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A Sketch Is Worth A Thousand Words

Vision is a sense deeply anchored in our mind. It not only allows us to "look," but far more valuable, vision helps us to "see." Thus, the skill of image making—sketching, painting, or photography—is a universally cherished art. In chemistry, molecular sketches and 3D representations are among the tools used to help us visualize and understand structures and reaction mechanisms. A sketch can also be a memorization technique, that teachers of all disciplines and grades use daily. In this issue of *CI*, two instances remind us that "a sketch is worth a thousand words." The first, extracted from Margolskee's contribution to a *PAC* special topic issue on the science of sweeteners, is appropriately sweet. And, it speaks for itself; see page 26. The second one, which I find delightful, comes from Professor Perrin's very private collection that was on display at the 16th International Conference on Physical Organic Chemistry (San Diego, CA, USA, August 2002); it is called *Distillation II*, see page 33. While *CI* is obviously not an artsy newsmagazine, I often feel that we should put more thinking into sketches, and use "images" to help overcome the complexities and difficulties of our common language. After all, this might also help to improve the "image" of chemistry!

Fabienne Meyers <fabienne@iupac.org>

Past-President's Column

What Lies Ahead for the Union

Having been involved in IUPAC for a long time, it is quite a new experience to realize that the present series of meetings in which I am involved will be my last. I was thinking about the changes that have occurred between the first General Assembly I attended (Lyon 1985) and the Ottawa event, which takes place in 2003. Much has happened, and the rate of change seems to be speeding up, but that is true for all organizations.

However, I wish to use the privilege of writing this column, not so much to look back, but to look forward. But first I want to pay tribute to those many volunteers who have worked so hard to bring about IUPAC's outstanding achievements in chemistry and the related sciences over its 80 plus years of existence. There is no doubt in my mind that some form of international collaboration and standard setting was essential for chemistry, which is the global enabling activity for so much science and technology.

But what lies ahead for the Union? What are the important tasks and problems that are now on our agenda? I will mention only four, though I am sure that many colleagues can list many more. I must remind you that the views I express are mine alone and are not necessarily shared by the Officers or the Bureau.

My first issue is what is often termed "the public appreciation of science and especially chemistry." We are all too aware that during our lifetimes of practicing our beloved science, the way that the "public" regards our efforts has changed from wonderment, admiration, and gratitude, to more critical, ungrateful (as we see it), and more inclined to blame us for environmental damage, poor health, "artificial" food, and more.

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Our first reaction to our realization that the public attitude was changing was to try to reason with people on a logical basis; it was much later that we realized that much of the concern was based on an emotional response, fed in part by a news media that seemed not to employ anyone with any scientific knowledge at all. So the industry, and then others, started to employ "experts" to advise on how the "public" (To paraphrase Einstein "the public is everyone but me.") could be persuaded that chemistry was not to blame for all our afflictions, but could indeed be part of the solutions.



Alan Hayes
IUPAC Past President

There have been several consequences of this adverse public view, one of the more serious being the marked fall off in many countries, particularly in Europe and the USA, of the number of young people who choose to study science and particularly the physical sciences. This is very worrisome both for mainstream science and because of how it will affect the future proportion of people who will have any awareness of the importance of scientific development to society.

Outlining the problem is always the easy bit of the process—What do we do about it? Well, IUPAC has several initiatives to counter the trend. One is the continuing CHEMRAWN program. The newly restructured Committee on Chemistry Education (CCE) has the subject of public appreciation as half of its remit. The Committee on Chemistry and Industry has built up a very significant collaboration with UNESCO on the DIDAC project, which continues to expand and is now a collaborative venture with CCE.

Further effort is needed and one approach is to attain some cooperation and coordination between industry, trade associations, and chemical societies. As often happens when a problem surfaces and develops, different groups each start their own programs. Therefore, it could be that better coordination could lead to more effective and efficient action.

Which leads me to my next issue, the relationship between IUPAC, national chemical societies, and regional associations. May I say at once that I am well aware, by personal experience, that there are several

national chemical societies with whom IUPAC has good, productive relationships, and that, so far as I am aware, all of the chemical societies support IUPAC. However, it has to be admitted that the fact that many of the member NAOs of IUPAC are not chemical societies can lengthen the lines of communication and give the societies the feeling that they are somewhat remote from the heart of IUPAC. This latter point is very important when we remember that the “new” IUPAC emphasizes ensuring a flow of good ideas for new projects to the various Divisions. Many of these project ideas should come via the chemical societies.

It is my view that the Union should liaise more actively, closely, and directly with the national chemical societies and the regional chemical federations. In this day and age when money is in even shorter supply and the pressure on people’s time is so great, it is of prime importance that each group of chemistry organizations be clear about what is their most effective sphere of action. For example, the regional federations do much that is “International”—perhaps IUPAC should become GUPAC, where G stands for “Global.”

Another group with whom I believe we should have a more productive relationship is industry. All the major chemical societies know that the majority of qualified chemists in their countries do not work in academia, yet all the top committees in those societies are populated by academics. This is not because colleagues from industry are excluded, it is largely because the pressures on the industrial people mean that they cannot afford the time. I believe that this is a partially short-term view and should be modified. On the positive side, there is good industry participation in the work of several IUPAC divisions (e.g., the Macromolecular, Chemistry and Human Health, Chemistry and the Environment, and the Chemical Nomenclature and Structure Representation Divisions).

However, I feel that the World Chemistry Leadership Meeting, which held its first meeting at the time of the Brisbane General Assembly, could benefit enormously if it became a forum that included senior representatives of the national chemical societies, regional associations, regional trade associations, and IUPAC. Such a biennial forum would be invaluable in its ability to set a general agenda for action on the agreed-upon major problems facing chemistry, and for helping to synergize strengths and capabilities. May I repeat what I have said many times before, that it is not my view that IUPAC should be representing industry, it has trade associations and its companies to do that, but we do have to recognize that the “A” in IUPAC does stand for “Applied,” and industry is where most application takes place.

Finally there is the issue of how IUPAC can help the beneficial development of chemistry in developing and

economically disadvantaged parts of the world. There are many gaps in IUPAC membership on the world map and by and large they correspond with the developing world. It would be good to get these countries into membership, but it is not easy. Lack of money for membership dues is one obvious factor, but there are others. The lack of educational infrastructure, “brain drain,” and the need for national investment in technology development are also very important factors. Also, even when we do manage to get some participation in the IUPAC programs from scientists in these countries, the difficulties they face, such as travel, are still enormous.

It is my view that the Union should liaise more actively, closely, and directly with the national chemical societies and the regional chemical federations.

IUPAC must solve the problem of involving many more of these countries in coordinating schemes whereby help can be given. Many young chemists have expressed surprise to me that IUPAC does not do more and I feel that we must be more creative. We have good relations with UNESCO UNIDO (United Nations Industrial Development Organization) and UNEP (United Nations Environment Programme), and we also have experience in raising money from various charitable foundations for CHEMRAWN conferences and other activities. I feel that we should focus more of our resources in this area.

So there we are; the ramblings of an old man coming to the end of his IUPAC “career.” Or the musings of an idealist who wishes that he had more years to serve? I haven’t even mentioned the problems of getting younger scientists involved, or of how we cope with keeping up the subscription and publications income, or the structure and function of the Bureau, etc.

My time in IUPAC has been satisfying and fun and I am convinced that the Union will make progress on all the issues that I have mentioned. I have been privileged to meet with lots of wonderful people—thanks for having me.

Dr. Alan Hayes is the current past president of IUPAC, and will retire as Officer at the end of 2003.

PEDECIBA—Programa de DEsarrollo de Ciencias BAsicas

A year ago, Uruguay became part of the IUPAC family, as the Chemistry Area of PEDECIBA became an Associate National Adhering Organization (ANAO). By becoming an ANAO, PEDECIBA provides a point of contact for the chemists in Uruguay and the global chemistry community. *CI* asked a Uruguayan member, Patrick Moyna, to review the origin of PEDECIBA and the significant role of chemistry in the organization.

Chemistry in Uruguay

by Patrick Moyna

In Uruguay, professional studies of pharmacy and chemistry started in the late 19th century at the Instituto de Quimica of the faculty of medicine. In 1929 these courses were combined with those of industrial chemistry (now chemical engineering) of the National Petroleum Company, and the new Facultad de Quimica y Farmacia (now Facultad de Quimica) was established. In the late 1970s the chemical engineering department moved to the Facultad de Ingenieria and became less chemistry oriented.

In spite of a national tradition of wide international contacts, the new college remained rather isolated from international associations. The graduating professionals joined either the Asociacion de Quimica y Farmacia del Uruguay (AQFU) or the Asociacion de Ingenieria Quimica del Uruguay (AIQU), while the small number of Masters and Doctoral graduates in chemistry failed to establish their own association. In the last two decades the AIQU became a member of EFCE (European Federation of Chemical Engineers) and AQFU became member of the International Union of Pharmacology (IUPHAR) although the pharmacy courses are still at the Facultad de Quimica. For this reason, although Uruguayan chemists were always very interested in IUPAC resolutions, there was no official link to the Union.

PEDECIBA Inception

In the early 1970s Uruguay went through a military coup that established a nondemocratic regime that ended in 1985. The small scientific community in Uruguay was concentrated at the University and was almost completely dispersed during those years. The situation troubled the director of the UNESCO regional office in Montevideo, and in the waning months of the regime he organized a committee with some of the few remaining local scientists to develop a program to resume scientific activity with the oncoming democratic government. The Program for the Development of Basic Sciences, (PEDECIBA, or Programa de DEsarrollo de Ciencias BAsicas,) was thus established in 1986 as a joint venture of the Ministry of Education, the National University, and UNESCO. The original

organization was comprised of five main Areas, representing the biological, chemical, physical, mathematical, and computational sciences. Each Area opened a register of active scientists, who were incorporated after presenting their curriculum vitae for evaluation. In this way each Area became a “sui generis” Academy, which included all active scientists working in Uruguay.

Each PEDECIBA Area has an honorary director and a standing committee of four other members, which decides on policies and programs to be developed and



calls for an annual registration of new members. Each committee, which serves for two years, also incorporates one representative of the post-graduate students. The honorary academic staff members (ASMs) are in categories similar to those of the national uni-

versity as full and associate professors and assistants, none of whom receive a salary from the PEDECIBA. Other members include doctoral and master's students, who can hold PEDECIBA bursaries. The ASMs are reevaluated periodically to ascertain their continued activity and productivity.

PEDECIBA was crucial to many Uruguayan expatriates who found ways of reestablishing contacts with their country, and who eventually returned. The national government took up the funding after some time, and established a yearly budget that has increased and decreased following the national financial fortunes. In spite of being very limited, this seed funding has allowed the Uruguayan groups to apply to international funding agencies, yielding a good record of results. Another positive result was that the different Areas applied different policies for their development, and the successful ones have been openly imitated, first by the sibling Areas, and later by the regular laboratories in colleges and ministries, making for a widespread improvement of research activities in the country.

This nonpolitical organization that is solely run by the end users (the scientists), has been much more efficient in improving scientific activities in the country than the “established” systems within the Ministries, or

the Consejo Nacional de Ciencia y Tecnología, or even the national university. Three external evaluations, in 1989, 1996, and 2001, have been instrumental in qualifying PEDECIBA's achievements as outstanding.

The Chemistry Area

As Chemistry was the only Area that was closely connected with an operating College, it could not quickly take advantage of the organizational and funding possibilities opened by the PEDECIBA. The Area began with a very small group of chemists, but it has progressed to include over 100 ASMs. The activities of the Area have helped to integrate chemists who are working outside the Facultad de Química, which is the only national university department where chemistry is taught. At present, there are members from 29 different laboratories, 16 are in the Facultad and 13 are from other colleges or national laboratories.

As a collateral result of the work of the Chemistry PEDECIBA, chemical research and research at the Facultad have progressed greatly. The post-graduate programs in chemistry have advanced both within PEDECIBA and at the university level: less than 5% of the staff at the Facultad had doctoral degrees when the PEDECIBA started in 1986, and now 59% has achieved that level; the number of publications of Chemistry ASMs was under one paper per year during the 1987-1995 period and climbed to over two per year in the 1996-2001 period; the Facultad is now responsible for the origin of over 20% of the total Uruguayan scientific productivity (according to the Institute of Scientific Information), although it gets less than 3% of the total national university's budget; many of these results are now going into local industries under an active PEDECIBA-sponsored academia-industry linked system.

The members of the Chemistry Area realized that Uruguay had no international linkages to IUPAC or other chemical societies and, after discussions with the PEDECIBA central committee, applied for ANAO status to IUPAC, suggesting that the other Areas associate with other members of ICSU. Although it is an unusual ANAO, the PEDECIBA has shown extremely positive results for the development of chemical sciences in Uruguay and has been able to expand the positive results outside its own operation. We hope to further improve by taking advantage of the new connections through IUPAC, learning what colleagues have done abroad, and contributing with our expertise to the further advancement of chemical sciences worldwide.

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www.rau.edu.uy/pedeciba

Snapshot of Uruguay

Nationality: *noun:* Uruguayan(s); *adjective:* Uruguayan

Language: Spanish

Land boundaries: total: 1 564 km

Border countries: Argentina 579 km, Brazil 985 km

Coastline: 660 km

Uruguay population: 3.1 million

Estimated number of research scientists: 1 100, including 300 in chemistry

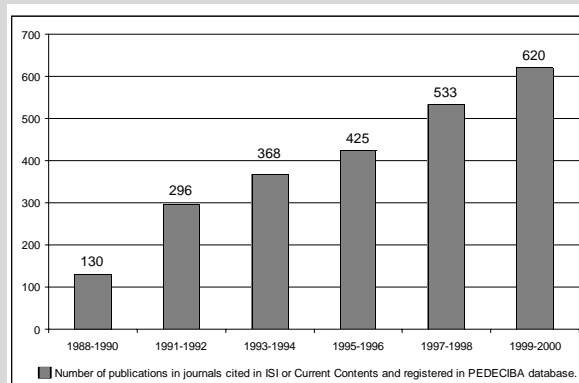
Estimated number of professional chemists: 2 100 (i.e., 1 200 chem. pharm. and 900 chem. eng.)

PEDECIBA (as of July 2002)

Postgraduate (M.Sc. and Ph.D.) students and graduates: 831

Total number of students and researchers: 756

Chemistry students and researchers: 195 (second after Biology with 390)



Number of times that Uruguayan research has been published in journals cited in ISI or Current Contents and registered in PEDECIBA database, 1988 to 2000.

Budget allocation over the period 1987-2002:

Equipment and publications: 58%

Human resources training: 27%

Administration: 10%

Supplies: 5%

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Scientific and Technical Information

IUPAC Representative's Report on the 2002 ICSTI General Assembly

by Wendy Warr

I have the pleasure to be IUPAC's representative to ICSTI, the International Council for Scientific and Technical Information <www.icsti.org>. ICSTI is a forum for interaction between organizations that create, disseminate, and use scientific and technical information. It is unique in its breadth of membership—primary and secondary publishers, database producers, government departments, national libraries, and users from across the world—because it represents such a broad range of interests in a multiplicity of scientific disciplines.

The ICSTI General Assembly is hosted by a different member organization each year. Recent meetings have been held in South Africa, the United States, Scotland, Taiwan, and Germany. Next year's meeting will be held in Canada. At this year's meeting there was a representative from every major land mass except Antarctica.

The 2002 Assembly was hosted in June by KTHB, the library of the Royal Institute of Technology in Stockholm, Sweden, which had celebrated the opening of a splendid new building the month before. The assembly hosts arranged for tours of the new facility and a visit to the Viking site of Birka. The Council Dinner was held in Stockholm City Hall, emulating the December 2001 Nobel Laureates' formal dinner. Such functions, which, in my opinion General Assembly hosts use legitimately and hospitably out of national pride, have led detractors to suggest that ICSTI is some sort of social club for those in the higher echelons of information organizations. This has certainly not been the case while IUPAC has been a member, although I have noticed a certain change in focus.

Some years ago, there was much discussion about the role of professional publishers and on copyright issues as publishers struggled to find new, money-making



Wendy Warr
and Tony Davies

arrangements in the changing world of electronic publishing. Nowadays, there is much more discussion about "free" information and how to provide access to those in the Third World. Indeed, at the Stockholm ICSTI meeting, the Swedish International Development Agency invited observers from the National Information System for Science and Technology in New Delhi, India, and from

the Sri Lanka Scientific and Technical Information Center. Access for all was also one of the main underlying themes at the second UNESCO/ICSU Conference on Electronic Publishing in Science, supported by ICSTI, and held in Paris in February 2001. A detailed report is available online. At the public conference in Stockholm, a representative of the Institute of Physics in Mexico also presented a paper on the "digital divide."

A one-day conference, open to the public, is held in conjunction with each ICSTI General Assembly. This year's theme was "Scientific information: the challenges of creating and maintaining access." Papers of particular

interest to me, personally, were presented by Uwe Assmann of Linköping University, on



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the second generation Web; by Ian Butterworth of Imperial College, London, on academic user behavior in accessing scholarly information; and by Mayur Amin of Elsevier Science, whose publisher viewpoint revealed some of the inconsistencies in user perceptions. The conference papers, or at least the presenters' slides, will appear in a next issue of ICSTI's journal *Forum*; see the Web site <www.icsti.org/forum>.

ICSTI also funds a number of projects under the auspices of its technical activities and information policy committees. One project worth mentioning here is Henry Kehiaian's "IUCOSPED" numeric data standardization effort. This work was supported in a small way by IUPAC about two years ago, and that was instrumental in raising further financial support from the International Council for Science (ICSU) and ICSTI. A final report is to be presented to the CODATA (ICSU Committee on Data for Science and Technology) General Assembly in October 2002. A Data Explorer portal, built on an Oracle database, will reportedly be made available at FIZ Karlsruhe.

ICSTI is currently very interested in ensuring that digital data is permanently archived. ICSTI, ICSU, and CODATA sponsored a seminar in February 2002 to consider the challenges. Tony Davies, secretary of the IUPAC Committee on Printed and Electronic Publication (CPEP), has written a useful article about this (see box below). Other projects, amongst many, have involved classifications and glossaries, knowledge management, the EU Copyright Directive, and work with the Ingenta Institute on access to journals through subscriptions and document delivery. In January 2003, ICSTI will be involved with two meetings on the public domain and open access to scientific and technical information generated by public institutions.

ICSTI's Secretariat is under new management and the organization's officers (who serve on a voluntary

basis) are actively ensuring that ICSTI's meetings and projects meet the rapidly changing needs and interests of its 50 or more member organizations. IUPAC and the International Unions of Physics and Crystallography are three of the nine members in the international category. I conclude that IUPAC and ICSTI continue to receive mutual benefits from the networking within this global community.

Wendy Warr <wendy@warr.com>, managing consultant at Wendy Warr & Associates in the United Kingdom, chairs the IUPAC Committee on Printed and Electronic Publications.



www.iupac.org/standing/on/icsti

Cometh A Digital Dark Age?

by Tony Davies

I was fortunate enough to represent IUPAC at the recent ICSTI (International Council for Scientific and Technical Information) seminar on the Digital Preservation of the Records of Science hosted by UNESCO in Paris over 14 and 15 February. The topics covered were an eye opener for an analytical spectroscopist. I had thought that over the years we had managed to supply our field with a range of widely implemented international data standards capable of guaranteed long-term digital archiving. I suppose I was rather proud of what we had achieved as a community of users, manufacturers, and industry. I now realize we are the lucky ones. The rest of the scientific world are currently running scared of what now appears to be the advent of the so-called "Digital Dark Ages." In this issue I will highlight the reasons for the meeting at UNESCO and what urgently needs to be achieved on a global scale.

There is a general worry in the international scientific community that the moves toward electronic production and presentation of sci-

entific data will lead to serious deficits in the archiving of the records of science. The first meeting on this topic was organized in January 2000 by ICSTI. A progress review in 2001 established the urgent need for a second meeting, which was hosted by UNESCO this February.

The objectives of the February meeting were outlined as follows:

- to ensure all the interests in digital preservation in science are aware of all current activities in the field
- to evaluate the needs for coordination of the efforts
- to create any necessary structures and work programs to ensure coordination of the activities

It was decided that future meetings should also deal with the following issues:

- What are the varieties and future uses of scientific and technological information that must and will be archived?
- What is the minimum amount of information (data fields) needed to locate and identify information and who is creating what kinds of standards related to location and basic identification?

- What business and information models are appropriate and how should access to the digital archives be arranged?
- Where are the common issues with the preservation of more general cultural archives and how can these be accommodated?

The Seminar

The seminar started with the usual welcoming speeches and an explanation of the interests of the sponsoring organizations. There then followed two days of specialist presentations from interested scientific organizations, international representative bodies, and renowned speakers from the scientific publishing industry.

For me, one of the most worrying revelations during the two-day meeting was the current acute fear amongst science historians, which was reported by William Anderson of CODATA. He used a phrase, which at the time was completely new to me, in revealing that there is imminent danger in the arrival of a new "Dark Age," wherein our scientific cultural heritage may be permanently lost through the exclusive use of electronic media. This Dark Age will become more severe when electronic laboratory notebooks finally became integrated into the normal working environment. The

danger of this new era was highlighted by an example of the problems archivists are now struggling with.

A worrying example was used to highlight the problem of archiving electronic material. Following the death of an eminent British scientist, his widow presented his archive material to the British Library for posterity. The problem was, however, that there is effectively no infrastructure available in this national archive for handling two old personal computers and boxes of old format disks!

The Debate on What to Archive?

A large amount of time was devoted to discussion on exactly what should be archived; however, no general agreement was reached. The data community (probably heavily influenced by the FDA 21 CFR Part 11 rules currently revolutionizing pharmaceutical IT) thought that all information needed to be stored, whereas the traditional archivists looked at the logistics

that electronic-only publications be archived. This international legal loophole urgently needs to be closed and will apparently be addressed during the Spanish presidency of the European Union. It will be interesting to see how the Council of Ministers deals with this thorny subject.

On an international level it was clear that the classic role of the librarian as archivist is outdated and being continually undermined by the digital presentation of scientific publications. An ever-increasing proportion of library budgets is being spent on digital-only subscriptions to peer-reviewed scientific journals. These electronic journals are maintained off-site and accessed through the Internet—often on a pay-per-view basis. The librarians cannot archive this material, as it never physically lands in the individual organizations. It was generally agreed that it is foolish to expect the publishers to take over the role of archivists and so another

What was strikingly clear was that the projects were not coordinated and any benefit would probably end with the funding.

Not Just a Problem for Scientists!

Having only just become aware of the phrase “Digital Dark Age,” you can imagine my complete surprise when browsing through one of the bookshops at Newark International Airport two weeks later, I discovered a brand new book *Dark Ages II—When Digital Data Die* by Bryon Bergeron, a teacher at Harvard Medical School and MIT (published by Prentice Hall PTR, Upper Saddle River, New Jersey 07458, USA, ISBN 0-13-066107-4, www.phptr.com). Much of this interestingly written book, which contains many anecdotes, directly addresses the problem of long-term data archiving. Written in clear, normal language, it is not a tacky techie tome for IT freaks. Instead, it has good advice for everyone from home computer users to managers of corporate networks. Bergeron

attacks “Bloatware” succinctly and provides many useful links to more detailed information sources such as the US NARA (National Archives and Records Administration) Center for Electronic Records guidelines. The table on page 9, extracted from the book, gives an idea of the level of the advice the book offers.



Unfortunately, we are currently in the situation that science archivists have well-established practices for handling paper legacies, but currently have terrible problems when presented with digital content.

and demanded that only selected content land in the electronic archives.

Although there is a legal requirement for publishers to deposit to their national archives all material printed in that particular country, there is no equivalent law requiring

mechanism needs to be put in place.

A series of presentations dealt with individual limited-term projects that were or had been run in various countries funded by the Mellon Foundation, the EU, and by different national governments.

Meeting Outcome

One of the messages that came out of the meeting was the clear need for a more active advocacy effort to make scientists aware of the encroaching danger and, especially, of the heritage value of their work, which they should be careful to

Expected Media Lifetimes under Ideal and Typical Conditions.
(Extracted and adapted from *Dark Ages II*, Chapter 3, page 82.)

Storage medium	Ideal lifetime (years)	Typical lifetime (years)	Comments
CD-R	5-100	2-30	Dye less stable than pits used in commercial CD-ROMs
CD-ROM	30-200	5-50	Uses pits on a metal surface to encode data-fragile surface
DVD	100	20	Higher density susceptible to environmental changes
DVD-R	20-30	10	As with CD-R less stable than commercial media
Hard disks	?100	10-20	Lifetime is down to stability of the mechanical parts
Magnetic tape	30-100	5-20	Rewind periodically to release tension
WORM	30-200	5-50	Formats not as standardized as for CD-ROMs and DVDs
Paper Buffered	?500	50-500	!
Photographic print	?200	?100	Assuming non-acid paper and stored out of light (non Polaroids!)
Microfilm	500	100-200	Standard for archives

make available to archivists. As digital preservation will not be a cheap exercise it was seen as important that the need be expressed at many levels in order to convince those who control the different budget sources of the vital nature of this work. ICSTI will take the lead in this area.

The different needs of the text archivists as opposed to the data archivists were clear to all by the end of the meeting. This was especially the case during discussions on metadata content. From my own recent experiences working with FDA 21 CFR part 11 compliance systems, I can see that the issues of exactly what metadata is worthy of storage and how to obtain it is still a critical factor in an industry well advanced in archiving digital content. Among those sciences just feeling their way into this field, there are those who cannot currently agree on what constitutes metadata!

I was surprised by the depth of thought given to this issue by many of the contributors to the seminar.

There were a number of well-constructed arguments, such as those presenting the desire for a “technology watch” on current archival computing systems. This technology watch will need to be established in order to warn in advance of

... there is no equivalent law requiring that electronic-only publications be archived.

upcoming mitigation needs when computer hardware or software on which the archives are reliant are about to become outdated.

Developing countries reported that they need help, not only in the area of the preservation of science information, but also with more exposure, which they currently lack.

Conclusions

Okay, all I can say is worry! Basically, we should all be rather worried about the current status of born-digital scientific information. Fortunately, the current precarious state of our science legacy has been spotted and there are now international initiatives underway at a political level to secure the significant funding required for establishing the necessary infrastructure. We can only hope that they are successful. Maybe by talking about the problems with our colleagues we can raise awareness and support those striving to find appropriate solutions.

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<www.spectroscopyeurope.com>.

Macromolecular Nomenclature and Terminology

A Brief History of IUPAC Activities

With the preparation of a revised edition of the so-called “Purple Book”—the *Compendium of Macromolecular Nomenclature*—well underway, the secretaries of the former IUPAC Commission on Macromolecular Nomenclature have drafted the commission’s history and reviewed 50 years of activities.

by *Máximo Barón, Norbert Bikales Bikales, Robert Fox, and William Work*

From the 1920s, as polymer science developed and came of age, so too a common language came into being through the efforts of individuals who recognized the need for such a language. They formed committees to consider issues that included not only systematic nomenclature, but terminology and definitions, symbols, and other matters that might affect communication. All of this effort forms a part of the prehistory of the work of the Macromolecular Division on Nomenclature and Terminology.

Subcommission on Nomenclature

IUPAC’s first report on macromolecular nomenclature was published in 1952 by the Subcommission on Nomenclature of what was then the IUPAC Commission on Macromolecules. That report,¹ which drew on the talents of such remarkable individuals as J. J. Hermans, M. L. Huggins, O. Kratky, and H. F. Mark, was a landmark in that, for the first time, it systematized the naming of macromolecules and certain symbols and terms commonly used in polymer science. It introduced the use of parentheses in source-based polymer names when the monomer from which the polymer is derived consists of more than one word, a practice that is now widely followed. The report also recommended an entirely new way of naming polymers based on their structure that included the suffix “amer,” a recommendation that has been almost totally ignored. After 10 years, the subcommission issued its second report,² which dealt with the then-burgeoning field of stereoregular polymers. A revision³ of definitions in the original report appeared four years later. In 1968, a summary report⁴ of the activities of the subcommission was published.

Commission on Macromolecular Nomenclature (Commission IV.1)

In 1968, the Commission on Macromolecular Nomenclature of the Macromolecular Division (Division IV) was established under the chairmanship of K. L. Loening. L. C. Cross was initially secretary and then R. B. Fox. A series of major documents was produced that shaped modern polymer language. Most

noteworthy was one that defined basic terms^{5,6} and another on structure-based nomenclature for regular single-strand polymers.^{7,8} The latter, originally developed by the Nomenclature Committee of the Polymer Division of the American Chemical Society and refined by the Commission, revolutionized polymer nomenclature by providing a systematic, consistent scheme particularly well adapted to indexing; it became the standard for *Chemical Abstracts* and major polymer journals throughout the world. A list of standard abbreviations was published⁹⁻¹¹ and later revised.¹²

As the 1970s came to a close, A. D. Jenkins assumed the chairmanship, with R. B. Fox continuing as secretary through 1979, to be succeeded by N. M. Bikales, who served until 1987. In the 1980s, the Commission produced a complete revision of the stereochemical definitions;¹³⁻¹⁴ terminology for molar masses in polymer science;¹⁵ an extension of structure-based nomenclature to inorganic and coordination polymers;¹⁶⁻¹⁷ the systemization of source-based nomenclature for copolymers;¹⁸ two key documents dealing with physicochemical terminology in the polymer field, one covering definitions for individual macromolecules, their assemblies, and dilute solutions¹⁹ and the other concerned with crystalline polymers;²⁰ a new method of classifying polymers;²¹ and a basic classification and definitions of polymerizations reaction.²² These documents were completed under the chairmanship of P. Kratochvíl, who assumed those duties in 1985; W. J. Work was elected

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Secretary in 1987. In 1991, the first edition of the *Purple Book*²³ was published. The compendium was the first major compilation of the commission and consisted of an introduction to macromolecular nomenclature and nine chapters corresponding to the then valid IUPAC recommendations.

The final decade of the century saw the activity of the Commission continue unabated. R. F. T. Stepto succeeded to the chairmanship in 1991, and he, in turn, was succeeded by M. Hess in 2000. M. Barón became secretary in 1998. Graphical representation of polymer structures was addressed for the first time in 1994.²⁴ In the course of this decade, a revised and enlarged glossary of basic terms²⁵ was published, along with definitive documents dealing with the terminology of polymer aging and degradation²⁶ and non-ultimate mechanical properties;²⁷ terminology concerned with liquid-crystal polymers was also published.^{28,29} In the field of structure-based nomenclature, the commission published recommendations covering regular double-strand polymers³⁰ and irregular single-strand polymers,³¹ and a revision of the commission's 1975 rules for structure-based nomenclature⁸ was completed.³² In 1997, a document concerned with a new area, source-based nomenclature for nonlinear macromolecules and macromolecular assemblies,³³ was published. A document on definitions relating to stereochemically asymmetric polymerizations³⁴ was prepared in 2000. A document on source-based generic nomenclature for macromolecules³⁵ was published in 2001.

At the end of the 1990s, the commission had formed active Working Parties considering many new aspects of polymer science. In various stages of preparation were documents concerned with the terminology or nomenclature of polymer composites and blends, inorganic composites, hyperbranched macromolecules, and cyclic macromolecules (including macromolecular rotaxanes and catenanes). Definitions in the fields of kinetics and thermodynamics of polymerization, and polymerization processes and polymers in dispersed systems were under consideration. A general guide to polymer terminology and nomenclature and a document on polymer class names were nearly complete.

Subcommittee on Macromolecular Terminology

Effective 1 January 2002, the Bureau and Council of IUPAC decided to form a new Division of Chemical Nomenclature and Structure Representation (Division VIII) to deal with nomenclature in an integrated manner across all branches of chemistry. In keeping with this change and the change to project-based funding, the Commission on Macromolecular Nomenclature decided to become the Subcommittee on Macromolecular Terminology of Division IV. The development was timely as it reflected the change in the emphasis of the work the commission was carrying out. Over the last

decade, under the chairmanship of R. F. T. Stepto and M. Hess, the majority of projects had been concerned with terminology, related particularly to polymer and polymer-based materials. However, the subcommittee also continues to work on macromolecular nomenclature in collaboration with the new Division VIII. With the current feasibility studies underway and the projects due to be completed, it may be expected that the next decade and beyond will see a continued proliferation of recommendations dedicated to the improvement of communication in polymer science.

Translations of Nomenclature and Terminology Recommendations

Although the nomenclature and terminology recommendations have all been published in English, those involved with the publishing have purposefully pursued their further dissemination and discussion in other languages, including Chinese, Croatian, Czech, French, German, Japanese, Korean, Polish, Portuguese, Russian, and Spanish. Over the years, there has been no doubt about the global influence of the recommendations on the language of chemistry. A list of translations can be obtained from <www.iupac.org/divisions/IV/compendium.html>.

A list of members of the commission can be obtained at <www.iupac.org/divisions/IV/IV.1/history.html>.

References

- 1 Report on Nomenclature in the Field of Macromolecules. *J. Polym. Sci.* **8**, 257-277 (1952). (now obsolete)
- 2 Report on Nomenclature Dealing with Steric Regularity in High Polymers. *J. Polym. Sci.* **56**, 153-161 (1962). (superseded by ref. 14)
- 3 Report on Nomenclature Dealing with Steric Regularity in High Polymers. *Pure Appl. Chem.* **12**, 645-656 (1966); *Macromol. Chem.* **82**, 1-15 (1965). (superseded by ref. 14)
- 4 Report of the Committee (*sic* Subcommittee) on Nomenclature of the International Commission on Macromolecules. *J. Polym. Sci.*, Part B, **6**, 257-260 (1968). (now obsolete)
- 5 Basic Definitions of Terms Relating to Polymers. IUPAC *Inf. Bull. Append.* No. **13** (1971). (superseded by ref. 24)
- 6 Basic Definitions of Terms Relating to Polymers 1974. *Pure Appl. Chem.* **40**, 477-491 (1974). (superseded by ref. 25)
- 7 Nomenclature of Regular Single-Strand Organic Polymers. IUPAC *Inf. Bull. Append.* No. **29**, (1972); *Macromolecules* **6**, 149-158 (1973); *J. Polym. Sci.*, Polym. Lett. Ed. **11**, 389-414 (1973). (superseded by ref. 32)
- 8 Nomenclature of Regular Single-Strand Organic Polymers (rules approved 1975). *Pure Appl. Chem.* **48**, 373-385 (1976). (superseded by ref. 32)
- 9 Recommendations for Abbreviations of Terms Relating to

- Plastics and Elastomers. *Pure Appl. Chem.* **18**, 581-589 (1969). (now obsolete)
- 10 List of Abbreviations for Synthetic Polymers and Polymer Materials. IUPAC *Inf. Bull. Append. No.* **12**, (1971). (superseded by ref. 12)
 - 11 List of Standard Abbreviations (Symbols) for Synthetic Polymers and Polymer Materials 1974. *Pure Appl. Chem.* **40**, 473-476 (1974). (superseded by ref. 12)
 - 12 Use of Abbreviations for Names of Polymer Substances (IUPAC Recommendations 1986). *Pure Appl. Chem.* **59**, 691-693 (1987).
 - 13 Stereochemical Definitions and Notations Relating to Polymers (provisional). *Pure Appl. Chem.* **51**, 1101-1121 (1979). (superseded by ref. 14)
 - 14 Stereochemical Definitions and Notations Relating to Polymers (IUPAC Recommendations 1980). *Pure Appl. Chem.* **53**, 733-752 (1981). (see also ref. 34)
 - 15 Note on the Terminology of the Molar Masses in Polymer Science. *Macromol. Chem.* **185**, Appendix to No. 1 (1984); *J. Polym. Sci., Polym. Lett. Ed.* **22**, 57 (1984); *J. Coll. Interface. Sci.* **101**, 277 (1984); *J. Macromol. Sci., Chem.* A21, 903-904 (1984); *Br. Polym. J.* **17**, **92** (1985).
 - 16 Nomenclature for Regular Single Strand and Quasi-Single-Strand Inorganic and Coordination Polymers (provisional). *Pure Appl. Chem.* **53**, 2883-2302 (1981). (superseded by ref. 17)
 - 17 Nomenclature for Regular Single Strand and Quasi-Single-Strand Inorganic and Coordination Polymers (IUPAC Recommendations 1984). *Pure Appl. Chem.* **57**, 149-168 (1985). (see also ref. 32)
 - 18 Source-Based Nomenclature for Copolymers (IUPAC Recommendations 1985). *Pure Appl. Chem.* **57**, 1427-1440 (1985).
 - 19 Definitions of Terms Relating to Individual Macromolecules, their Assemblies, and Dilute Solutions (IUPAC Recommendations 1988). *Pure Appl. Chem.* **61**, 211-241 (1989).
 - 20 Definitions of Terms Relating to Crystalline Polymers (IUPAC Recommendations 1988). *Pure Appl. Chem.* **61**, 769-785 (1989).
 - 21 A Classification of Linear Single-Strand Polymers (IUPAC Recommendations 1988). *Pure Appl. Chem.* **61**, 243-254 (1989).
 - 22 Basic Classification and Definitions of Polymerization Reactions (IUPAC Recommendations 1994). *Pure Appl. Chem.* **66**, 2483-2486 (1994).
 - 23 *Compendium of Macromolecular Nomenclature*, Blackwell Scientific Publications, Oxford, 1991. (contains 9 chapters that are, respectively, reprints of refs. 6, 14, 19, 20, 8, 17, 18, 21, and 12).
 - 24 Graphic Representations (Chemical Formulae) of Macromolecules (IUPAC Recommendations 1994). *Pure Appl. Chem.* **66**, 2469-2482 (1994).
 - 25 Glossary of Basic Terms in Polymer Science (IUPAC Recommendations 1996). *Pure Appl. Chem.* **68**, 2287-2311 (1996).
 - 26 Definition of Terms Relating to Degradation, Aging, and Related Chemical Transformations of Polymers (IUPAC Recommendations 1996). *Pure Appl. Chem.* **68**, 2313-2323 (1996).
 - 27 Definitions of Terms Relating to the Non-Ultimate Mechanical Properties of Polymers (IUPAC Recommendations 1997). *Pure Appl. Chem.* **70**, 701-754 (1998).
 - 28 Basic Definitions of Terms Relating to Low-Molar-Mass and Polymer Liquid Crystals (IUPAC Recommendations 2001). *Pure Appl. Chem.* **73**, 845-895 (2001).
 - 29 Basic Definitions of Terms Relating to Polymer Liquid Crystals (IUPAC Recommendations 2001). *Pure Appl. Chem.* **74**, 493-509 (2002).
 - 30 Nomenclature of Regular Double-Strand (Ladder and Spiro) Organic Polymers (IUPAC Recommendations 1993). *Pure Appl. Chem.* **65**, 1561-1580 (1993).
 - 31 Structure-Based Nomenclature for Irregular Single-Strand Organic Polymers (IUPAC Recommendations 1994). *Pure Appl. Chem.* **66**, 873-880 (1994).
 - 32 Nomenclature of Regular Single-Strand Organic Polymers (IUPAC Recommendations 2001). *Pure Appl. Chem.*, in press.
 - 33 Source-Based Nomenclature for Non-Linear Macromolecules and Macromolecular Assemblies (IUPAC Recommendations 1997). *Pure Appl. Chem.* **69**, 2511-2521 (1997).
 - 34 Definitions Relating to Stereochemically Asymmetric Polymerizations (IUPAC Recommendations 2001). *Pure Appl. Chem.* **74**, 915-922 (2002).
 - 35 Source-Based Generic Nomenclature for Macromolecules (IUPAC Recommendations 2001). *Pure Appl. Chem.* **73**, 1511-1519 (2001).

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www.iupac.org/divisions/IV/IV.1

Aligning the Revised Red and Blue Books and Preparing for IUPAC Preferred Names

by Ture Damhus

At the 2001 IUPAC General Assembly in Brisbane, Australia, the former Commissions on Nomenclature of Organic and Inorganic Chemistry (CNO and CNIC, respectively) began discussions on a project to avoid conflict between the preferred names for organic nomenclature and the revision of inorganic nomenclature. The project arose from the fact that CNO was working on a revision of the "Blue Book" and its supplemental *Guide*—to become one revised Blue Book—and CNIC was working on a revision of the "Red Book." (See box below.)



Ture Damhus

The need for alignment of these two areas of nomenclature was clear given that the revised Blue Book had as a main feature the introduction of *preferred names*. That is, among the various names that can often be constructed for a given compound using the nomenclature principles endorsed by IUPAC, one name was to be designated the preferred one, ready to offer to users who would like to have always just one name. It turned out that a number of inorganic compounds were also represented with preferred names in the drafts of the revised Blue Book. This requires a bit more of an explanation.

The main principle of organic nomenclature as laid out in the Blue Book is that of naming compounds on the basis of parent compounds by applying standard operations, mainly substitution, whereby the parents are modified in order to arrive at the structure of the compound being named. This is *substitutive nomenclature*. (Examples include 'trichloroacetic acid', where the numerical prefix 'tri' together with the prefix 'chloro' indicates substitution of the three methyl group hydrogen atoms in acetic acid by chlorine, and 'butan-2-ol', obtained by modifying the parent name 'butane' by introducing the 'ol' suffix and the locant '2'.)

Many parent compounds are hydrides, such as butane and naphthalene, and a number of them are inorganic

hydrides, i.e., they do not contain carbon, such as gallane (GaH_3) and selenane (SeH_2). Other parent compounds are organic or inorganic oxoacids, such as acetic acid, CH_3COOH , and phosphonic acid, $\text{PH}(\text{O})(\text{OH})_2$. The parent names are important for the naming of organic derivatives and thus had a prominent place in the drafts of the revised Blue Book. However, the former Commission on Nomenclature of Inorganic Chemistry felt that it was premature to designate the inorganic parent names themselves as preferred. The revised Red Book will not contain preferred names for the simple reason that the working group does not think the chemistry community is ready to select preferred names for inorganic compounds at large. The choice will often be difficult for inorganic compounds; compare examples given below.

The general problem of selecting parent structures and the desire to extend the naming principles of coordination chemistry to broader areas of inorganic chemistry had led inorganic chemists to favor *additive nomenclature* over substitutive nomenclature. Additive names specify compounds according to the way they are formally assembled from particular building blocks (*central atoms* and *ligands*).

A simple example may illustrate the general points made above. Take a neutral molecular compound like PCl_5 . Traditionally, it would be named 'phosphorus pentachloride'. This type of name will be called a *compositional* name (of binary type) in the revised Red Book. By systematic additive nomenclature, its name is 'pentachloridophosphorus'. (In the revised Red Book, ligands in additive names now carry the 'ido' ending rather than just the 'o' ending used before.) By substitutive nomenclature, starting from the parent hydride PH_5 , its name becomes 'pentachloro- λ^5 -phosphane'. Now, which of the three names does one want to choose as the preferred one? The first name is what everybody uses. The next two belong to two different systematic approaches, one of which prevails in inorganic chemistry, the other in organic chemistry. Neither of the two systems can be

Red Book—*Nomenclature of Inorganic Chemistry (Recommendations 1990)*, Leigh, G. J. (Blackwell Science, 1990, ISBN 0-63202-4941)

Blue Book—*Nomenclature of Organic Chemistry*, Rigaudy, J. and Klesney, S. P. (Pergamon, 1979, ISBN 0-08022-3699)

Supplement—*Guide to IUPAC Nomenclature of Organic Compounds (Recommendations 1993)*, Panico, R.; Powell, W.H.; and Richer, J.-C. (Blackwell Science, 1994, ISBN 0-63203-4882)

The revisions of these books should be completed in 2003.

extended to all of chemistry without creating sometimes extremely cumbersome and unfamiliar-looking names. Division lines have to be drawn through chemistry and most probably also through inorganic chemistry, and this will require more careful thinking than the Red Book group presently has time for. It is generally anticipated in IUPAC that a new project will be set up to address the issue of inorganic preferred names once the Red Book revision has been finished.

For organometallic compounds (compounds with a bond from a carbon atom to a metal atom), the question arises whether to use substitutive or additive nomenclature. Consider $\text{Pb}(\text{C}_2\text{H}_5)_4$. By substitutive nomenclature, the name is 'tetraethylplumbane', with reference to the parent hydride plumbane, PbH_4 , and the additive name is 'tetraethyllead' (or tetraethanidolead). Which one should be preferred? In the alignment project, there was support for a proposal made by W. H. Powell that prescribes where to draw the line between organometallic compounds that will have preferred substitutive names and those that will have preferred additive names. This proposal is being discussed among members of the Chemical Nomenclature and Structure Representation Division (Div. VIII) Advisory Committee and will probably be incorporated into the Blue Book and Red Book more or less in its present form.

In conclusion, the 'ane' hydride names are needed for a number of preferred organometallic names and, within inorganic chemistry, for constructing substitutive names that may or may not end up being preferred names in the future, depending on where the borderline is drawn between substitutive and additive nomenclature. Therefore, those parent hydride names will be given both in the Red Book and Blue Book. As an interesting aside, there was a problem in giving an 'ane' name to indium trihydride, InH_3 . The name 'indane' is occupied for a particular parent ring system in organic chemistry. The name 'indiane' would present problems when derived names containing the sequence '. . . indiene' could be misinterpreted as indicating the presence of two double bonds. The latter is maybe less of a problem, but nevertheless, the proposal being considered at present is the name 'indigane', which should not lead to confusion and which is in accord with the historical origin of the word 'indium' as related to an indigo-blue spectral line.

There are organic derivatives of inorganic parents that present a particular problem. Consider a compound like $\text{C}_2\text{H}_5\text{As}(\text{Cl})(\text{OH})\text{S}$. It could be named *substitutively* on the basis of the parent hydride AsH_3 , λ^5 -arsane. It could also be named additively. However, neither of these options is chosen in practice. There is an extensive system of names for derivatives of certain inorganic oxoacids whereby this compound would be named 'ethylarsonochloridothioic acid'. This name is based on the

substitution of a hydrogen atom by an ethyl group, and the replacement of the oxo group and one hydroxy group in the parent arsonic acid, $\text{HAs}(\text{O})(\text{OH})_2$, by sulfur and chloride, respectively. There are related oxoacids called

$\text{As}(\text{O})(\text{OH})_3$	arsenic acid or arsonic acid
$\text{AsH}(\text{O})(\text{OH})_2$	arsonic acid
$\text{As}(\text{OH})_3$	arsenous acid, arsorous acid
$\text{AsH}(\text{OH})_2$	arsonous acid
$\text{AsH}_2(\text{O})\text{OH}$	arsinic acid
$\text{AsH}_2(\text{OH})$	arsinous acid

which are all needed as parents when naming various organic derivatives according to this particular type of nomenclature called *functional replacement nomenclature*. The problem with these oxoacid names from the inorganic point of view is that they stem from an antiquated system for indicating oxidation states using the endings 'ous' and 'ic'. Compare with names like 'ferrous' and 'ferric', which were officially abandoned about 50 years ago (although they are difficult to get entirely rid of!) in favor of indications of oxidation state by Stock numbers (iron(II) oxide, etc.) or by charge numbers (iron(2+) oxide, etc.), because the 'ous' and 'ic' names were ambiguous. (The name 'ferric' only says it is a higher oxidation state than 'ferrous', but not *which* oxidation state.) There is no way to know what 'arsinous acid' is unless you are given a table of formulas to memorize it from, whereas the additive name 'dihydrodihydroxidoarsenic', although a bit longer, immediately tells you that the structure is $\text{AsH}_2(\text{OH})$. (But the latter name cannot be used as a parent name in functional replacement nomenclature.)

It was therefore not acceptable to institute the 'ous' and 'ic' names as preferred names for the oxoacids themselves. The agreement was made in the alignment project that these names are kept available as parent names for giving preferred names to the organic derivatives, but no decision was made regarding the status of the parent names themselves. Having said this, a number of names are of course in daily use all over chemistry (e.g., sulfuric acid, arsenic acid) and the Red Book team has no intention to prohibit the use of those well-entrenched names. They will be given in the revised Red Book alongside systematic additive names (which may or may not end up being the preferred ones later).

The Red Book chapter on substitutive nomenclature, in a draft form, was also reviewed in the alignment project. The process here consisted not just in naming specific compounds, but in inspecting the rules and ensuring they were consistent with the rules for substitutive nomenclature given in the Blue Book. And finally, a number of names of organic ligands needed for the Red

Book were checked for consistency with the (new) Blue Book rules.

The formal name of this project, # 2001-031-1-800, is "Alignment of nomenclature in areas of overlap between the preferred names for organic nomenclature and the revision of the nomenclature of inorganic chemistry." The project task group consisted of Henri Favre and Warren H. Powell, who represented the task group revising the Blue Book that will replace the 1979 Blue Book and the 1993 Guide; Gerry P. Moss, who represented the IUBMB-IUPAC Joint Commission on Biochemical Nomenclature; and Richard Hartshorn and myself (task group chairman), who represented the team working on a revision of the Red Book that will replace the 1990 version. At its meetings, the group also had participation from Neil G. Connelly, editor in chief of the revised Red Book; Herbert D. Kaesz, the last chairman of the former Commission on Nomenclature of Inorganic Chemistry where the Red Book revision proj-

ect was initiated; and Alan D. McNaught (ADM), president of Division VIII on Chemical Nomenclature and Structure Representation. ADM also hosted the meetings at the facilities of The Royal Society of Chemistry in Cambridge.

I would like to thank Warren H. Powell and Alan McNaught for helpful comments on a draft of this article.

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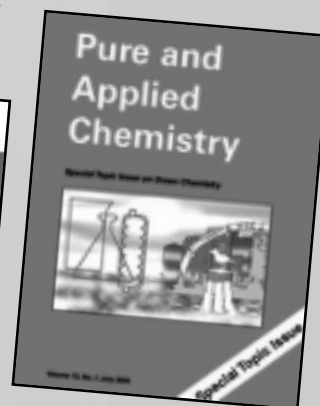
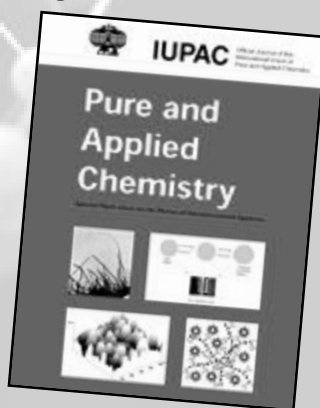
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IUPAC News

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by Fabienne Meyers

Since we work hard at making [iupac.org](http://www.iupac.org) up to date, versatile, and accurate, last summer I thought that I would enter the site in a contest for "Best Chemical Sites on the Web," sponsored by ChemIndustry.com Inc.; John Wiley & Sons, Inc.; and the Royal Society of Chemistry,

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UK. I had nothing to lose and hoped to get a little feedback. On 1 September 2002, the winners and honorees were announced, and I am pleased to report that www.iupac.org was chosen as an honoree in the "Portals and Information Hubs" category.

The awards recognize unique and noteworthy Internet resources for chemists, chemical engineers, and chemical industry professionals in three categories: "Online Courses and Tools," "Portals and Information Hubs," and "Corporate Sites." The sites must be in English and free to users. An international panel of 16 distinguished judges in various chemical fields selected the winners. In the category "Portals and Information Hubs," there were 41 contestants. The winner in this category was the NIST Webbook, which is a comprehensive database of chemical data. We can be proud of putting [iupac.org](http://www.iupac.org) in the good company of a number of resourceful sites. See for yourself the following list:

The Winner:


Webbook, a comprehensive database of chemical data provided by NIST <webbook.nist.gov>

Category Honorees:

- Chemweb, a chemistry community portal <www.chemweb.com>
- SpecialChem, a polymer additives focused online service <www.specialchem.com>
- Integrated Spectral Data Base System for Organic Compounds, by the National Institute of Advanced Industrial Science and Technology, Tsukuba, Ibaraki, Japan <www.aist.go.jp/RIODB/SDBS/menu-e.html>
- MatWeb, a searchable database of chemical names and properties <www.matWeb.com>
- SIS, a chemical information portal by the National Library of Medicine <chem.sis.nlm.nih.gov>
- The portal of the International Union of Pure and Applied Chemistry <www.iupac.org>
- The chemistry portal of the American Chemical Society <www.chemistry.org>

The official announcement and more information about the contest can be found at <www.chemindustry.com/contest>.

Questions, comments about the IUPAC Web site, please contact Fabienne Meyers <fabienne@iupac.org>.




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Awards and Honors

Dana Knox Receives the Franzosini Award

Paolo Franzosini, professor of Physical Chemistry at the University of Pavia, Italy was an enthusiastic supporter of the Solubility Data Project. He had almost completed Volume 33 of the *Solubility Data Series* when he died suddenly on 24 January 1985. His colleagues Paolo Ferloni, Alberto Schiraldi, and Giorgio Spinolo efficiently completed the volume. In 1988, Franzosini's wife, with the encouragement of his colleagues, very generously donated the payments for Volume 33 to the Solubility Data Commission (V.8) to establish the Franzosini Award. The award is given to a promising young contributor to the Solubility Data Project (SDP) to help them attend, in even years, the International Symposium on Solubility Phenomena (ISSP) and, in odd years, the annual meetings of the commission. As of

Franzosini Award are listed in the table below.

The Franzosini Award of 2002 was given to **Dr. Dana Knox** in appreciation of his continuous contributions to the Solubility Data Project. His expertise in solution thermodynamics, including better representation of high-pressure phase equilibria, such as supercritical solubilities has led to the following project on Solids and Liquids in Supercritical Carbon Dioxide, which belongs to the section on Solubility Data Related to Industrial Processes. See the Web site for the project description <www.iupac.org/projects/2002/2002-045-1-500.html> or page 20, under "New Solubility Data Projects."



Dr. Dana Knox

Carbon dioxide itself is an important industrial solvent. The corresponding volume will contain comprehensive compilations and evaluations of the existing data on the solubility of solids and liquids in supercritical CO₂. Processing using supercritical fluids is an increasingly important area worldwide. Such processes, with their significant variation in solubility with pressure, permit the accomplishment of many processes that would be otherwise very difficult to achieve. Further, systems that employ carbon dioxide as the solvent are particularly attractive as CO₂ is environmentally friendly.

Dr. Knox is associate professor of Chemical Engineering and Environmental Science within the Department of Chemical Engineering at the New

Jersey Institute of Technology (USA).

Franzosini Award Winners*

Year	Venue	Recipient	Promoter
1989	15th meeting, Lund, Sweden	Rumen Duhlev (Bulgaria)	Chr. Balarew
1990	16th meeting, Troy, NY, USA 4th ISSP	Pirketta Scharlin (Finland)	R. Battino
1991	17th meeting, Hamburg, Germany	A. Pacheco Tanaka (Peru)	A. Namor
1992	18th meeting, Moscow, Russia 5th ISSP	Stefan Gradinarov (Bulgaria)	Chr. Balarew
1993	19th meeting, Lisbon, Portugal	Michel Ferriol (France) and Teresa Calvet (Spain)	M.-Th. Cohen-Adad
1994	20th meeting, Buenos Aires, Argentina 6th ISSP	Erich Königsberger (Austria)	H. Gamsjäger
1995	21st meeting, Guildford, UK	Felix José Sueros (Peru)	A. Namor
1996	22nd meeting, Leoben, Austria	_____	_____
1997	23rd meeting, Geneva, Switzerland	_____	_____
1998	24th meeting, Niigata, Japan 8th ISSP	Lan-Chi Tran-Ho (Austria)	H. Gamsjäger
1999	25th meeting, Berlin, Germany	Chiara Milanese (Italy)	A. D'Aprano
2000	26th meeting, Hammamet, Tunisia 9th ISSP	Vladimir Zbranek (Czech Republic)	J. Eysseltová
2001	27th meeting, Brisbane, Australia	Justin Salminen (Finland)	P. Scharlin
2002	1st meeting SSED, Varna, Bulgaria 10th ISSP	Dana E. Knox (USA)	R. P.T. Tomkins

*established by Mrs. M. C. Franzosini in 1998 at the 14th SDP meeting, Surrey, UK.

2002, the chair of the new Subcommittee on Solubility and Equilibrium Data (SSED) receives nominations for the award (The capital is held by IUPAC and the IUPAC Secretariat does the accounting.). The recipients of the



www.iupac.org/divisions/V/502

IUPAC Projects

New SIT Software Makes Speciation Calculations Easier

Metal ion speciation in environmental systems is a hot topic because speciation is strongly linked to bioavailability. For labile systems, the speciation can be determined by equilibrium modelling calculations to give the well known "speciation diagram," a plot of composition (species concentration) vs. pH or composition vs. metal/ligand ratio.

Speciation calculations require values for the stability constants of all the species that may form from the system components. These values must be valid at the ionic strength of the medium concerned. Here is a major problem: the vast majority of equilibrium constants have been determined at a fixed ionic strength that is typically much higher (ca. 0.1-1.0 M) than applies in freshwater environmental systems (<0.02 M).

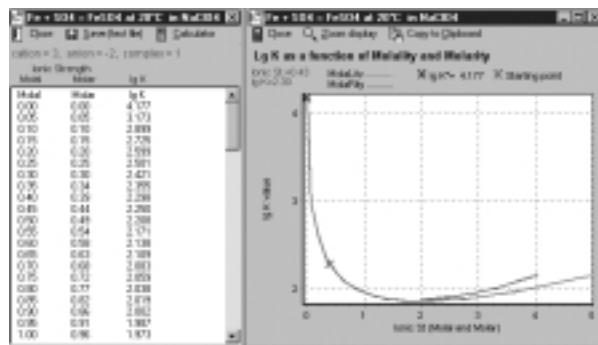
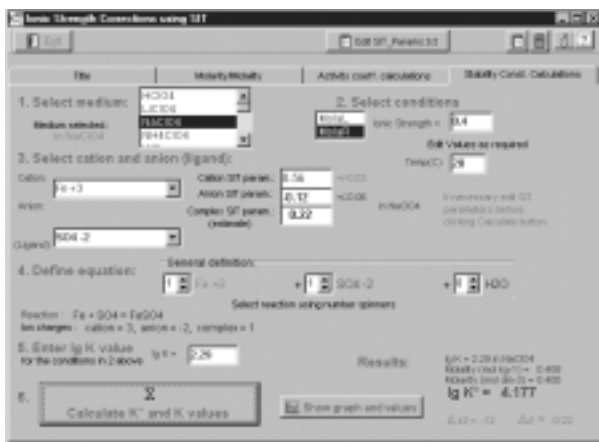
To correct the stability constants to the required ionic strength one must be able to calculate the activity coefficients of all species in the equilibrium reaction. These corrections may be quite large (e.g., $\log K_1$ for the reaction $\text{Fe}^{3+} + \text{nta}^{3-}$ is 16.26 for $I=0.10$ M NaClO_4 and the value calculated for $I=0.001$ M is 17.89).

The second problem is that not all equations for activity coefficient calculations (e.g., Debye-Hückel and Davies [eqn. 1]) are valid to such high ionic strengths:

$$\log \gamma_i = -Az_i^2\{1/2/(1+1/2)-0.3I\} \quad (1)$$

Specific Interaction Theory, or **SIT** (and Pitzer parameters), provides a valid tool for calculating stability constants over a wide range of ionic strengths. The calculations are not trivial; they require a database of ionic coefficients, $\epsilon_{M,X}$, for each ion-ion interaction:

$$\log \gamma_M = -Az_i^2\{1/2/(1+1.5I^{1/2})+\epsilon_{(M,X)}m_X\} \quad (2)$$



Now for the easy and exciting part! An IUPAC project, undertaken by L. D. Pettit of Academic Software, has produced the SIT program that will calculate:

- ionic activity coefficients in a user-specified medium, up to 5.0 molal
- stability constants in the range 0-5.0 m, based on published values at a single ionic strength
- molarity from molality, and vice versa

This is an enormous asset for those involved in speciation calculations. It is a user-friendly program that is now in the public domain at <www.iupac.org/projects/2000/2000-003-1-500.html>. Interested persons are invited to test the SIT program and send comments to the author. The program includes a comprehensive, but not exhaustive, file of SIT parameters. The file can be edited, but if users have access to reliable SIT parameters that are not included, please send these to the author at <www.acadsoft.co.uk> so that the release version of the program can be updated for all to benefit.

The SIT program can be readily applied to industrial processes for which stability constants may be required at very high ionic strengths.

Two other IUPAC products will assist in the understanding and application of stability constants. The IUPAC Stability Constant database, **SC-database**¹ should be a starting point for stability constant data. It links data directly to the program **SPECIES** that will calculate speciation curves. The **HELP** files in the database provide definitions and information about temperature, ionic strength, and solvent effects. For a much wider discourse, the program **Sol-Eq**² explains the principles of solution equilibrium and explores many applications in environmental, biological, and industrial systems. It includes a primer on how to do your own speciation calculations.

1 **SC-database**, Stability Constants Database; IUPAC, Academic Software. 2001.

2 Sol-Eq. Solution equilibria: Principles and Applications. Academic Software. 2001.

Both of these programs are available to order via <www.acasoft.co.uk>.

Reviewed by Kip Powell, vice president, Analytical Chemistry Division.

 www.iupac.org/projects/2000/2000-003-1-500.html

Recommendations for NMR Measurements of High pK Values and Equilibrium Constants in Strongly Basic Solutions

Nuclear Magnetic Resonance (NMR) is a well-established, powerful method for monitoring the dissociation of acidic groups. Chemical shift-pH titration is widely used with potentiometric measurements within $2 < \text{pH} < 12$ and also as an alternative to the glass electrode at high ($\text{pH} > 12$) and low ($\text{pH} < 1$) pH-range. In the former case an excellent agreement between potentiometric and NMR equilibrium data obtained in the same background medium could be observed. For extremely high and low hydrogen ion concentrations it is believed that NMR provides more accurate data.

Unlike “normal” procedure, the chemical shift-pH titration of highly basic solutions normally requires a complete change of the background electrolyte composition (e.g., 1 M NaCl to 1 M NaOH). Moreover, frequently a titration under variable ionic strength has to be used in order to measure anomalously high (low) pK values. At the same time, little is known about the NMR chemical shift sensitivity of different nuclei to the effects that are not associated with particular chemical protonation/deprotonation equilibrium (e.g., to the “indifferent” supporting electrolyte concentration and a drastic variation of its composition as well as to the presence of internal reference and uncontrolled $\text{D}_2\text{O}/\text{H}_2\text{O}$ ratio).

At high pH such background electrolytes as sodium and potassium salts form undissociated NaOH and KOH species. Usually this process is not accounted for in acidity constants calculations. Another problem with these salts is a complex formation with an acid under the study. This normally leads to a significant decrease in pK values.

At the same time, the comparison of pK values for different acids requires the data obtained under similar conditions (e.g., $I=0.1$ M or 1.0 M). This raises the problem of high pK value measurement at a common ionic strength with reasonable accuracy.

Everyday practice reveals a large diversity of experimental approaches to the chemical shift-pH titration

procedure: internal (external) references; D_2O , H_2O or $\text{D}_2\text{O}/\text{H}_2\text{O}$ solvents; titration at a constant (variable) ionic strength; use of different nuclear. As a result, a large disagreement for high (low) pK data could be observed.

A recent IUPAC project is intended to indicate some real and possible sources of errors in chemical shift-pH titration at high (low) pH range and to formulate some recommendations for this procedure.

For more information, contact the Task Group Chairman K. Popov <ki-popov@mtu-net.ru>. Additional task group members are H. Rönkkömäki and L. H. J. Lajunen.

 www.iupac.org/projects/2001/2001-038-2-500.html

Performance Evaluation Criteria for Preparation and Measurement of Macro- and Microfabricated Ion-Selective Electrodes

During the past several years, the application of microfabrication technologies of practical microsensor devices has entered the field of biology and medicine and is beginning to serve as the driving force for discoveries in cell biology, neurobiology, pharmacology, and tissue engineering. In parallel, the methodology of ionophore-based liquid membrane ion-selective electrodes (ISEs) has now entered the arena of trace analysis and precision science due to the latest updated and upgraded research and development of this method. This circumstance has made it necessary to also upgrade and update the evaluation criteria for the preparation and measurements of ISEs, primarily microfabricated ISEs and potentiometric cells. This is in fact the purpose of this project.

There are more or less generally accepted evaluation criteria for ISEs. Some of those are summarized in *Pure and Applied Chemistry* documents (*PAC* 1994, **66**, 2527; *PAC* 1995, **67**, 507).

In this new document, we will deal with the specialties of macro- and microfabricated ISE sensors; standard procedures for the microfabricated devices are much more critical compared to macroelectrodes. In addition, some evaluation criteria for the micro reference electrodes are of the same importance. Items we will discuss include the following:

- conditioning of the multilayered sensor system (sensing membrane, underlying hydrogel; and eventually biocompatible coating) before use to reach high stability readings, due to water transport through the membrane
- conditioning overnight or storage in humid atmosphere

- conditioning and calibration before and after the measurement
- effect of osmotic pressure (give a procedure, how to measure)
- shelf and use lifetime (effect of storage); estimation of the residual lifetime in vivo and in vitro
- added-site optimization for selectivity and as requisite for Nernstian response
- electrode construction including microfabrication, FET covered with membranes, and Ppy electrode covered with membranes
- response time as well as detection limit
- microfabricated inner- and outer-reference electrodes

We will correct the inconsistencies in the previous document (*PAC* 1994, **66**, 2527) (e.g., the definition of the calibration plot, which contradicts the convention related to the determination of pH). Finally, we will discuss the latest results concerning the lower detection limit, true selectivity coefficients, and twice Nernstian slopes, etc.

For more information, contact the Task Group Chairman Yoshio Umezawa
umezawa@chem.s.u-tokyo.ac.jp.



New Solubility Data Projects

One of the major functions of the IUPAC Subcommittee on Solubility and Equilibrium Data (formerly IUPAC Commission V.8) is to publish authoritative texts on all aspects of solubilities. The main output of this subcommittee is the ongoing series of volumes in the IUPAC-NIST *Solubility Data Series*, or simply the *SDS*. The priority subjects to be pursued over the next three years within the framework of this Solubility Data Project were approved by the Analytical Chemistry Division on 2 July 2002. In this context, compilations and evaluations of experimental solubility data in the following three fields are in progress:

1) Solubility Data of Compounds Relevant to Mobility of Metals in the Environment

Solubilities in aqueous media of sparingly soluble metal salts such as carbonates play an important role in chemical processes. Solubility phenomena (i.e., dissolution and precipitation reactions) frequently control procedures for preparing, separating, and purifying chemicals. Moreover, interactions of the hydrologic cycle with the cycle of rocks, as well as the naturally occur-

ring dissolution of minerals in water and their precipitation on the ocean floor and in sediments of rivers and lakes, can often be simply described in terms of solubility equilibria.

In addition, solubility measurements have been shown to be a powerful tool for the determination of thermodynamic properties of sparingly soluble metal salts. The total concentration of alkaline earth and transition metals in carbonate-bearing natural waters is predominantly determined by the solubilities of the respective hydroxides, oxides, hydroxide carbonates, and neutral carbonates. A careful determination of thermodynamic data of sparingly-soluble metal salts is an essential prerequisite for the geochemical modeling of the release of trace elements from waste repositories. Clearly, a comprehensive compilation and evaluation of the existing solubility data is an invaluable basis for all sorts of predictive models in this field. Presently three volumes are in preparation: 1) alkaline earth metal carbonates; 2) metal carbonates (Mn, Fe, Co, Ni, Cu, Zn, Ag, Cd, Hg, Pb); and 3) inorganic actinide compounds.

2) Solubility Data Related to Oceanic Salt Systems

The oceanic salt system comprises the ions Na^+ , K^+ , Mg^{2+} , Ca^{2+} , Cl^- , and SO_4^{2-} . Extended evaporitic deposits in Europe (Germany, Netherlands, Spain, France, Poland, Russia); North America (Canada); South America (Brazilia); Africa (Congo); and Asia had been formed from these ions during the evaporation-crystallization processes of seawaters in geological times. Geological surveying of these deposits, potash mining, rock salt mining, fertilizer production, and usage of rock salt mines as repository for nuclear or chemical wastes require the exact knowledge of solubility equilibria in the multicomponent oceanic salt system within a broad range of temperatures. At present, solution mining of magnesium chloride for magnesium metal production is performed or is in the planning stage in a number of places (Netherlands, Congo, Thailand, and Uzbekistan). In addition, evaporation and aerosol formation from oceans are important controlling factors for the world's



Solubility data is essential to industries such as rock salt mining.

climate. In order to formulate material and energy exchange models, it is crucial to understand the coupling of evaporation and crystallization processes within the droplets transported into the upper atmosphere. Climate changes from past time periods are manifested in the complex evaporitic deposition patterns, which are interpreted on the basis of the solid-liquid equilibria of the multicomponent oceanic salt system.

Presently two volumes are under way: 1) binary systems containing sodium, potassium, and ammonium sulfate; and 2) magnesium chloride-water and calcium chloride-water and their mixtures.

3) Solubility Data Related to Industrial Processes

Gas solubility is one of the fundamental properties of various gas absorption processes in the chemical industry. The removal of carbon dioxide from gas mixtures is a necessary and expensive step in many processes. It is of particular importance, for example, in the purification of ammonia synthesis gas, in the synthesis of liquid fuels from coal, and in the upgrading of fuel gases. Absorption with suitable solvents provides a convenient method for the removal of CO₂. In enhanced oil recovery, carbon dioxide is used to displace the hydrocarbons from the reservoir and the solubility of CO₂ in the hydrocarbons is important to ensure that miscibility occurs, with a concomitant increase in the oil recovered. In addition, processing using supercritical fluids is an increasingly important area worldwide. Systems that employ carbon dioxide as the solvent are particularly attractive as CO₂ is environmentally friendly.

The availability of accurate and reliable information on the equilibrium solubility of CO₂ in absorbing solvents as a function of temperature and pressure is of utmost importance in the rational design of gas-treating units. Such data will allow more economical construction and more nearly optimum operation of gas-treating plants. Thus, compiled and evaluated data on the solubility of CO₂ in various industrially important aqueous solvents and solvent mixtures are very much sought after.

Presently, three volumes are in preparation: 1) CO₂ in aqueous nonelectrolyte solutions; 2) CO₂ and the lower alkanes at pressures above 2 bar: part 1, methane to butane; and 3) solids and liquids in supercritical CO₂.

Because of the diversity of industrial processes sometimes pending problems have to be tackled when there is sufficient individual expertise and interest from contributors. Thus, volume four concerning the solubility of lead sulfate is in preparation. Lead sulfate in aqueous and non-aqueous solvents continues to present problems in the design and manufacture of the still very important lead-acid batteries.

Acetonitrile is one of the best extractive distillation solvents for separation of close boiling paraffinic and olefinic hydrocarbons. As the chemical process industry seeks more efficient and less energy-intensive separation techniques, liquid-liquid extraction based on selec-

tive solubilities is becoming more common. Volume five, which is being produced, covers this issue.

Reviewed by Heinz Gamsjäger, chairman of Subcommittee on Solubility and Equilibrium Data.



www.iupac.org/divisions/V/502

Concepts and Structure for Requests in Clinical Laboratories

Laboratory medicine measurements and other examinations are made in the context of requests from physicians and reports back to the physicians. The request for measurements and examinations is typically embedded in a request to the laboratory phrased in the medical language of the requester and using conceptual dimensions and granularity levels appropriate to a particular patient's case and the discipline of the requester. Requests usually are formatted within the framework of an electronic healthcare record system (or as a paper request) and are transmitted using an electronic health care information system carried via a communication standard protocol (i.e., HL-7 or Med-RPT). In this project, a solution for the problem of dealing with the request concept in at least three contexts—healthcare information system, communication standard, and clinical laboratory—will be sought.

The strong context dependency of the part of the request containing the medical information and questions asked is in contrast to the part dealing only with measurements or other examinations, but the two are clearly related. The project is set up to define concepts and outline structures for requests in laboratory medicine, taking into consideration the former commission's nomenclature and syntactic rules that are meant to promote and maintain scientifically and conceptually sound ways of expressing the outcome of measurements and other examinations in laboratory medicine.

For more information, contact the Task Group Chairman Urban Forsum <urban.forsum@ihm.liu.se> or visit the Nomenclature, Properties, and Units in Laboratory Medicine subcommittee Web page at <www.iupac.org/divisions/VII/VII.C.1>.



[www.iupac.org/projects/2001/
2001-058-1-700.html](http://www.iupac.org/projects/2001/2001-058-1-700.html)

Properties and Units for Transfusion Medicine and Immunohaematology

Unambiguous expression of properties will assist in fulfilling safety and legal requirements in the handling of

blood products intended for transfusion and organs intended for transplantation. The C-NPU (Committee on Nomenclature, Properties and Units)—maintained as a joint activity of the International Federation of Clinical Chemistry and Laboratory Medicine (IFCC) and IUPAC—has as its main task to promote and maintain scientifically and conceptually sound ways of expressing the outcome of measurements and other examinations in laboratory medicine. The NPU coding scheme and vocabulary, based on the international system of units, concepts theory, and high-level international standards, is the main outcome and should be the cornerstone for expressing measurements within international communication standards. Thus, the task in this project is to work out properties and units for transfusion medicine and tissue typing based on the former C-NPU concepts and syntactic rules.

It is a characteristic of the fields of transfusion medicine and tissue typing that the properties examined may involve both nominal, ordinal, differential, and rational scales. Thus, the project will establish the metrological and logical basis for expressing such properties. In addition, the necessary international coding scheme identifiers and code values will have to be chosen as required by interlaboratory transmission between databases. In this respect, active collaboration and/or endorsement by the International Society of Blood Transfusion will be sought.

For more information, contact the Task Group Chairman Urban Forsum <urban.forsum@ihm.liu.se>



[www.iupac.org/projects/2001/
2001-059-1-700.html](http://www.iupac.org/projects/2001/2001-059-1-700.html)

Global Use of the C-NPU Concept System for Properties in Toxicology

The objective of this project is to work out properties and units for global use of the C-NPU (Committee on Nomenclature, Properties and Units) concept system and syntactic rules for properties in toxicology.

The C-NPU, maintained as a joint IFCC-IUPAC activity for two decades, has as its main task to promote and maintain scientifically and conceptually sound ways of expressing the outcome of measurements and other examinations in laboratory medicine. The NPU coding scheme and vocabulary, based on the SI system, concepts theory, and high-level international standards, is the main outcome and should be the cornerstone for expressing measurements within international communication standards.

During the first meeting (3-4 August 2002), a first draft by J. H. Duffus was discussed that involved properties in toxicology based on the general structure elaborated by C-NPU. The C-NPU concept system was proven to be appropriate for that purpose as demonstrated by a large number of typical examples. For the next meeting (5-6 December 2002), a draft comprehensive list will be prepared for discussion and after corrections it will be distributed for comments among appropriate organizations and individual specialists.

For more information, contact the Task Group Chairman W. R. Külpmann <kuelpmann.wolf@mh-hannover.de>



[www.iupac.org/projects/2001/
2001-066-1-700.html](http://www.iupac.org/projects/2001/2001-066-1-700.html)

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Highlights from Pure and Applied Chemistry

Presenting recently published IUPAC technical reports and recommendations

Definitions Relating to Stereochemically Asymmetric Polymerizations (IUPAC Recommendations 2001)

by K. Hatada, J. Kahovec, M. Barón, K. Horie, T. Kitayama, P. Kubisa, G. P. Moss, R. F. T. Stepto, and E. S. Wilks
Pure and Applied Chemistry, Vol. 74, No. 6, pp. 915-922 (2002)

Asymmetric polymerization has been of interest to many academic and industrial polymer scientists, but IUPAC has made no explicit reference to the classification and definitions of reactions involving the asymmetric synthesis of polymers. This document presents definitions concerned with asymmetric and related polymerizations, with examples included to clarify the meaning of the definitions.

Asymmetric polymerization is defined as “A polymerization that proceeds in an unsymmetrical manner in terms of chirality under the influence of chiral features present in one or more components of the reaction system.”

The asymmetric polymerizations embrace two main categories, “asymmetric chirogenic polymerizations”

and “asymmetric enantiomer-differentiating polymerizations,” which are defined as follows:

Asymmetric chirogenic polymerization: An asymmetric polymerization in which the polymer molecules formed contain one (or more) new type(s) of elements of chirality not existing in the starting monomer(s). (See example below.)

Asymmetric enantiomer-differentiating polymerization: An asymmetric polymerization in which, starting from a mixture of enantiomeric monomer molecules, only one enantiomer is polymerized. (See example below.)

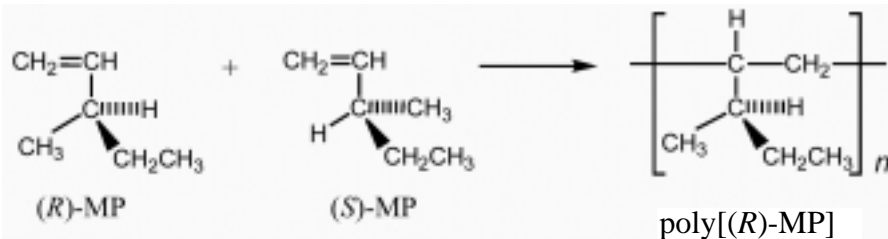
Some asymmetric chirogenic polymerizations give helical polymer molecules of only one screw sense that usually show optical activity due to the helicity. These polymerizations are termed “asymmetric helix-chirogenic polymerizations.”



www.iupac.org/publications/pac/2002/7406/7406x0915.html



An example of asymmetric chirogenic polymerization: Polymerization of penta-1,3-diene by 1,4-addition with an optically active catalyst gives an optically active polymer comprising configurational repeating units with predominantly one type of chirality center.



An example of asymmetric enantiomer-differentiating polymerization: Polymerization of racemic 3-methylpent-1-ene (MP) using an optically active catalyst may give an optically active polymer by a polymerization that is partially asymmetric; preferential consumption of one of the two enantiomers leaves a monomer mixture having optical activity.

Potentiometric Selectivity Coefficients of Ion-Selective Electrodes

Part II. Inorganic Anions (IUPAC Technical Report) by Y. Umezawa, K. Umezawa, P. Bühlmann, N. Hamada, H. Aoki, J. Nakanishi, M. Sato, K. P. Xiao, and Y. Nishimura *Pure and Applied Chemistry*, Vol. 74, No. 6, pp. 923-994 (2002)

Part III. Organic Ions (IUPAC Technical Report) by Y. Umezawa, P. Bühlmann, K. Umezawa, and N. Hamada *Pure and Applied Chemistry*, Vol. 74, No. 6, pp. 995-1099 (2002)

An earlier IUPAC data compilation of potentiometric selectivity coefficients, $K_{A,B}^{\text{pot}}$, for ion-selective electrodes (ISEs) was published in 1979 (*Pure Appl. Chem.* **51**, 1913-1980 [1979]). It covered $K_{A,B}^{\text{pot}}$ data reported from 1966 to 1977 and was later followed by another extensive compilation of such data in a handbook from CRC Press (Y. Umezawa [ed.], *Handbook of Ion-Selective Electrodes: Selectivity Coefficients*, CRC Press, Boca Raton, FL [1990]). The latter covered most of the $K_{A,B}^{\text{pot}}$ data reported from 1966 to 1988. An updated compilation produced in 1998 was limited to a number of particularly selective ionophores (P. Bühlmann et al., *Chem.*

Rev. **98**, 1593-1687 [1998]). Very recently, a data compilation of selectivity coefficients for ionophore-based cation-selective electrodes was published as part I of this series (*Pure Appl. Chem.* **72**, 1851-2082 [2000]).

These two most recent reports compile the latest $K_{A,B}^{\text{pot}}$ data for liquid-membrane ISEs for inorganic-anions (part II) and organic ions (part III) based on neutral and charged ionophores, reported between 1989 and the end of 1998. Moreover, this new compilation also contains some older data that had not been included in the CRC handbook. The presented $K_{A,B}^{\text{pot}}$ data are listed together with the methods and conditions for their determinations; also tabulated are response slopes, linear concentration (activity) ranges, chemical compositions, and ionophore structures for the corresponding ISE membranes. Selectivity coefficients can be measured with different methods that fall into two main groups, namely (1) mixed solution methods, and (2) separate solution methods. The details of the definition of each method have been briefly discussed in the first part of this series.



www.iupac.org/publications/pac/2002/7406/7406x0923.html

www.iupac.org/publications/pac/2002/7406/7406x0995.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*. There is currently one document available for review:

Definitions of Terms Related to Polymer Blends, Composites and Multiphase Polymeric Materials

The document defines the terms most commonly encountered in the field of polymer blends and composites. The scope has been limited to mixtures in which the components differ in chemical composition or molar mass and in which the continuous phase is polymeric. Incidental thermodynamic descriptions are mainly lim-

ited to binary mixtures although, in principle, they could be generalized to multi-component mixtures.

The document is organized into three sections. The first defines terms basic to the description of polymer mixtures. The second defines terms commonly encountered in descriptions of phase domain behaviour of polymer mixtures. The third defines terms commonly encountered in the descriptions of the morphologies of phase-separated polymer mixtures.

Comments by 31 March 2003

To Dr. William J. Work

1288 Burnett Road

Huntingdon Valley, PA 19006 USA

E-mail: wjwork@comcast.net



www.iupac.org/reports/provisional/abstract02/work_310303.html

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Applications from candidates under age 40 are welcomed. Scientists from academia, government, or industry may submit applications directly to the address below. Those accepted will be expected to submit an abstract of a poster or paper to be presented at the Congress. Such abstracts will be subject to adjudication as will all other submissions for presentation at the meeting. Estimates of the economy airfare to and from the Congress should also be provided. There is no specific application form, but applicants are required to provide:

- a letter of application
- a brief curriculum vitae
- a confirmation of their current status and affiliation
- a publication list
- a letter of support from the appropriate department head, dean, or laboratory supervisor

The deadline for receipt of applications is 30 November 2002.

Applications should be sent to:

Dr. Hamid Jorjani
National Research Council of
Canada
Building M 58, Montreal Road
Ottawa, Ontario K1A 0R6,
Canada
E-mail: <Hamid.Jorjani@nrc.ca>

<www.iupac.org/news/archives/2002/39thCongress-yc.html>

New Books and Publications

The Science of Sweeteners

A special topic issue of *Pure and Applied Chemistry*, Vol. 74, No. 7, 2002
IUPAC, 2002.
(ISBN 0-09678550-4-7)

A recent Special Topic Issue of *Pure and Applied Chemistry* was devoted to the “**Science of Sweeteners.**” The issue derives from the 2nd International Symposium on Sweeteners, which was held 13-17 November 2001 in Hiroshima, Japan under the auspices of IUPAC. (The 1st symposium was held July 1997 in Jerusalem, Israel.)

The health problems caused by the extensive use of sweeteners in the human diet still persist. Ingestion of excessive high-calorie saccharides such as sucrose, glucose, and fructose has been linked to dental caries, diabetes, hyperlipidemia, obesity, and many dietary-dependent diseases. Consequently, the development of safe, low-calorie, noncariogenic sweeteners has been the focus of intense (and sometimes controversial) scientific, commercial, and public interest.

In light of their tremendous potential commercial and medical benefits, compounds from a variety of chemical categories have been investigated as “sugar substitutes.” Synthetic heterocyclic compounds, saccharides, halogenated saccharides, sugar alcohols, plant glycosides (terpenoids, steroids, and phenolics), peptides, and proteins have been examined.

Research on sweeteners encompasses a diverse set of scientific disciplines involving physiology, molecular biology, synthetic chemistry, structural chemistry,

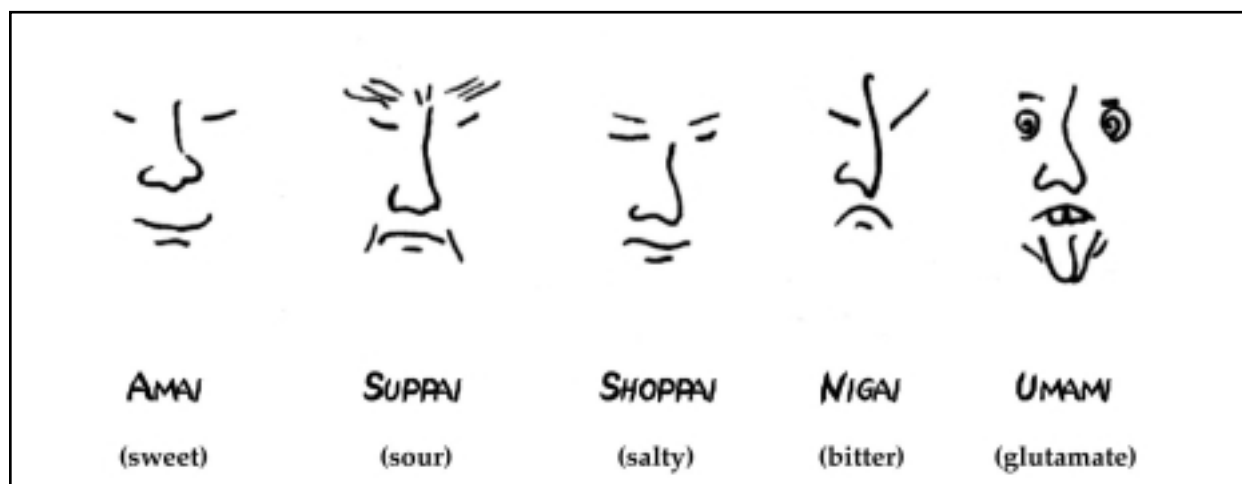
enzyme chemistry, food chemistry, pharmacology, nutritional science, preventative medicine, and dental science. Because of this diversity in research disciplines, it has been difficult for individual scientific societies to comprehensively deal with sweeteners. Adding to the complexity of the problem, legislation on the commercial use of sweeteners varies from country to country. Therefore, there have been numerous national symposia and scientific publications focusing on select aspects of sweeteners.

The aim and purpose of this symposium was to bring together scientists and technologists from a variety of disciplines from all over the world. The goal of this diverse assembly was to allow the participants to get a comprehensive perspective on sweetener research. Ultimately, it is hoped that this will lead to new approaches and contribute to further progress on sweeteners.

The symposium was chronologically divided into four sessions. The first day concentrated on the topics of chemoreception and biochemical aspects of receptors. The second day was directed mainly toward naturally intense sweeteners, including design and synthesis. The third day was spent on the topics of oligosaccharides and sugar alcohols, and the last day was devoted to the potential role of sweeteners in the etiology and prevention of disease.

The symposium comprised 11 invited lectures, 20 symposium lectures, 10 contributed papers, and 28 poster contributions. There were 181 participants from 21 countries. Ample time was provided for fruitful discussions of the comprehensive science of sweeteners.

Besides the main sponsor, IUPAC, extensive support



Cross-modality representation of human taste qualities. Psychophysical studies suggest that human taste sensation can be divided into five distinct categories: amai (sweet), suppai (sour), shoppai (salty), nigai (bitter) and umami (glutamate). Modified from the original silkscreen by John Lennon. Figure reproduced from Margolskee, *Pure and Applied Chemistry* Vol. 74, No. 7, pp. 1125-1133 (2002)

was obtained from the many sponsors as indicated in the individual abstracts. This issue is the result of an invitation to participants to submit for publication articles based on their presentations. It reflects well the panorama of subjects covered in the symposium with respect to both fundamental aspects and the importance of current and new research on the development of sweeteners. The topics covered vary from receptor studies to natural sweeteners to design and synthesis of sweeteners to industrial applications.

This issue was coordinated by professor J. Bull, IUPAC special topics editor and professor Mugio Nishizawa, conference editor. Preface by Kazuo Yamasaki, Symposium chairman, and Osamu Tanaka, Planning Committee chairman.

 www.iupac.org/publications/pac/2002/7407

Ionic Polymerization

Nikos Hadjichristidis and Hermis Iatrou (symposium editors)


Macromolecular Symposium, Vol. 183.

Wiley-VCH, 2002, pp. 1-210.

(ISBN 3-527-30473-8)

The IUPAC International Symposium on Ionic Polymerization (IP'01)—the fourth in the series after Istanbul (1995), Paris (1997), and Kyoto (1999)—was held in Crete, Greece, in October 2001. The major topics of the symposium included anionic and cationic polymerization, both vinyl and ring opening, as well as living radical, metathesis, metal-coordination, template and enzymatic polymerization. One day of the symposium was devoted to polymer physical chemistry and physics. Most of the invited lectures and selected papers are compiled in this issue of *Macromolecular Symposia*, which provides an excellent overview of current research in this area.

The Crete Symposium was the first to incorporate lectures on polymer physical chemistry and physics. There were altogether over 240 active participants from about 30 countries. In total, 66 invited lectures, 29 oral lectures, and 91 posters were presented.

 www.iupac.org/publications/macro/2002/183_preface.html

Green Chemistry in Africa

P. Tundo and L. Mammino (editors)

INCA, 2002.

(ISBN 88-88214-07-0)

IUPAC has always been keen on promoting the advancement of science in developing countries. A

recent contribution in this regard is *Green Chemistry in Africa*, the fifth volume in the green chemistry series. As the book points out, Africa's vast abundance of natural resources offers valuable opportunities for African countries to pursue novel routes to sustainable processes. Focusing on the search for such routes as alternatives to Western methodologies—and expanding their benefits—is an exacting and exciting challenge that can render African countries extremely competitive at the international level.

The book grew out of the work of IUPAC's Interdivisional Subcommittee on Green Chemistry, which organized the "Workshop on Green Chemistry Education," held in September 2001 in Venice in collaboration with INCA (Italian acronym for the Interuniversity Consortium "Chemistry for the Environment"). The proceedings of this conference—published as the third volume of the green chemistry series—represented the "state of the art" on green chemistry education. It included a number of recommendations for strengthening the diffusion of the chemical sciences into society through cleaner technologies. One of the most pressing recommendations was the following:

"To disseminate Green Chemistry educational materials and techniques to both developed and developing nations."

Accordingly, the subcommittee proposed the preparation of a collaborative volume on green chemistry in Africa, with the specific aim of offering university lecturers a useful tool for their teaching activities. The proposal was accepted by IUPAC and the book was pub-




Some of the book's authors convening in Pretoria, South Africa (25-28 May 2002) for the first editing.

From left: Lilians Mammino, Pietro Tundo, Egid Mubofu, Joseph Gaie, and Salie Lwenje.

lished in collaboration with INCA—a nonprofit organization that encourages the diffusion of knowledge, with particular emphasis on the importance of the chemical sciences to protecting the environment. In order to pursue its mission, INCA is involved in a wide range of activities that span from research to publishing.

Green Chemistry in Africa originates from the passionate work of academicians based in African institutions and it aims at familiarizing African students with the principles of clean and sustainable chemistry. The book is meant as an introduction to the challenges of green chemistry. Its primary objective is to highlight the major roles of chemistry in the study of the problems that were discussed at the World Summit on Sustainable Development (held 26 August to 4 September 2002 in Johannesburg, South Africa) and in the design of valuable solutions for those same problems. The Subcommittee on Green Chemistry hopes that this book will attract researchers' and students' attention to the importance of chemistry to sustainable development.

 www.iupac.org/publications/books/author/tundo.html

Vermeer's Camera: Uncovering the Truth Behind the Masterpieces

Philip Steadman
Oxford University Press, 2002 (ISBN 0-19-280302-6)

Reviewed by Hans Bouma

Do you like detective stories? No, not the ones in which the blood flows in liters but the real ones, in which the detective, after finding a nail clipping and a postage stamp of 39 eurocents is able to infer that the suspect's alibi is faulty. Or are doctoral dissertations more in your line? Are you interested in art? And you are involved in education in one of the sciences?

Well, then you must not go past this book. It explains, step by step, with compelling logic, that Vermeer used a

camera obscura for his paintings, in which room this happened, and which dimensions lens the camera had, how the painter employed them, and how in that way the paintings were produced. From the two dimensions of the paintings, Steadman is able to derive the three dimensions of Vermeer's world.

In nine chapters the logic line is drawn: first the camera obscura, then Vermeer with testimonies that he worked with a camera obscura, an idea of the room-studio and of the way the objects (their dimensions verified and compared with reality) are grouped in this room, the reconstruction, and the new evidence then forthcoming. To make sure, the author also deals with the arguments which are contrary to the idea of the camera with Vermeer, and he outlines the influence of it on his style of painting.

Now here you can see how fertile the application of science to objects of art is, this time not in connection with restorative activities, but to penetrate more deeply into the work. Not all questions can be solved, as Steadman honestly admits. But he also shows which tricks in perspective are applied by the painter, and, in the last chapter, he succeeds in penetrating into the artist's soul.

There is an elaborate account in notes and an impressive list of references. The author, too, gives the impression that he is well versed in 17th century Delft and in Holland in general, and that renders the book even more readable. He even is able to report that the bricks used in the houses around the Delft market had, in those times, a length of 16 centimeters.

You can sense that I am terribly enthusiastic. My only refutation that I deemed a length of 1.80 metres for a seventeenth century Dutchman quite sturdy is disproved by clear evidence in the book.

A book about paintings by a great researcher of a great painter. Cordially recommended!

Hans Bouma is an IUPAC Fellow and former member of the Committee on Teaching of Chemistry.

 www.oup-usa.org/isbn/0192803026.html

Reports from Conferences

Bioinformatics 2002: North-South Networking

by Prasit Palittapongarnpim

Bioinformatics is rapidly emerging as a new branch of science. It is widely believed that scientists in developing countries will be able to significantly contribute to the progress of this field since the capital investment needed for bioinformatics research may be much small-

er than for experimental biological sciences. However, the advancement of bioinformatics science in developing countries requires not only competent human resources, but also good ideas and problems. Without good communication with state-of-the-art experimental laboratories, there is a clear danger that small bioinformatics teams in developing countries may try to address irrelevant questions. Without good communication with state-of-the-art bioinformatics laboratories, there is a danger of using suboptimal technology to address the problems. To avoid these dangers, there must be forums

where bioinformatics scientists in developing countries interact with their counterparts in developed countries, as well as with biologists from various disciplines. This can be done through scientific publications as well as meetings and seminars.

There are several good international bioinformatics conferences. The fact that they are mostly organized in the developed world limits the access of scientists from developing countries. Moreover, there are problems that are of urgent importance for developing countries, such

as those relating to agriculture and biodiversity. From 6-8 February 2002, the International Conference on

Bioinformatics 2002: North-South Networking (INCOB2002) was held in Bangkok to provide a forum for facilitating these interactions.

Conference participants attended several interesting lectures on the current status of bioinformatics, as well as research presentations by scientists from more than 20 countries. The papers describing the works of several plenary speakers are published in *Pure and Applied Chemistry*, Vol. 74, No. 6, pp. 881-914. INCOB2002 has been such a successful event in establishing understanding between scientists with different backgrounds that participants agreed to hold similar meetings every one or two years. These meetings, as well as communication of research through publications such as *PAC*, will be among the essential components for generating more interaction between bioinformatics scientists around the world. With these interactions, the successful spread of bioinformatics in developing countries will finally be realized.

Prasit Palittapongarnpim of the National Center for Genetic Engineering and Biotechnology in Pathumthani, Thailand, is a member of the Organizing Committee and is conference editor.



www.iupac.org/publications/pac/2002/7406

CHEMRAWN XIV Follows Up With Green Chemistry Activities

by *R. Pariser*

In May 2002 in Bangkok, Thailand, there were two green chemistry activities. First, from 27-28 May, the U.S. team conducted a green chemistry training workshop at Chulalongkorn University. This workshop, organized by the Thai Chemical Society, was designed to expose students and faculty from across Southeast Asia to the concepts, principles, and methodologies of green chemistry. There were 90 registrants for the meeting, a majority of whom were from Thailand, but participants also came from Australia, Indonesia, Vietnam, India, and Malaysia.

The workshop was supported by the IUPAC Chemistry Research Applied to World Needs (CHEMRAWN) XIV program. The sessions provided the necessary foundations for ongoing development and initiatives in regional/country green chemistry education.

Among the subjects covered were the following:

- how to create national green chemistry programs
- current environmental and human health issues that pose a challenge for sustainability
- history of world approaches to dealing with threats to the environment, ecosystems, and biosphere
- definitions and 12 principles of green chemistry

Workshop instructors included Dennis L. Hjeresen, director of the Green Chemistry Institute (GCI); Paul T. Anastas, director of environmental programs at the White House Office of Science and Technology; Mary M. Kirchhoff, assistant director of GCI and international workshop coordinator; and John Warner, chairman of the chemistry department at the University of Massachusetts, Boston. The coordinator in Thailand was M. L. Siripastra Jayanta from the chemistry department of Chulalongkorn University.

Immediately following the workshop, the instructors attended the International Conference and Exhibition on Pure and Applied Chemistry (PACCON 2002)—a regional chemistry conference for Southeast Asia. All delivered invited speeches on different aspects of green chemistry and sustainable development. Dr. Hjeresen received a plaque from the Thai Minister of Science, Technology, and Environment recognizing the contribution of the ACS Green Chemistry Institute to environmental chemistry in Southeast Asia.

While in Bangkok, Dr. Hjeresen also signed an agreement creating a Thai chapter of the GCI. The chapter, located at Chulalongkorn University, will coordinate green chemistry education and research and development efforts with other universities in Thailand and across Southeast Asia. The chapter was created in association with the Thai Chemical Society and is the 23rd international GCI Chapter. The chapter contact will be Dr. Supawan Tuntayanont, vice president of the Thai Chemical Society and a professor at the university.

After the workshop, CHEMRAWN coordinators received follow-up information and programming requests from Thailand, Malaysia, the Philippines, and Vietnam. The meeting has also stirred discussion in Australia and a grant application to IUPAC to fund a Southeast Asia Green Chemistry network.

Rudolph Pariser is coordinator for CHEMRAWN XIV on Green Chemistry, and an IUPAC Fellow.



www.iupac.org/standing/chemrawn.html

Functional π -Electron Systems

by Günter Wulff

Over 600 people from 29 nations attended the 5th International Symposium on Functional π -Electron Systems (F π 5), which took place in Ulm/Neu-Ulm, Germany, from 30 May to 4 June 2002.

The symposium was organized under the guidance of the chairmen, Professor Peter Baeuerle (University of Ulm) and Professor Klaus Müllen (Max Planck Institute for Polymer Research, Mainz). It was the fifth consecutive congress in the series, which was founded by one of the honorary presidents, Professor Zen-ichi Yoshida (Kyoto, Japan) in 1989.

The two main objectives were to combine chemistry, physics, biology (in particular), and applications of functional π -electron systems on the one hand, and to strengthen interactions between academia and industrial research laboratories on the other hand. This was realized in two key note lectures by the Nobel Laureates, Professor Alan J. Heeger (University of California, Santa Barbara, USA), who spoke about "Photo-voltaic cells and biosensors using luminescent conjugated polymers" and Professor Jean-Marie Lehn (University of Strasbourg, France), who spoke about "Self-organization of functional architectures from heteroaromatic components." In addition, the plenary lectures by 42 distinguished invited scientists, 63 invited short lectures, and more than 300 poster presentations underlined the importance of functional π -systems in today's research.

The scientific program of F π 5 covered all highlights and aspects of functional π -electron systems of current interest and provided the absolute state of the art and information on further developments in this highly interdisciplinary field at all levels.

Plenary lectures covered the following topics:

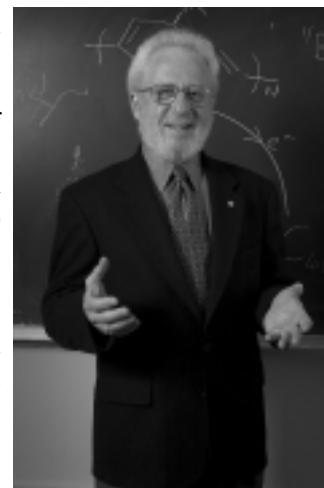
- Synthesis: F. Diederich (Switzerland), H. Hopf (Germany), A. Hirsch (Germany), R. McCullough (USA), A.-D. Schlüter (Germany), J. Siegel (USA), V. Snieckus (Canada)
- Structure-property relationships: J.-L. Brédas (USA), A. Osuka (Japan), J. Roncali (France), Y. Shirota (Japan), T. Swager (USA), D. Zhu (China)
- Nanostructures: T. Aida (Japan), J.M.J. Fréchet (USA), G. Wulff (Germany)
- Supramolecular organization: H. Anderson (England), B. Feringa (Netherlands), M. Fujita (Japan), E.W. Meijer (Netherlands), R.J.M. Nolte (Netherlands), J.-P. Sauvage (France), F. Stoddart (USA)
- Organic electronic devices and molecular electronics: Z. Bao (USA), T. Bjornholm (Denmark), R.

Friend (England), G. Malliaras (USA), Y. Wada (Japan)

- Biological systems: C. Braeuchle (Germany), T. Carell (Germany), F. Garnier (France), D. Oesterhelt (Germany), T. Yanagida (Japan), I. Willner (Israel)
- Probing and imaging: F. DeSchryver (Belgium), T. Jung (Switzerland), J.P. Rabe (Germany), H.-W. Spiess (Germany)
- Industrial aspects: S. Farid (USA), P. Kirsch (Germany), S. Kirchmeyer (Germany), E. Winkler (Germany)

A special highlight was a special lecture, which included experiments, given by Professor D. Haarer (Germany) on "Goethe's theory of colors, experiments, and poetry."

On the evening before the official opening of the symposium, a special presentation called "From the nobel prize to high-tech: polymers which conduct and emit" was made to 200 members of the public and press. The event, which took place in the "Stadthaus" of Ulm, featured leading scientists from industry and the two chairmen of F π 5,



Professor Alan Heeger

who presented and demonstrated the application of semiconducting polymers in organic light emitting devices, organic transistors and integrated circuits, organic photovoltaic cells, and molecular electronics. Finally, Nobel Laureate, professor Alan Heeger gave concluding words and offered a promising future outlook for the field.

The symposium definitely was a complete success and the series will be continued in 2004. At the closing ceremony, professor G. Malliaras (Cornell University, USA), one of the coming chairmen, presented details about F π 6, the 6th International Symposium on Functional π -Electron Systems which will be held in Ithaca, New York (USA), in June 2004.

Günter Wulff is a professor at Heinrich Heine University Duesseldorf, Germany, and an IUPAC Fellow.



www.uni-ulm.de/fpi5

by David StC Black

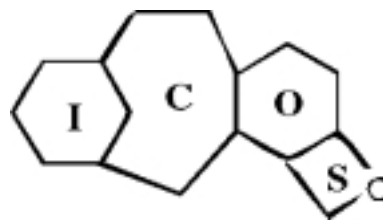
The field of organic synthesis has always been at the center of chemical science. As such, the series of International Conferences on Organic Synthesis, initiated and sponsored by IUPAC, continues to thrive. The 14th conference (ICOS-14) was held from 14-19 July 2002 in Christchurch, New Zealand.

Because it is desirable to develop as wide a geographical spread of influence for the conferences, to act as stimulants for the outgrowth of new chemistry, the decision was made to hold ICOS-14 in New Zealand. Professor Margaret Brimble (University of Auckland) enthusiastically took up the baton as conference chair and Professor Jim Coxon (Canterbury University at Christchurch) stepped in as co-chair. Christchurch was chosen as the venue because of superior conference facilities.

There is always a risk in locating conferences in the southern hemisphere because serious travel leads to uncertain attendance. However, those who brave and endure such travel are sometimes well rewarded. That was certainly the case with ICOS-14, where the organizers provided a superb combination of chemistry, efficiency, and hospitality for the almost 500 participants. The event was boosted by a particularly large and stimulating contingent from Japan; however, the low participation level of North American chemists was disappointing.

The scientific program embraced all aspects of modern synthetic organic chemistry. There were 11 plenary lectures, the Thieme/IUPAC award lecture, approximately 20 invited section lectures, and a series of 6 mini symposia woven into the program, which was arranged with two parallel sessions for the shorter lectures. The plenary speakers were as follows: Yoshito Kishi (Harvard) on halichondrin synthesis; Ben Feringa (Groningen) on asymmetric catalysis; K. C. Nicolaou (Scripps) on total synthesis; Koichi Narasaka (Tokyo) on azaheterocycles from oximes; William Roush (Michigan) on allylorganometallic reagents; Tohru Fukuyama (Tokyo) on synthesis of vinblastine; Jonathan Ellman (Berkeley) on new synthetic methodology for nitrogen-containing compounds; Albert Padwa (Emory) on cascade processes for heterocycles; Keisuke Suzuki (Tokyo Institute of Technology) on pericyclic routes to natural polyarenes; John Wood (Yale) on synthetic approaches to CP-263,114; and Stephen Martin (Texas) on synthesis of C-arylglucosides.

The Thieme/IUPAC prize was awarded to Erick Carreira (ETH Zurich) who lectured on asymmetric synthesis made simple. The mini symposia were in the areas of synthesis of bioactive molecules, combinatorial chemistry, stereoselective synthesis, green chemistry,



metal mediated synthesis, and automation in synthesis. A selection of plenary lectures will be published in *Pure and Applied Chemistry*, for which Professor Andrew Abell is acting as conference editor. A feature of the conference was the outstanding array of 267 posters presented mainly by a large and enthusiastic group of international graduate students, who also contributed greatly to the lively ambience of the meeting.

The organizers are to be congratulated for producing such a superb meeting in every respect. ICOS-15 will be held in Nagoya, Japan, from 1-6 August 2004 under the co-chairmanship of Minoru Isobe and Hisashi Yamamoto.

David StC Black of the University of New South Wales is vice president of the IUPAC Division of Organic and Biomolecular Chemistry and chairman of the subcommittee on Organic Synthesis.



www.conference.canterbury.ac.nz/icos14

Solubility Phenomena—Application for Environmental Improvement

by J. W. Lorimer

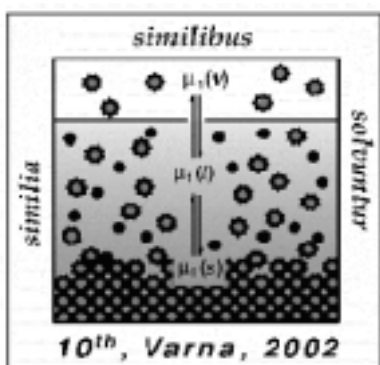
The 10th International Symposium on Solubility Phenomena was held at the Home of Scientists “Frédéric Joliot Curie” in the Sts. Constantine and Helen resort complex north of Varna in Bulgaria on the Black Sea, from 21 to 26 July 2002. Unlike previous symposia which consisted of invited lectures and papers given in non-overlapping sessions, this symposium was accompanied by a Workshop on Solubility Phenomena—Application for Environmental Improvement, whose sessions were held in parallel with the symposium, except for one joint session. One hundred-eighty participants from 37 countries took part. Of the scientific participants, 50 were from Bulgaria and 117 from elsewhere.

The new Subcommittee on Solubility and Equilibrium Data of the IUPAC Analytical Chemistry Division met over the two days prior to the symposium, with Professor Heinz Gamsjäger (Austria) as the chair. The symposium and workshop were chaired by Professor Christo Balarew,

with Dr. Stefka Tepavitcharova as scientific secretary; both are from the Bulgarian Academy of Sciences.

The symposium and workshop were organized by the Bulgarian Academy of Sciences, the Subcommittee on Solubility and Equilibrium Data, and the International Centre of Black Sea Studies. IUPAC was the major sponsor of the symposium as part of the IUPAC program to provide financial support for international symposia in developing and economically disadvantaged countries. Support was also received from the Bulgarian Academy of Sciences; the UNESCO Regional Bureau for Science in Europe, Venice; and the U.S. Army Research Development and Standardization Group, UK. Sponsors for the Workshop, in addition to the Bulgarian Academy of Sciences and UNESCO, were the International Centre of Black Sea Studies, Athens; the European Commission, Directorate General Research; Intergovernmental Oceanographic Commission, Paris; International Ocean Institute, Malta; Cesum-BS, Centre of Excellence, Varna; Chernomorski Solnizi AD, Burgas; and Black Sea Technological Company, Varna. The symposium and workshop received good coverage in the local Varna press and on Bulgarian radio.

The opening ceremonies were presided over by Professor Balarew, symposium chair. Professor Ivan Gutzow (Bulgaria) gave the opening plenary address on "Solubility and Crystallization in Biological Fluids and the Problems of Life and Health," a topic that served as an excellent introduction to both the symposium and workshop.



The Symposium was organized in 12 sessions divided among the four sections: Quantitative Structure-Solubility Relationships; Solubility Diagrams, Phase Relationships, and their Application; Application of Solubility Data for Environmental Improvement of Polluted Waters and Soils; and Application of Solubility Data in Marine-Type Solutions and Industrial Waste Treatment. Fourteen plenary lectures and 21 contributed papers made up these sessions, and 47 posters were presented during two evenings. The contributions themselves covered a wide spectrum of solubility phenomena, from fundamentals of dissolution processes through new data and modelling of solubility

processes to many applications.

The workshop was organized in six sessions divided among the three sections: Pollution Level and Pollution Sources of Danube, Dnieper, Dniester, Bug, and Other Rivers Flowing into the Black Sea; Black Sea Fluxes, Monitoring of the Black Sea (including a roundtable discussion); and Reinforcement of Regional Participation in Integrative European Programmes for Solving Ecological Problems (with a roundtable discussion on regional cooperation). Three plenary lectures, 25 contributed papers, and 28 posters were presented. The plenary lectures given at both the symposium and the workshop are to be published in *Pure and Applied Chemistry* under the editorship of David Shaw (USA).

The extensive participation of delegates from countries with Black Sea coastlines, as well as of those from countries that have historical, economic, and political connections with the Black Sea, was a noteworthy feature of the workshop. The workshop thus provided a valuable forum for scientific workers to meet one another and to learn of the several national and international programs that are addressing the many problems connected with the ecological health of the Black Sea.

Participants enjoyed a half-day excursion to Balchik, followed by a memorable dinner at the Ethnographic Complex "Chiflika" in the village of Chukurovo in the Dobrich region.

J. W. Lorimer is a professor at the University of Western Ontario, Canada, and a long-time IUPAC member.



Physical Organic Chemistry

by Tom Tidwell

From 4-9 August 2002 at the University of California, San Diego, 280 chemists from 30 countries assembled for "Structure and Mechanism in Organic Chemistry," the 16th International Conference on Physical Organic Chemistry, which was sponsored by IUPAC. The meeting featured 34 plenary and invited lectures, 93 contributed lectures, and 128 posters.

The local organizer was Professor Charles L. Perrin, who is also chair of the Subcommittee on Structural and Mechanistic Chemistry of the IUPAC Organic and Biomolecular Chemistry Division. A social and cultural program included a welcoming reception, visits to the Mt. Palomar Observatory and the San Diego Zoo, city and harbor tours, and a banquet at the Birch Aquarium of the Scripps Institute for Oceanography.

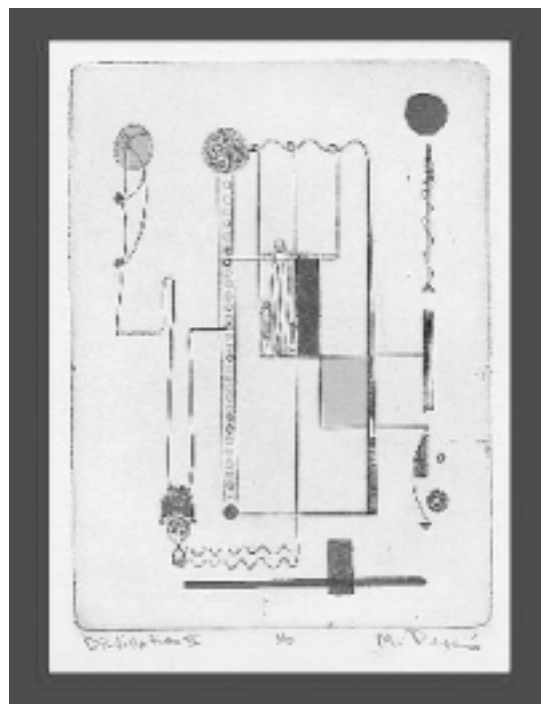
The University of California at San Diego (UCSD) is now more than 40 years old, and the faculty has included

nine Nobel Prize winners in the sciences. The most recent is Walter Kohn, a 1998 winner in chemistry who developed DFT computational methods at UCSD before moving to U.C. Santa Barbara. Barry Sharpless, a 2001 winner in Chemistry, is at the nearby Scripps Research Institute. The San Diego campus is situated in a lovely environment on the Pacific Ocean, in an area that has become a leading center of the biotechnology industry in the United States. In addition to a benign summer climate, the university has excellent conference facilities, with low-cost student residences available for participants.

The topics presented at the five-day meeting emphasized the diversity of modern research in structural and mechanistic chemistry, with particular emphasis on understanding chemical reactivity, intermolecular recognition, supramolecular chemistry, biological systems, and materials. A key topic was nanotechnology, including lectures on photochemically activated molecular-level devices (Vincenzo Balzani, Bologna, Italy); dynamics of contractile catenanes and rotaxanes (Jean-Pierre Sauvage, Strasbourg, France); synthesis and operation of a molecular motor (Ben Feringa, Groningen, Netherlands); and millimeter-scale self-assembly and potential applications (George Whitesides, Harvard). Another key topic was the analysis of the relation between structure and biochemical function, including lectures on hydrogen tunneling in enzyme-catalyzed reactions (Judith Klinman, U.C. Berkeley); kinetics of self-replicating systems and self-assembly of nanoobjects based on nucleic acids (Gunther von Kiedrowski, Bochum, Germany); genetic selection as a tool for mechanistic enzymology (Donald Hilvert, ETH, Zürich, Switzerland); chemical methods for modulating cell-surface architecture (Carolyn Bertozzi, U.C. Berkeley); single-molecule studies of the mechanism of protein unfolding (Jane Clarke, Cambridge, U.K.); and the thermodynamics of some



Conference participants outside the meeting room: Left to right; John Toscano (Johns Hopkins U., Baltimore), Peter Chen (ETH, Zurich), Charles L. Perrin (UCSD, Chair of Organizing Committee), JoAnn DeLuca (Central Washington U.), and John Baldwin (Syracuse U.)



Distillation II by Marilyn H. Perrin—Since it has been an ICPOC tradition to include artwork in conference programs, Professor Perrin chose one of his wife's pieces for all to enjoy. This piece can be viewed in color at <http://chem-faculty.ucsd.edu/perrin/icpoc>.

reactions of NO and NADH (Jin-Pei Cheng, Nankai University, China). Other presentations dealt with gas-phase and solution reactivity and structure, including catalysis of electron-transfer processes (Shunichi Fukuzumi, Osaka); low-coordination silicon compounds (Yitzhak Apeloig, Haifa, Israel); salt effects on conformations of heterocycles (Eusebio Juaristi, Mexico); mass spectrometric detection of organometallic intermediates in new catalytic processes (Peter Chen, ETH, Zurich); and synthesis of novel cyclopropane derivatives (Armin de Meijere, Gottingen, Germany).

This symposium continues an impressive series of scientific presentations, following the trajectory of the plenary lecture by K. R. Seddon at the 15th Conference in 2000 in Göteborg, Sweden. That lecture was published in *Pure and Applied Chemistry* in 2001 and was ranked in the top 10 requested articles from the Chemical Abstracts document service. The 17th conference is scheduled for Shanghai in 2004, and is expected to continue to showcase the growth and development of this field.

Tom Tidwell, University of Toronto, is president of the IUPAC Division of Organic and Biomolecular Chemistry.



chem-faculty.ucsd.edu/perrin/icpoc

Conference Announcements



designates IUPAC sponsorship

11th International Conference on Polymer Characterization (POLYCHAR-11) 6-10 January 2003, Denton, Texas, USA

This continuing series of conferences has been held annually at the University of North Texas since 1992. The conference focus is on characterization on the one hand and synthesis, processing, manufacturing, and properties on the other, with an emphasis on predictions of service performance. All polymer-based materials, including thermoplastics, thermosets, heterogeneous and molecular composites, blends, polymer melts, and solutions are covered.



Research presentations are in both oral and poster format. Topic areas include the following:

- predictive methods
- polymerization
- polymer liquid crystals
- mechanical properties and performance
- dielectric, electrical, and magnetic properties
- surfaces and interfaces
- rheology, solutions, and processing
- characterization and structure-property relations
- recycling
- international education and scientific information

Contact: POLYCHAR-10
University of North Texas, P.O. Box 305310, Denton, TX 76203-5310, USA
Fax: +1 940 565 4824
E-mail: polychar@marta.phys.unt.edu



www.unt.edu/POLYCHAR



6th Annual UNESCO School & IUPAC Conference on Polymer Properties 14-17 April 2003, Mpumalanga, South Africa (UNESCO Introductory Course, 10-11 April 2003)

This continuing series of schools and conferences, held annually, has the following goals:

- to expose Africa to macromolecules and materials technology that is applicable to their economies
- to create a virtual teaching encyclopedia CD-ROM for teaching in developing countries, where books, journals, and teaching material preparation are not available

The primary focus will be on the following:

- characterization of polyolefins and emulsions from newest synthetic techniques (e.g., metallocenes and living-free radical)
- catalysts and polymer synthesis (including combinatorial chemistry) hyphenated HPLC techniques, morphology, and ultrasonics

The scientific program will comprise plenary and invited lecturers, as well as other oral and poster presentations. Delegates are invited to submit contributions to the organizers.

Contact: Professor R. D. Sanderson
UNESCO Associated Centre for Macromolecules and Materials, Institute for Polymers Science, University of Stellenbosch Private Bag X1, Matieland 7602, South Africa
Tel.: +27 21 808 3174
Fax: +27 21 808 4967
E-mail: rds@sun.ac.za



www.sun.ac.za/unesco/Conferences/Homepage.htm



International Symposium on Ionic Polymerization 30 June-4 July 2003, Boston, USA


This symposium represents the 16th in the series of biannual symposia which began with the first "International Symposium on Cationic Polymerization" that was held in Akron, Ohio in 1976. This symposium will provide state-of-the-art presentations (oral and poster) describing both recent advances in anionic, cationic, and ring-opening polymerization research as well as recent developments in the industrial applications of these synthetic methodologies to prepare commercially useful polymeric materials.

Contact: Professor R. P. Quirk
Department of Polymer Science, The University of Akron, Akron, Ohio 44325-3909
Tel.: +1 330 972 7510
Fax: +1 330 972 5290
E-mail: quirk@polymer.uakron.edu

Also see page 27 for the IP'01 related publication, *Macromolecular Symposia*, Vol. 183.



www2.uakron.edu/cpspe/iupac/ip2003.htm

 22nd Discussion Conference of
P.M.M. on Spectroscopy of Partially
Ordered Macromolecular Systems
21–24 July 2003, Prague, Czech Republic

This conference continues in the tradition of the Prague Meetings on Macromolecules, organized since 1967. It will deal with various aspects of detection and evaluation of order emerging in systems of synthetic as well as natural macromolecules in bulk or solution by molecular spectroscopy. The conference will also tackle relative ordering on various scales accessible to molecular spectroscopy, in particular molecular (preferred conformations, increased persistence length, ordering of low-molecular-weight ligands and counterions), supramolecular (complex formation, short-range ordering interactions) and supermolecular or phase-like (micelles, microphases and other nanostructures, micro-

scopic domains in polymer blends, etc.). Main methods probing into emerging order, discussed at the conference, will be high-resolution liquid- and solid-state NMR (spectra, relaxation, spin-diffusion, self-diffusion, etc.) and vibrational spectroscopy (infrared, Raman, micro-Raman imaging, etc.).

Contact Dr. Drahomir Vyprachticky
Institute of Macromolecular Chemistry, Academy of Sciences of the Czech Republic, Heyrovskeho nam. 2, CZ-162 06 Praha 6, Czech Republic
Tel.: +420 2 204 03251
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E-mail: sympo@imc.cas.cz



www.imc.cas.cz/sympo/22discon.html

Calendar of IUPAC Sponsored Conferences

Visit www.iupac.org for complete information and further links

NEW designates a new conference since the last issue

2002

Polymer Science and Technology

2–5 December 2002

IUPAC Polymer Conference on the Mission and Challenges of Polymer Science and Technology, Kyoto, Japan.

Prof. Seiichi Nakahama, Faculty of Engineering, Tokyo Institute of Technology, 2-12-1 Ohokayama, Meguro-ku, Tokyo 152-8552, Japan

Tel.: +81 3 5734 2138

Fax.: +81 3 5734 2887

E-mail: snakahama@aist.go.jp

2003

Polymer Characterization

6–10 January 2003

11th Annual Course on **NEW** Polymer Characterization and 11th POLYCHAR World Forum on Polymer Applications and Theory, Denton, Texas, USA.

Dr. Witold Brostow, Department of Materials Science, University of North Texas, Denton, Texas, 76203-5310 USA

Fax: +1 940 565 4824

E-mail: polychar@marta.phys.unt.edu

Clinical Laboratory

6–7 February 2003

2nd European Symposium on Clinical Laboratory and In Vitro Diagnostic Industry, Barcelona, Spain

Prof. Xavier Fuentes Arderiu, Ciutat Sanitària i Universitària de Bellvitge Servei de Bioquímica Clínica

L'Hospitalet de Llobregat, Catalonia, E-08907 Barcelona, Spain

Tel.: +34 93 260 7644

Fax: +34 93 260 7564

E-mail: xfa@csub.scs.es

Flow Analysis

17–21 February 2003

The 9th International Conference on Flow Analysis, Geelong, Victoria, Australia.

Dr. Daryl J. Tucker, School of Biological and Chemical Sciences, Deakin University, Geelong, Victoria 3127 Australia.

Tel.: +61 3 5227 2325

Fax: +61 3 5227 1040

E-mail: tucker@deakin.edu.au

Heterocyclic Chemistry

10–12 March 2003 (Pre-conference 9 March 2003)

4th Florida Heterocyclic Conference, Gainesville, Florida, USA.

Prof. Alan R. Katritzky, University of

Florida, Dept. of Chemistry, PO Box 117200 Gainesville, FL 32611, USA

Tel.: +1 352 392 0554

Fax: +1 352 392 9199

E-mail: katritzky@chem.ufl.edu

Polymer Properties

10–11 April 2003

UNESCO Introductory Course 14–17 April 2003

6th Annual UNESCO School & IUPAC Conference on Polymer Properties, Mpumalanga, South Africa.

Prof. R.D. Sanderson, UNESCO Associated Centre for Macromolecules and Materials Institute for Polymers Science, University of Stellenbosch, Private Bag XI, Matieland 7602, South Africa

Tel.: +27 21 808 3174

Fax: +27 21 808 4967

E-mail: rds@sun.ac.za

100 Years of Chromatography

13–18 May 2003

3rd International Symposium on Separations in BioSciences (SBS '03), follow up to the International Symposia Series "Biomedical Applications of Chromatography and Electrophoresis," Moscow, Russia.

Prof. Vadim A. Davankov,

Nesmeyanov Institute of Organo-Element Compounds, Vavilov str., 28, 119991, Moscow, Russia.
Tel./Fax: +7 095 135 6471
E-mail: davank@ineos.ac.ru

High Temperature Materials

19–23 May 2003

11th International Conference on High Temperature Materials Chemistry (HTMC XI), Tokyo, Japan.

Prof. Michio Yamawaki, University of Tokyo, Department of Quantum Engineering, 7-3-1 Hongo, Bunkyo-ku, Tokyo 113-8656, Japan
Tel.: +81 3 5841 7422
Fax: +81 3 5841 8633
E-mail: yamawaki@q.t.u-tokyo.ac.jp

Macromolecule Metal Complexes

20–24 May 2003

Xth International Symposium on Macromolecule Metal Complexes (MMC-X), Moscow, Russia.

Prof. Valerii V. Lunin, Department of Chemistry, Moscow State University, Leninskie Gory, Moscow, 119899, Russia.
Tel.: +7 095 939 5377
Fax: +7 095 932 8846
E-mail: kar@petrol.chem.msu.ru

Ionic Polymerization

30 June–4 July 2003

International Symposium on Ionic Polymerization, Boston, MA, USA.

Prof. R. P. Quirk, Department of Polymer Science, The University of Akron, Akron, OH 44325-3909, USA.
Tel.: +1 330 972 7510
Fax: +1 330 972 5290
E-mail: quirk@polymer.uakron.edu

Organo-Metallic Chemistry

6–10 July 2003

12th IUPAC International Symposium on Organo-Metallic Chemistry Directed Towards Organic Synthesis (OMCOS-12), Toronto, Ontario, Canada.

Prof. Mark Lautens, Department of Chemistry, University of Toronto, Toronto, ON M5S 3H6, Canada
Tel: +1 416 978 6031
E-mail: omcos@chem.utoronto.ca

Spectroscopy of Macromolecular Systems

21–24 July 2003

22nd Discussion Conference of P.M.M.on Spectroscopy of

Partially Ordered Macromolecular Systems, Prague, Czech Republic.
Dr. Drahomir Vyrachticky, Institute of Macromolecular Chemistry, Academy of Sciences of the Czech Republic, Heyrovskeho nam. 2, CZ-162 06 Praha 6, Czech Republic

Tel.: +420 2 204 03251
Fax: +420 2 353 57981
E-mail: sympo@imc.cas.cz

IUPAC 42nd General Assembly

8–17 August 2003

Ottawa, Ontario, Canada.

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

IUPAC 39th Congress

10–15 August 2003

Chemistry at the Interfaces, Ottawa, Canada.

National Research Council Canada, Montreal Road, Building M-19, Ottawa, ON, Canada K1A 0R6
Tel.: +1 613 993 0414
Fax: +1 613 993 7250
E-mail: iupac2003@nrc.ca
<www.iupac2003.org>

See enclosed booklet for Preliminary Program

Young chemists !! Watch out for deadline—See page 25

Colloquium Spectroscopicum Internationale

7–12 September 2003

33rd Colloquium Spectroscopicum Internationale 2003, Granada, Spain.

Prof. Alfredo Sanz-Medel, Department of Physical and Analytical Chemistry, University of Oviedo, C/Julian Claveria, 8 E-33006 Ovido, Spain
Tel.: +34 985 103474
Fax: +34 985 103125
E-mail: asm@sauron.quimica.uniovi.es

General and Applied Chemistry

21–26 September 2003

XVII Mendeleev Congress on General and Applied Chemistry, Kazan, Tatarstan, Russia.

Prof. Alexander I. Kononov, A.E.

Arbuzov Institute of Organic and Physical Chemistry, Kazan Scientific Center of Russian Academy of Sciences, Arbuzov Str., 8, Kazan 420088, Tatarstan, Russia.
Tel.: +7 (8432) 739 365
Fax: +7 (8432) 752 253
E-mail: arbuzov@iopc.knc.ru

Medicinal Chemistry

15–18 October 2003

Polish-Hungarian-German-Italian Joint Meeting on Medicinal Chemistry, Krakow, Poland.

Prof. Zdzislaw Chilmoczyk, Drug Institute, Chemska 30/34, PL-00-725 Warsaw, Poland
Tel.: +48 22 851 52 29
E-mail: chilmon@il.waw.pl

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To apply for IUPAC sponsorship, conference organizers should complete an Advance Information Questionnaire (AIQ). The AIQ form is available at <www.iupac.org> or by request to the IUPAC Secretariat, and should be returned between 2 years and 12 months before the conference. Further information on granting sponsorship is included in the AIQ and available online.

Visas

It is a condition of sponsorship 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.

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please visit the IUPAC Web site at www.iupac.org/news/prize.html
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