference series decline after 20–30 years, the CSI series is still vigorous, probably because it is a truly international series of conferences. In Antwerp, as in previous conferences, there were participants from about 40 countries and from all continents.

The most recent CSI conferences took place in Granada, Spain (2003), Pretoria, South Africa (2001) and Ankara, Turkey (1999). The next one will be organized in Xiamen, China, from 24–28 September 2007, while in 2009, the event will take place in Budapest, Hungary. The conference alternates, in principle, between Europe and other parts of the world.

Following the tradition of the preceding CSI conferences, emphasis was placed on new developments and applications of spectroscopy in all branches of analytical chemistry. At this conference there were almost 300 participants, and more than 300 abstracts were received for oral and poster contributions. The topics included new research of various spectroscopic techniques and methodologies (such as atomic plasma spectrometry, molecular spectroscopy, organic and inorganic mass spectrometry, X-ray spec-



## Conference Call

trometry, hybrid techniques, laser spectroscopy, imaging techniques, quality control, and chemometrics), as well as applications of spectroscopy in, among others, micro-, surface and interface analysis, speciation, proteomics, environmental and geochemical analysis, and archaeometry and cultural heritage.

The program included 5 invited plenary lectures (by Y. Baba, M. Blades, D. Günther, G.M. Hieftje, and R. Niessner), 8 invited keynote lectures (by A. de Juan Capdevilla, M. Höhn, J. Kolar, A. Laskin, N. Omenetto, C. Gruening, K. Shimizu, and F. Vanhaecke), 120 oral contributions in 20 parallel sessions introduced by the invited speakers, and 3 poster sessions. Two vendor sessions were arranged as well.

During the opening ceremony, the CSI-XXXIV Award was given to Yoichi Gohshi, whose professional career has been of impressive relevance both to X-ray spectrometry and to analytical science in Japan. Gohshi retired recently from the National Institute for Environmental Studies in Tsukuba, Japan, and earlier from the University of Tokyo. This award was sponsored by Wiley, publisher of scientific books and of the journal *X-Ray Spectrometry*, for which Gohshi served for many years as editor for Japan. The laudation for the award was given by Jun Kawai from Kyoto University, one of Gohshi's famous students. After receiving his award, Gohshi highlighted some of his research over the decades.

Furthermore, at the conference dinner, three poster prizes, sponsored by Elsevier, were awarded to Kouichi Tsuji (Osaka City University, Japan), David De Muynck (Ghent University, Belgium) and Gerardo Gamez (Indiana University, USA), and their coworkers.

Besides the interesting scientific contributions, the participants of the CSI-XXXIV conference did find opportunities to sample some of Antwerp's cultural and historical treasures and some of its gastronomy and lifestyle. The city of Antwerp, in addition of hosting one of the most important harbors, the second largest petrochemical complex, and the most important diamond center in the world, also has a unique late medieval historical center, the home of Rubens, and numerous fine museums. The conference itself was held in the medieval "Elzenveld" conference center, which was originally a hospital when built in 1238. It was given to the city of Antwerp by Napoleon was turned into a conference center in 1989. The CSI participants enjoyed the quiet environment and beautiful gardens of the complex, which were especially attractive in the nice summer weather.

The homepage of CSI-XXXIV, including its detailed scientific program, can still be viewed at <[www.csixxiv.ua.ac.be](http://www.csixxiv.ua.ac.be)>. The Website of the next conference in China in 2007 is already in place at <[www.csixxv.org](http://www.csixxv.org)>.

René Van Grieken <[rene.vangrieken@ua.ac.be](mailto:rene.vangrieken@ua.ac.be)> is a professor in the Department of Chemistry, University of Antwerp, Belgium. He served as chairman of CSI-XXXIV.

## ThermoML: New IUPAC Standard for Thermodynamic Data Communications

by Michael Frenkel

A one-day symposium on **ThermoML: Purpose, Structure, and Applications** was held on 27 March 2006 in Atlanta, Georgia, USA, as part of the 231st National Meeting of the American Chemical Society. Speakers from the USA, Canada, UK, Germany, Netherlands, and New Zealand represented all components of the global data delivery process based on ThermoML (Markup Language for Thermodynamics).

Introductory remarks for the symposium were given by Bryan R. Henry, IUPAC president (University of Guelph, Canada); Daniel Friend, acting chief of the Physical and Chemical Properties Division, U.S. National Institute of Standards and Technology; and Catherine T. Hunt, president elect of ACS (Rohm and Haas Company). The announcement of ThermoML as a new IUPAC standard was made on 27 March 2006 by IUPAC President Bryan R. Henry during a special "ThermoML" reception co-sponsored by IUPAC, NIST, FizChemie Berlin (Germany), and Elsevier (Netherlands).

Thermodynamic property data represent a key resource for development and improvement of all chemical process technologies. However, rapid growth



*Michael Frenkel, conference organizer, opens the ThermoML symposium. Seated at the table (from left) are Catherine Hunt, Bryan Henry, and Daniel Friend.*

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*Bryan Henry (left), IUPAC president, announces ThermoML as a new IUPAC standard for thermodynamic data communications during the "ThermoML" reception. He is joined by Michael Frenkel.*

in the number of custom-designed software tools for engineering applications has created an interoperability problem between the formats and structures of thermodynamic data files and required input/output structures for the software applications. Establishment of efficient means for thermodynamic data communications is absolutely critical for provision of solutions to such technological challenges as elimination of data processing redundancies and data collection process duplication, creation of comprehensive data storage facilities, and rapid data propagation from measurement to data-management system and from data-management system to engineering application. Taking into account the diversity of thermodynamic data and numerous methods of their reporting and presentation, standardization of thermodynamic data communications is very complex.

In 2002, IUPAC approved project 2002-055-3-024, "XML-Based IUPAC Standard for Experimental and Critically Evaluated Thermodynamic Property Data Storage and Capture," and established a task group to carry out the project. Michael Frenkel, USA, was the chair of this group, whose members included John Dymond, UK; Erich Königsberger, Australia; Kenneth Marsh, New Zealand; Stephen Stein, USA; and William Wakeham, UK. This project was completed with the establishment of the new IUPAC standard for ThermoML. The full description of ThermoML was published in the March 2006 issue of *Pure and Applied Chemistry*, and the ThermoML namespace has been established on the IUPAC Website.

Michael Frenkel <[frenkel@boulder.nist.gov](mailto:frenkel@boulder.nist.gov)> acted as symposium organizer; for details on the session program see <[www.iupac.org/symposia/2006/ThermoML-symposium.html](http://www.iupac.org/symposia/2006/ThermoML-symposium.html)>. For more information on this project see <[www.iupac.org/namespaces/ThermoML](http://www.iupac.org/namespaces/ThermoML)>.

## Advanced Materials and Polymer Characterization

*by Michael Hess*

The 14th POLYCHAR Conference—Annual World Forum on Advanced Materials was held in Nara, Japan, from 17–21 April 2006 during the Japanese cherry blossom season. One day prior to the main conference, a Short Course on Polymer Characterization was held, which was an educational project of the IUPAC Polymer Division (IV). The organization committee was led by Masaru Matsuo, Nara Women University, chair, and co-chairs Kohji Tashiro, Toyota Technical Institute, Tokyo, and Yoshiyuki Einaga, Nara Women's University.

The annual POLYCHAR conferences have been IUPAC-sponsored for several years and are well-known among scientists interested in the properties and characterization of polymers and the synthesis, processing, and manufacturing of novel polymers. The conference was subdivided into 10 sections:

- Predictive Methods
- Synthesis
- Nanomaterials and Smart Materials
- Mechanical Properties and Performance
- Dielectric and Electrical Properties
- Surfaces, Interfaces, and Tribology
- Rheology, Solutions, and Processing
- Biomaterials and Tissue Engineering
- Natural and Biodegradable Materials and Recycling
- Characterization and Structure—Property Relationships

Due to the high number of participants, two parallel sessions had to be organized for the conference. This is usually not the case with POLYCHAR conferences.



*Paul J. Flory Laureate Koichi Hatada (right) receiving his award from Moshe Narkis.*

## Conference Call

However, this event attracted 240 participants from 35 countries, who presented about 270 contributions (oral and 2 poster sessions). Many students also attended the presentations. It is not so much the intention of the conference to have a high number of participants and parallel sessions but rather to attract young scientists and advanced and graduate students and give them the opportunity to meet with colleagues and well-known scientists to exchange experiences, make contacts and present their results to the scientific community.



*Paul J. Flory Laureate Witold Brostow (right) receiving his award from Moshe Narkis.*

The conference is also the platform for the prestigious Paul J. Flory Research Award, which that was jointly awarded to Witold Brostow, University of North Texas, Denton—for his work on the prediction of long-term reliability of viscoelastic materials and discoveries in tribology—and Koichi Hatada, Fukui University of Technology—for his spectroscopy and other research presented in 390 publications, and also for his efforts to encourage interest among children in materials science and engineering.

Although encouraged by the organizers to present oral contributions, many students' presentation were found in the two poster sessions comprising 136 excellent contributions. Of these presentations, three were

recipients of the IUPAC Student Poster Awards:

- Steven Lamoriniere, Imperial College London (advisor Alexander Bismarck), for his work on composites reinforced with carbon nanotubes
- Kyota Miyamoto, Kyushu University, Fukuoka (advisor Atsushi Takahara), for results on surface and interface structures of blend thin films
- Yumiko Nakano, Nara Women's University (advisors Yuezhen Bin and Masaru Matsuo), for her results on carbonization of poly(vinyl alcohol) films containing carbon fillers and metal dioxides

It is difficult to select particular contributions from the multitude of excellent oral and poster contributions from universities, research institutes, and industry without overlooking important contributions. The full conference program is available at [www.nara-wu.ac.jp/polychar-14/index.html](http://www.nara-wu.ac.jp/polychar-14/index.html).

The Short Course on Polymer Characterization has been an integral part of the conference from the very beginning and is held the day before the conference. The course offers condensed presentations by well-known specialists who provide basic information for students and newcomers in the field and who update participants on popular characterization techniques. A nice feature of the course is that the lecturers are available to participants during the whole conference. Due to the support of the IUPAC Polymer Division, it was possible to waive the fee for the 40 participants.

POLYCHAR-15 will be held in April 2007 in Rio de Janeiro, Brazil. POLYCHAR-16 will be held in Lucknow, India, in January 2008.

Michael Hess <[hi259he@uni-duisburg.de](mailto:hi259he@uni-duisburg.de)> is a professor at the Universität Duisburg-Essen, in Duisburg, Germany. He is a member of the IUPAC Polymer Division and its subcommittee on Polymer Terminology and subcommittee on Polymer Education.



*After conference excursion of the POLYCHAR 14 participants to the cherry blossoms in the Yoshino mountain area.*



# Food and Drug Administration—100 Years of Service

by *Laure Joumel*

On 16 May 2006, the Food and Drug Administration's (FDA) tour of the United States in celebration of its 100th anniversary stopped by the Chemical Heritage Foundation in Philadelphia. Around 250 people came to celebrate and hear speakers from the FDA and the industry consider the history of the administration. Dr. Andrew von Eschenbach, acting commissioner of the FDA, presented his vision for the agency.

The FDA's centennial provides a good opportunity to reflect on its history. The agency, part of the U.S. Department of Health and Human Services, regulates food, drugs, cosmetics, medical devices, dietary supplements, biologics, and blood products.

Suzanne White Junod, FDA historian, provided some perspective on FDA's past, and Peter Barton Hutt, senior counsel for the law firm Covington and Burling and former legal counsel for the FDA, considered "the 10 most important turning points in FDA history."

According to the speakers, the beginnings of drug regulation in the United States can be traced to an 1862 meeting between President Abraham Lincoln and the chemist Charles Wetherill that led to the creation of the Division (later Bureau) of Chemistry within the Department of Agriculture. This year's centennial celebrates the anniversary of the 1906 Food and Drugs Act, signed by President Theodore Roosevelt, which according to Hutt, marked the birth of premarket drug approval. The act also became known as the Wiley Act for the chief chemist's long-standing efforts to secure a law.

In 1927, the bureau was divided into two parts: the Food, Drug, and Insecticide Administration and the Bureau of Chemistry and Soils. Three years later, the

word "Insecticide" was dropped and the Food and Drugs Administration gained its present name.

The 1906 act was extended in 1938 after a health

scandal. A raspberry-flavored sulfa elixir that was not tested before being launched on the market caused the death of more than 100 people. The elixir was mostly composed of diethyl glycol—now known to be poisonous. Due to public outrage, the FDA obtained the right to control every new drug. A second scandal would reinforce the power of the FDA. In 1962, the drug Thalidomide caused an international scare when it was found to cause deformities in babies whose mothers had used it during their pregnancy. After this event, pharmaceutical companies have had to prove to the FDA the safety as well as efficacy of all products they produce.

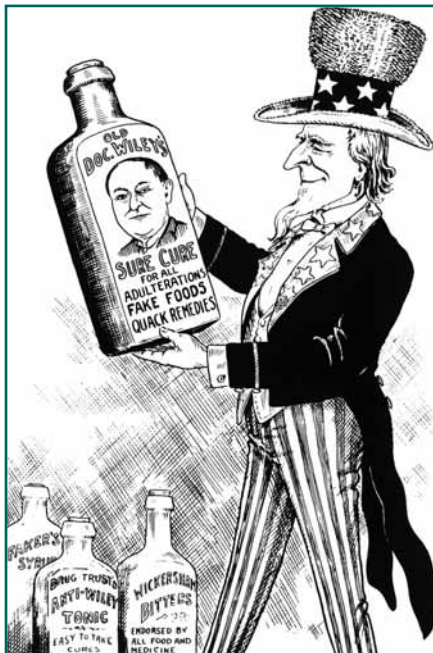
Recent developments in U.S. food and drug regulation include the 1990 requirement that all food packaging have nutrition labeling and health claims. The FDA has introduced measures to allow faster approval for some drugs

and its staff has increased. The Prescription and User Fees Act of 1992 asked companies to pay fees for every new drug application. More recently, government pressure on the FDA to help consumers choose heart-healthy food, resulted in a 2003 measure requiring food producers to note the presence of "trans fat" in their products.

In the realm of drug advertising, the agency has seen its regulatory power reduced despite the vision of the FDA. Since 1997, companies have been able to spend less ad time or space reviewing the side effects of the drugs they market. It is interesting to note that in most countries in Europe and in Asia advertising for prescription drugs is forbidden.

## To Better Communication

Since the Prescription and User Fees Act of 1992, the FDA has been financially dependent on the drug



*J.F. McPhee's 1906 cartoon reflected public expectations concerning the "Wiley Act." The new law, it was hoped, would put a stop to food adulteration and the marketing of quack remedies. Courtesy FDA History Office.*

## Conference Call

industry. During this same period, public suspicion of the drug regulation system has seemed to grow after drugs with dangerous side effects were approved by the FDA. In particular, the Vioxx controversy has Americans asking for more transparency. “We want more information” hears Steven Galson, director of the FDA center for Drug Evaluation and Research.

In 1999, Merck received authorization to sell rofecoxib (Vioxx), a nonsteroid anti-inflammatory drug. In April 2000, a study requested by Merck revealed an increase of myocardial infarcts among people taking the drug. Despite this, Vioxx was still prescribed by doctors. In 2001, *The Journal of the American Medical Association* published a meta analysis that pointed out the risk of infarcts. In response, the FDA warned Merck that their ads were untrue and in 2002 cautioned doctors against the use of Vioxx for patients with coronary disease. However, it was not until 2004 that the drug was withdrawn from the market.

Could another “Vioxx situation” occur? “This controversy about Vioxx has already resulted in large changes” said Galson. “We need to improve FDA communication about emerging drugs,” he said and added, “Even with perfect information and improved analysis there will be disagreement.”

### Toward Individualized Prescriptions

One of the goals of FDA and industry is to better envisage drugs’ side effects. “We want to be able to predict if this drug is or is not for you” said Ronald Krall, senior vice president of worldwide development for GlaxoSmithKline. The aim is to establish a bridge between a study conducted on a sample of the population before commercialization and the real-market population. “By now, we can predict the side effects. We can tell, in some cases, this drug might [cause] nausea or somnolence or sweating,” said Krall. But the goal is to target the patient. Predicting if this patient, in particular, is going to have this side effect and not another one, is the aim, he said. And in the future, companies will correlate one side effect with the other, according to Krall, so the prescription will be individualized.

### Food Issues

Robert Brackett, director of the FDA’s Center for Food Safety and Applied Nutrition, reminded the audience that “76 millions food-borne illnesses, 325 000 hospi-



Courtesy FDA History Office.

talizations, and 5 000 deaths” occur each year in the United States because of food intoxication. He explained how the role of FDA changed after the Pasteurized Milk Ordinance of 1924 because the philosophy of the public changed. Today, we are more aware about nutrition and labeling, but new diseases and ways of transmission have been introduced. New products on the market, like mangos or bean-sprouts, call for new ways of controlling food-borne pathogens.

Acting Commissioner von Eschenbach—who was named one of the 100 most influential people in the world in a May 2006 issue of *Time* magazine—concluded the anniversary day by summarizing his wishes for the future of the FDA and introducing The Oncology Biomarker Qualification Initiative. This collaboration among the FDA, National Cancer Institute, and the Center for Medicare and Medicaid Services is intended to provide modern tools to define biomarkers. According to Eschenbach, these biomarkers will allow the creation of a healthcare and healthcare delivery system in the United States in which medicine will be personalized.

Laure Joumel <laurejoumel@gmail.com> is a freelance writer. She spent part of her summer at the Chemical Heritage Foundation reviewing the Ray G. Neville Collection in the Othmer Library.



[www.chemheritage.org/events/fda](http://www.chemheritage.org/events/fda)  
[www.fda.gov/centennial](http://www.fda.gov/centennial)

An article by John P. Swann titled “How Chemists Pushed for Consumer Protection—the Food and Drugs Act of 1906” was published in *Chemical Heritage*, 24:2, summer 2006, p. 6.

# Mark Your Calendar

Upcoming IUPAC-sponsored events  
See also [www.iupac.org/symposia](http://www.iupac.org/symposia)  
for links to specific event Web site

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 IUPAC poster prizes to be awarded

## 3-7 September 2006 • Polymer Networks • Sheffield, UK

*Functional and Biological Gels and Networks: Theory and Experiment*

Prof. J. L. Stanford, School of Materials, University of Manchester, Grosvenor Street, Manchester M1 7HS, United Kingdom, Tel.: +44 0161 306 3573, E-mail: [john.stanford@manchester.ac.uk](mailto:john.stanford@manchester.ac.uk)

## 3-8 September 2006 • Radical Polymerization • Il Ciocco/Castelvecchio Pascoli, Italy

*International Symposium on Radical Polymerization: Kinetics and Mechanism*

Prof. Michael Buback, Institut für Physikalische Chemie, Universität of Göttingen, Tammannstraße 6 D-37077 Göttingen, Germany, Tel.: +49 5-513-931401, Fax: +49 5-513-93144, E-mail: [mbuback@gwdg.de](mailto:mbuback@gwdg.de)

## 9-13 September 2006 • Chemical Biology • Antalya, Turkey

*9th Eurasia Conference on Chemical Sciences—Innovations in Chemical Biology at the Bridge of Eurasia*

Prof. Bilge Sener, Department of Pharmacognosy, Gazi University, Maltepe, TR-03360 Ankara, Turkey, Tel.: +90 312 212 22 67, Fax: +90 312 213 39 21, E-mail: [bilgesen@gazi.edu.tr](mailto:bilgesen@gazi.edu.tr)

## 10-15 September 2006 • Green Chemistry • Dresden, Germany

*First International IUPAC Conference on Green-Sustainable Chemistry*

Prof. Pietro Tundo, Dipartimento di Scienze Ambientali, Ca' Foscari, University of Venice, Calle Larga S. Marta, Dorsoduro 2137, I-30123 Venezia, Italy, Tel.: +39 41 2348642, Fax: +39 41 2348620, E-mail: [tundop@unive.it](mailto:tundop@unive.it)

## 18-22 September 2006 • High Temperature Materials • Vienna, Austria

*12th International Conference on High Temperature Materials Chemistry (HTMC XII)*

Prof. Dr. Adolf Mikula, Währingstr. 42, A-1090 Vienna, Austria, Tel.: +43 4277 52606, Fax: +43 4277 52679, E-mail: [Adolf.Mikula@univie.ac.at](mailto:Adolf.Mikula@univie.ac.at)

## 27-29 September 2006 • Occupational Health and Safety • Nairobi, Kenya

*Occupational Health and Safety Management in East Africa*

Mr. Kelvin Khisa, Kenya National Cleaner Production Centre, P.O. Box 1360, Nairobi, 00200, Kenya, Tel.: +254 20-604870, Fax: +254 20-604871, E-mail: [kkhisa@cpkenya.org](mailto:kkhisa@cpkenya.org)

## 10-13 October 2006 • Advanced Polymers • Busan, Korea

*Advanced Polymers for Emerging Technologies*

Prof. Sung Chul Kim, Department of Chemical Engineering, Korea Advanced Institute of Sci. & Tech., 373-1 Guseongdong, Yuseong-gu, Daejeon 305-701, Korea, Tel.: +82 42 869 3914, Fax: +82 42 869 8435, E-mail: [kimsc@kaist.ac.kr](mailto:kimsc@kaist.ac.kr)

## 16-20 October 2006 • Chemistry for Life • Havana City, Cuba

*27th Latin American Congress on Chemistry and 6th International Congress of Chemistry and Chemical Eng.*

Prof. Alberto J. Núñez Sellés, Center of Pharmaceutical Chemistry, Sociedad Cubana de Química, Ave 21 & 200, Rpto. Atabey, Apdo. 16042 Havana, CP 11600, Cuba, Tel.: +53 7 218 178, Fax: +53 7 273 6471, E-mail: [alberto.nunez@cqf.sld.cu](mailto:alberto.nunez@cqf.sld.cu)

## 20-23 November 2006 • Polymers for Advanced Applications • Stellenbosch, South Africa

*9th Annual UNESCO/IUPAC Conference on Macromolecules: Polymers for Advanced Applications*

Prof. Ron D. Sanderson, Department of Chemistry and Polymer Science, University of Stellenbosch Private Bag X1, Matieland, 7602, South Africa, Tel.: +27 21 808 3172, Fax: +27 21 808 4967 E-mail: [rds@sun.ac.za](mailto:rds@sun.ac.za)

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 IUPAC poster prizes to be awarded

## 1-2 March 2007 • Clinical Laboratory • Barcelona, Spain

*Fourth European Symposium on Clinical Laboratory and In Vitro Diagnostic Industry,*

Dr. Josep M. Queralto, Hospital de la Santa Creu i Sant Pau, Servei de Bioquímica, Av. S. Antoni M. Claret, 167 Barcelona, 08025, Spain, Tel.: +34 932919022, Fax: +34 932919196, E-mail: [jqueralto@santpau.es](mailto:jqueralto@santpau.es)

## 15-21 April 2007 • Phosphorus Chemistry • Xiamen, China

*17th International Conference on Phosphorus Chemistry*

Prof. Yufen Zhao, Xiamen University, Department of Chemistry, Xiamen, China 361005, Tel.: +86 5922185610 Fax: +86 5922186292, E-mail: [yfzhao@xmu.edu.cn](mailto:yfzhao@xmu.edu.cn)

## Mark Your Calendar

### 21-25 May 2007 • Mycotoxins and Phycotoxins • Istanbul, Turkey

*XIth International Symposium on Mycotoxins and Phycotoxins*

Dr. Hamide Z. Senyuva, Tubitak-Atal, Konya Yolu No. 67, Besevler, 06530, Ankara, Turkey,  
Tel.: +90 312 2124620/ext.14, Fax: +90 312 2123749, E-mail: hamide.senyuva@tubitak.gov.tr

### 26-30 June 2007 • Advanced Materials • Kharkiv, Ukraine

*Modern Physical Chemistry for Advanced Materials (MPC'07)*

Prof. Yuriy Kholin, Materials Chemistry Department, V.N. Karazin Kharkiv National University, Svobods Square 4, Kharkiv 61077, Ukraine, Tel.: +380 57 707 51 26, Fax: +380 57 705 12 61, E-mail: kholin@univer.kharkov.ua

### 16-20 July 2007 • Solution Chemistry • Perth, Australia

*30th International Conference on Solution Chemistry*

Prof. Glenn Hefter, School of Mathematical and Physical Sciences, Murdoch University, Murdoch, WA 6150 Australia, Tel.: +61 8 9360 2226, Fax: +61 8 9360 1711, E-mail: g.hefter@murdoch.edu.au

### 22-27 July 2007 • Novel Aromatic Compounds • Awaji City, Japan

*12th International Symposium on Novel Aromatic Compounds (ISNA-12)*

Prof. Yoshito Tobe, Division of Frontier Materials Science, Osaka University, Toyonaka, Osaka University, Japan, Tel.: +81 6 6850 6225, Fax: +81 6 6850 6229, E-mail: tobe@chem.es.osaka-u.ac.jp

### 2-6 August 2007 • Organometallic Chemistry • Nara, Japan

*14th International Symposium on Organometallic Chemistry Directed Towards Organic Synthesis (OMCOS-14)*

Prof. Koichiro Oshima, Department of Material Chemistry, Graduate School of Engineering, Kyoto University, Kyoto-daigaku katsura, Nishikyo-ku, Kyoto 615-8510, Japan, Tel.: +81-75-383-2437, Fax: +81-75-383-2438, E-mail: oshima@orgrxn.mbox.media.kyoto-u.ac.jp

### 4-12 August 2007 • IUPAC 44th General Assembly • Torino, Italy

IUPAC Secretariat, Tel.: +1 919 485 8700, Fax: +1 919 485 8706, E-mail: secretariat@iupac.org

### 5-11 August 2007 • IUPAC 41st Congress • Torino, Italy

Chemistry Protecting Health, Natural Environment, and Cultural Heritage  
E-mail: IUPAC.2007@unito.it <www.iupac2007.org>



### 2-7 September 2007 • Ionic Polymerization • Bayreuth, Germany

*International Symposium on Ionic Polymerization*

Prof. Axel Müller, MC II / NW II, Universität Bayreuth, D-95440 Bayreuth, Germany, Tel.: +49-921-553399, Fax: +49-921-553393, E-mail: axel.mueller@uni-bayreuth.de

### 23-28 September 2007 • Transactinide Elements • Davos, Switzerland

*Third International Conference on the Chemistry and Physics of the Transactinide Elements (TAN'07)*

Prof. H.W. Gäggeler, Paul Scherrer Institut, Radio- und Umweltchemie, CH-5232 Villigen, Switzerland, Tel.: +41 (0)56 310 24 01, Fax: +41 (0)56 310 44 35, E-mail: heinz.gaeggeler@psi.ch

## Visas

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

## How to Apply for IUPAC Sponsorship

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

<[www.iupac.org/symposia/application.html](http://www.iupac.org/symposia/application.html)>.