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Applied Chemistry (IUPAC)

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Reflecting on IUPAC Projects

China's Petrochemical Technologies

Introducing EuCheMS

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From the Editor

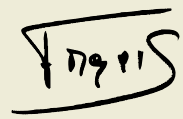
"Think IUPAC"

—these words were a call by former IUPAC Secretary General Ted Becker for readers of this magazine to consider in what ways the Union might enhance its contributions to the chemical sciences. In his editorial published in the January 2001 issue, Becker stressed that even scientists with no long-term affiliation with IUPAC may well be interested in tackling a project. Becker's editorial appeared during a transition period from which IUPAC emerged with a fully phased in project system.

Since that time, "Think IUPAC Project" has been a recurring topic of discussion for all constituencies of the Union. Last year, the *Vice President's Critical Assessment* also focused on the topic. Despite all this, it remains critical that we keep promoting the project system, encouraging scientists from all horizons to come forward with new ideas. If you are a member or fellow of IUPAC, you know that the system is actually quite simple. On the other hand, if you have never participated in an IUPAC project before, a simple description of the system might be very helpful. Let Gus Somsen, current chairman of the Project Committee, take you on a tour of the IUPAC project system (page 2). His experience with and perspective on IUPAC make his piece a "must read" if you are thinking of embarking on an IUPAC project.

If you would like more specific examples of IUPAC projects, visit the IUPAC website where each project is listed with a short description, a progress report, and information on outcomes if applicable. All current and completed projects (about 400 have been initiated since 1999) are kept online for reference. In this issue, you can turn to page 12, and see information about new, current, and complete projects and related initiatives.

Your inquiries are always welcome, and each task group invites your comments. Your participation can start here.



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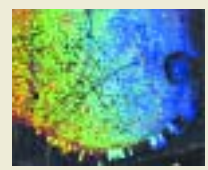

Cover: Jeremy G. Frey <j.g.frey@soton.ac.uk>, University of Southampton (UK), collected images for a UK EPSRC-funded project for the Public Appreciation of Science. **Bright Reflections** ***(From W.S. Brocklesby) is a SNOM (Scanning Near-field Optical Microscopy) image of a nanostructure surface generated by electrodeposition through polymer spheres. This image shows the iridescence of a promising low-technology route to making interesting grainy metals.***

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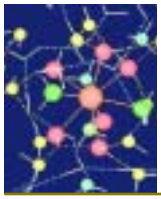

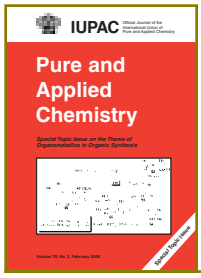

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The IUPAC Project System Revisited

by Gus Somsen

About five years ago, IUPAC was busy implementing a novel way to carry out part of its work: the so-called project system. This system opened the possibility for any scientist worldwide to participate in an activity funded by IUPAC. At the last IUPAC General Assembly in 2005, Vice President Bryan Henry reported that this project system is functioning very well, maybe even better than expected. Although many scientists have experience with the system, it seems appropriate to highlight some of its ins and outs for those who might be interested but are not familiar with how it actually works.

IUPAC is an organization dealing with the chemical sciences in an international context. Consequently, all of its projects have international aspects. In practice this means that the objective of an IUPAC project can be realized only by cooperation among expert scientists from several countries. To illustrate the different activities that take place during IUPAC projects, examples of several types of projects will be given.

Traditionally, IUPAC plays a leading role in the international standardization of nomenclature and terminology. At present, IUPAC is involved in developing a way to express chemical structures in a standard computer-readable format that provides lots of information, like bonds, tautomeric state, and stereochemistry of a compound. Other projects are dedicated to the standardization of experimental methods and procedures, so that around the globe results of experiments can be compared on the same basis. To this end, IUPAC realized recently a uniform scale for the quantity pH, where in the past, countries were accustomed to using different scales.

Many efforts are aimed at compiling critically evaluated data in areas like thermodynamics and kinetics. In many areas of the chemical sciences there is a desperate need for reliable numerical data that are selected and checked by a worldwide group of experts working together on a project.

One of the long-range goals of IUPAC is to contribute to the enhancement of chemistry education and the public appreciation of chemistry. Projects in this direction are highly welcome. A recent successful project is the Young Ambassadors of Chemistry, where teachers are trained to develop the communicative skills of young people to become ambassadors for chemistry. In 2005, this program made stops in Argentina, Russia, and Taiwan.

These examples show that any problem or subject requiring the development of a consensus among the worldwide family of chemical scientists may be an IUPAC project. However, there are some restrictions. General research is excluded, even if it is realized by a broad international team. The same is true for scientific conferences of a general nature. For these meetings, IUPAC offers the possibility to apply for IUPAC sponsorship. Sponsorship does not mean financial support, but it provides proof of the quality of the conference, which may enable the organizers to attract funding from other sources. Issues that concern one country or a small number of countries do not qualify to be IUPAC projects. Finally, the project system excludes publication of a journal or magazine, as well as granting of scholarships.

Proposals for funding through the project system are subject to two types of critical review, one from inside IUPAC, the other from external referees. A broad spectrum of the chemical sciences is covered by IUPAC divisions and standing committees. Each project proposal that is submitted will be reviewed by at least one of these bodies. If more divisions and standing committees are interested, they are involved also in the proposal review. When the proposal is accepted by a division committee or standing committee, the views of several knowledgeable scientists outside IUPAC will be sought. On the basis of the internal and external reviews the decision will be made to embark on the project. The division or standing committee will then arrange for modest financial support from its budget for projects. In cases in which the project is interdisciplinary or requires funding beyond the

The project system provides an oppotunity for the Union to enhance its contributions to the development of the chemical sciences.

The Project System

budget of the relevant committee, the decision is referred to another body, the Project Committee.

Project proposals can be submitted at any time by anyone. The Secretariat provides the administrative support associated with proposal submissions and reviews. Information on IUPAC projects can be found on the IUPAC website <www.iupac.org>. There, one can find pages on "Guidelines for IUPAC Projects," the "Project Review Procedure," and "Frequently Asked Questions on Project Submission and Approval Process." From the same website, a *Project Submission Form* can be downloaded. Other pages provide "Guidelines for the Completion of the Project Submission Form."

IUPAC tries to restrict the processing time between the submission of a proposal, and the decision about it, to four months. However, much depends on the completeness of the information provided by the submitter. An important item is the way in which the result of the project will be disseminated, since only after adequate dissemination can a project be considered to be finished. In addition, detailed information on the project budget will help the reviewing body significantly in reaching a final decision in a timely manner.

For the realization of a project, a task group is formed consisting of scientists who are experts in the subject of the project proposal. The task group members

should be active participants, communicating predominantly by e-mail. The management of the project is the joint responsibility of the relevant division or standing committee and the task group chairman. Mostly, the final result of a project is a publication, a recommendation, a technical report, or a database. The project is finished when the dissemination plan is implemented. The task group exists during the lifetime of the project and is disbanded after its completion.

The project system provides an opportunity for the Union to enhance its contributions to the development of the chemical sciences. To this end, the worldwide participation of scientists is extremely important. In the project system it is possible for anyone to participate, regardless of nationality. One of the long-range goals of the Union is to maximize diversity in membership. For IUPAC committees, membership is restricted to scientists from countries that are members or associated members of the Union; within the project system the geographic representation in task groups has no limits. Anyone can submit project proposals and serve in task groups. Hopefully, many will do so.

Gus Somsen <somsen@few.vu.nl> is a long-time member of IUPAC. He was once president of the Physical Chemistry Division and an elected member of the Bureau. He currently serves IUPAC as chairman of the Project Committee.

China's Petrochemical Technologies*

by Jiming Wang

After the establishment of the People's Republic of China, the country's petrochemical industry started from scratch but developed fast. Due to dramatic growth, particularly in the two decades since opening to the outside world, China has become one of the major petrochemical producers.

By the end of 2004, China's primary crude distillation capacity had reached 315 million metric tons per year (mmtpa) (second worldwide), ethylene production had reached 6.085 mmtpa (third worldwide), synthetic resin 19.50 mmtpa (second worldwide), synthetic fibre 13.10 mmtpa (first worldwide), and synthetic rubber 1.39 mmtpa (fourth worldwide). In 2004, China's refining throughput totaled 270 million tonnes, with 160 million tonnes of gasoline, diesel, and kerosene products, meeting domestic demand both in volume and in quality. Ethylene production in 2004 was 6.27 million tonnes, satisfying 38.5 percent of direct and indirect needs for ethylene.

The reform and restructuring of the Chinese economy initiated in 1998 led to the establishment of several dominant state-owned enterprises in different sectors of the petrochemical industry, thus creating an interim system and mechanism for a future market economy. SINOPEC and China National Petroleum Corporation (CNPC), ranked 31st and 46th respectively in Fortune 500 for 2004, are a testimony to the increasing competitive power of state-owned enterprises.

In recent years, restructuring and technology advances have intensified in China's petrochemical industry, with improved industry layout and expanded scale. The construction of world-scale refineries with integrated refining and chemical operations has been accelerated, with eight refineries reaching ten-million-tonne capacity, including Zhenhai, Dalian, and Maoming. A number of refining and chemical complexes have been developed, such as Yanshan Petrochemical, Shanghai Petrochemical, Yangzi Petrochemical, and Daqing Petrochemical. The completion of joint ventures with YPC-BASF, SECCO, and CNOOC-SHELL for ethylene production will further optimize the industry layout and product mix, gradually increasing industry concentration. Through increasing investment and technology revamping, China has been able to improve the quality of its refined oil products, narrowing the gap between domestic and international standards. On 1 July 2005 China implemented a nationwide automotive gasoline standard equivalent to Euro II. In addition, Beijing has started to apply the Euro III-equivalent standard for auto-use gasoline and diesel.

Years of unremitting research and development efforts have enabled China to develop its own technology leading to intellectual property rights in a number of core technologies. A series of unique refining technologies, including heavy oil catcracking, hydrocracking, hydrofining, residue hydrotreating, and hydro-upgrading, have been successfully developed and deployed. In chemical production, improvements have been developed and commercialized in ethylene cracking; in the production of acrylonitrile, ethylbenzene/styrene, polypropylene, SSBR [Solution Styrene Butadiene Rubber], and SBS [Styrene Butadiene Styrene]; in toluene disproportionation and transalkylation, aromatics extraction, and C5 extraction. Some of these improved technologies have also been licensed overseas. China is now 85 percent self-sufficient in manufacturing and supplying catalysts for refining and chemicals.

Petrochemical Technology—The Current Situation in China

China has made remarkable progress in petrochemical technology along with its industrial development. For more than 50 years, especially since the establishment of the former China Petrochemical Corporation in 1983, a technology R&D system has existed that inte-

*This paper is based on the author's plenary lecture presented at the 40th IUPAC Congress in Beijing, China on 15 August 2005.

grates research institutes, colleges and universities, and industrial enterprises. Guided by the motto "Prosper the Petrochemical Industry, Science and Technology Take the Lead," technological innovation was promoted based on licensed foreign technologies and a large number of patented technologies subsequently developed in China. This drive toward innovation has strongly bolstered China's petrochemical industry and is constantly driving it forward.

Through R&D and innovation, China has developed unique processes and catalyst technologies for clean fuels production, heavy and sour crude processing, and integration of refining and chemical production. China is also capable of building refineries with ten-million-tonne capacities with the self-developed technologies and equipment.

In clean fuels production, China has improved not only the conventional hydrocracking and hydrotreating technologies, but also a series of desulfurization and olefin reduction technologies for catalytic gasoline. These include medium-pressure hydro-upgrading and hydrotreating for diesel fuel; catalysts for diesel hydrotreating; new technologies for FCC [fluid catalytic cracking] gasoline desulphurization, such as FCC gasoline selective HDS [hydro desulfurization], FCC gasoline HDS, and olefin removal; flexible FCC gasoline olefin removal technologies and a supplemental reactor for upgrading and olefin removal; and a series of catalysts and co-catalysts that reduce the olefin content in FCC gasoline for the production of cleaner burning fuels. These technologies are helping to meet the goal of providing high-quality clean fuels for the 2008 Beijing Olympics and 2010 Shanghai World Expo.

In residue processing, improved technologies include residue catcracking, hydrotreating, and decoking. The self-developed Daqing vacuum residue FCC encompasses several leading technologies, lifting the ratio of vacuum residue in FCC feed to as high as 85 percent, or even 100 percent in some cases. This achievement allows China to process heavy crude and to utilize the residue resources. In addition, the patented fix-bed residue hydrotreating technology and relevant catalysts can effectively remove sulfur, nitrogen, and metals in the residue and fully convert sulfur-containing residue. Its successful commercialization marks a breakthrough in China's sour-crude processing technology, enabling China to process imported high-sulfur crude. Self-developed processes and catalysts for residue hydrotreating account for more than 90 percent of the market share in China.

In refining and chemical integration, a series of technologies for maximum chemical feedstock production have been developed, such as DCC (catcracking for maximum propylene production), maximum gasoline and LPG production, maximum iso-olefin production, maximum iso-paraffin production, hydrocracking to produce high-quality feedstock for reforming and cracking, and low-pressure combination-bed catalytic reforming for aromatics.

Improvements to other refining technologies, such as isomerization, hydrogenation, sulfur recovery, and technologies for high-class lubricants and asphalt have been developed. The Great Wall premium-quality lubricant was used in China's Shengzhou V Spaceship, and Donghai high-class asphalt was used in the Shanghai International Circuit's Formula-1 race track.

Through intensified technology transfer and innovation, China has developed and commercialized many patented chemical technologies, some of which have been licensed to overseas market.

With respect to basic organic feedstock, ethylene, butadiene, toluene disproportionation and transalkylation, and ethyl benzene/styrene technologies have been developed. The self-developed ethylene cracker, which is widely commercialized in China, achieves world-leading marks on technical and economic indices. The jointly-developed 100 kta cracker with ABB Lummus has been widely applied. The self-devel-

oped complete ethylene technology proved successful in revamping and expanding Tianjin and Zhongyuan ethylene facilities, demonstrating that China is able to build large-scale ethylene facilities independently with its own technologies.

With respect to other organic feedstock, acrylonitrile, purified terephthalic acid, cumene, caprolactam, ethylene glycol, and C5 extraction technologies have been developed. For caprolactam, China has developed and commercialized cyclohexane biomimetic catalytic oxidation, cyclohexanone oximation, and a magnetic stabilized fluid bed caprolactam purification process. This is the only brand new caprolactam process in the world.

In synthetic materials, loop-process polypropylene [PP], SBS/SSBR technologies have been developed and N catalyst for PP and SBS technology have been transferred overseas. N catalysts and NG catalysts for PP have been applied to large-, medium-, and small-scale PP facilities in China, delivering international-level performance.

China has developed a number of technologies for catalyst manufacturing. Catalyst technologies for catcracking, hydrofining, hydrocracking, residue hydrotreating, catalytic reforming, PP, polyethylene, ethylene oxide/ethylene glycol, AN, toluene disproportionation, and transalkylation have reached world-leading levels. Presently, 85 percent of the catalysts, solvents, and agents used in refining and chemical enterprises are domestically manufactured and supplied, with some exported as well.

Prospects for China's Petrochemical Technology

China has clearly developed a blueprint for constructing a moderately prosperous society in the first two decades of this century. Guided by this blueprint, China's goal is to sustain its healthy and fast economic growth, which should translate into sustained demand growth and huge potential for petrochemicals and other energy-related raw materials. This in turn will encourage the development of core and proprietary petrochemical technologies in the following areas.

1. China should further develop deep processing through innovation, such as hydrocracking, to increase product yield, to efficiently utilize this valuable crude resource, and convert it into transport fuels and chemical feedstock to the maximum extent possible. Clean-fuels production technologies should be developed to make it possible to meet the clean-fuels production requirements while using increasing amounts of low-cost feedstock. The target is to implement Euro III equivalent auto-use gasoline and diesel standards in China in 2010.

2. China should develop maximum low-carbon olefin and aromatics production technologies, utilizing the synergy of integrated refining and chemical operation. The refining industry should be restructured to revamp existing enterprises and increase their scale and integration. China should increase the number of ten-million-tonne capacity refineries and mega-tonne ethylene crackers in the Yangtze River Delta, Pearl River Delta, and Bohai Bay area, tapping the synergy of integration and optimization and improving competitive power.

3. The target for petrochemical technology development should be to address the needs of economic development. Therefore, ethylene and polyolefin technologies and other core and proprietary technologies should be intensely developed to reach world-leading levels, enabling the construction of large ethylene sites and major chemical complexes. New product development and product mix restructuring should be market oriented. While increasing production volume, the industry should also develop new products, upgrade product quality, increase the proportion of high-end products such as performance compounds of synthetic resins, and differential synthetic fibers, so as to sharpen its competitive edge in the marketplace.

4. China should comprehensively improve the industry's automation, optimize facilities in real time, and widely promote network technology. Petrochemical enterprises should implement enterprise resource planning and other IT construction measures, thus integrating human resources, operation management, and technology and optimizing information flow, materials flow, and cash flow. In this way, IT can strongly support the enterprise's operations and decision-making processes and facilitate the intelligence and modernization of the enterprise.

5. China should develop and promote efficient technologies and low pollution emissions. The industry should limit the generation of pollution at the source, increase production of clean fuels and green petrochemicals, and strengthen the control and recycling of pollutants.

Only with constant innovation can we succeed in developing new petrochemical technologies and meeting the changing and ever-higher requirements of the world economy and international community. As China's petrochemical enterprises pursue innovation, they seek to enhance the exchange and collaboration with international peers. We are committed to the harmonized development of the human society and our globe.

Jiming Wang is vice chairman of the Board of Directors and President of SINOPEC, Corp., China Petroleum & Chemical Corporation.

www.sinopec.com

The European Association for Chemical and Molecular Sciences

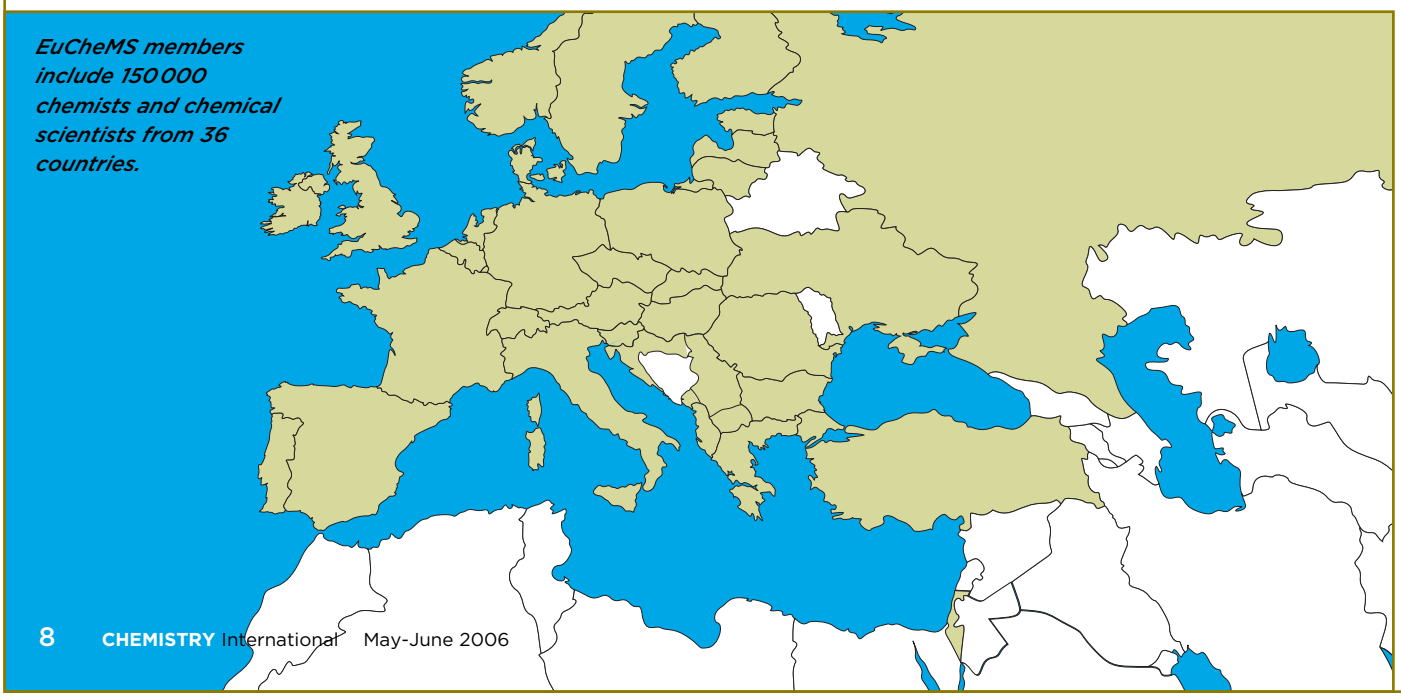
by Gábor Náray-Szabó

The chemists and chemical scientists of the Federation of European Chemical Sciences (FECS) have decided to take the lead in redefining our central science. Recently, FECS changed its name to the European Association for Chemical and Molecular Sciences (EuCheMS) to signal its transformation from an old club of committed scientists into a professional organization representing chemistry throughout Europe. The name change also reflects the organization's newfound determination to form alliances with other scientific disciplines that have an interest in molecules. Molecular biology, drug research, materials science, chemical engineering, and several other important new fields grew out of chemistry—a fact that is easily understood if one considers that all these disciplines focus on properties, interactions, and the engineering of molecules.

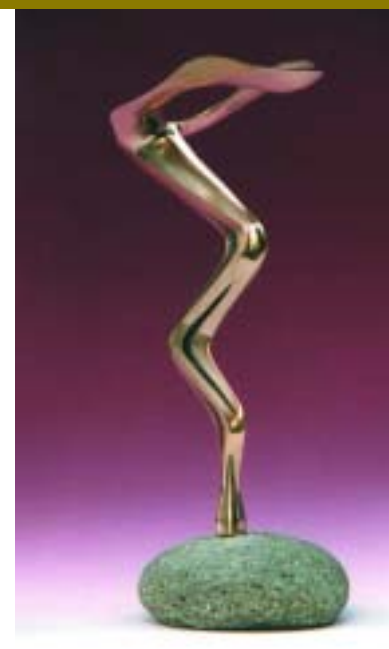
With the expansion of the European Union and recognition of the need for more cooperation among chemists, the members of EuCheMS have developed a vision for raising the stature and influence of the discipline. The idea is that if we represent our discipline at the European level more intensively, we will gain influence in legislation and we will put pressure on politicians to understand the vital role of chemistry in our knowledge-based society. Because the civil sector plays an increasingly important role in Europe, strong chemical societies, like the Gesellschaft Deutscher Chemiker (Germany) or the Royal Society of Chemistry (UK), together with EuCheMS can gain more publicity and influence.

An important challenge for the chemical community is to attain the right place for molecular sciences. In cooperation with representatives of other molecular disciplines and industries we should make clear to the public that chemistry plays a central role in everyday life. We all know that chemistry is essential to all branches of the natural sciences and to all but a few industries. For example, the molecular basis of life cannot be understood without a basic and thorough education in chemistry. Machinery requires paints and varnishes. Electronics production requires detailed knowledge of the chemical properties of complicated materials. Drug research is dependent on the molecular concept. Even archaeology and astronomy rely on chemical considerations. Clearly, we enjoy the benefits of thousands of chemical substances. It is important to convince all players, especially the public, but also scientists, engineers, and administrators, that without a broad knowledge on molecules the quality of our everyday lives would be diminished.

Despite the numerous applications of chemicals in everyday life—or perhaps because of over usage—the



EuCheMS members include 150 000 chemists and chemical scientists from 36 countries.



The Flavor of Rose, a sculpture by Béla Vízi, is the logo of the 1st European Chemistry Congress. Vízi, a retired chemistry professor of Veszprém University, Hungary, made the original of bronze and marine pebble stone. Standing 17-cm tall, the sculpture was inspired by the molecular shape of phenylethyl alcohol, a constituent of rose oil.

public image of chemistry is rather poor, which is something we have to change with full energy. We have to convince the laymen that chemistry does its best not *against*, but *for* society. Chemicals can become harmful if handled without appropriate expertise, but this can be avoided if more people—from pupils to teachers to employees to executives—can acquire some basic chemistry knowledge. In order to achieve this, we have to encourage more interest in chemistry. For example, its popularity could be enhanced by presenting meaningful experiments in schools and broadcasting fascinating programs on television.

About a year ago an editorial published in *Chemical & Engineering News* discussed whether or not the American Chemical Society should change its name—one it has had for more than 100 years. Clearly, our colleagues on the other side of the Atlantic are well aware of current trends: The molecular concept has gradually became so important that broad expert groups involved in any aspect of the molecular approach demand to have their own identity and a separate representation of interests.

Chemistry, like mathematics, penetrated into a great number of other disciplines, enriching them with the molecular concept and broadening their radius of action. However, chemistry, like math, may be absorbed by these disciplines, which would leave only a fraction of "pure" chemists on the scene. This is not desirable, since it is obvious that we, chemists, know the most about molecules and are best suited to transfer this knowledge to others. Several scientists who deal continuously with molecules call themselves molecular physicists, physiologists, pharmacologists, or materials scientists, but we have to underline that a considerable amount of their knowledge is related to the molecular concept. Therefore, by explicitly mentioning the term "molecular," the new name of the European chemists' association demonstrates our commitment to maintaining alliances among these various disciplines.

An outstanding opportunity to bring together European chemists and molecular scientists, as well as to raise public interest, will be the 1st

EuCheMS is a nonprofit association that promotes cooperation in Europe between nonprofit scientific and technical societies and professional institutions in the field of chemistry/chemical sciences whose membership consists largely of individual qualified chemists/chemical scientists and whose interests include the science and/or practice of chemistry/chemical sciences.

EuCheMS was founded in 1970 and currently has 50 member societies in 36 countries, which together represent over 150 000 individual chemists/chemical scientists. EuCheMS is an Associated Organization of IUPAC.

Divisions and Working Parties organize scientific and educational events on

- Analytical Chemistry
- Chemical Education
- Chemistry and the Environment
- Chemistry and Life Sciences
- Chemistry in Microsystems
- Computational Chemistry
- Food Chemistry
- History of Chemistry
- Organometallic Chemistry

EuCheMS is sponsoring the 1st European Chemistry Congress, 27-31 August 2006, Budapest, Hungary.

President: Professor Giovanni Natile (Italian Chemical Society)

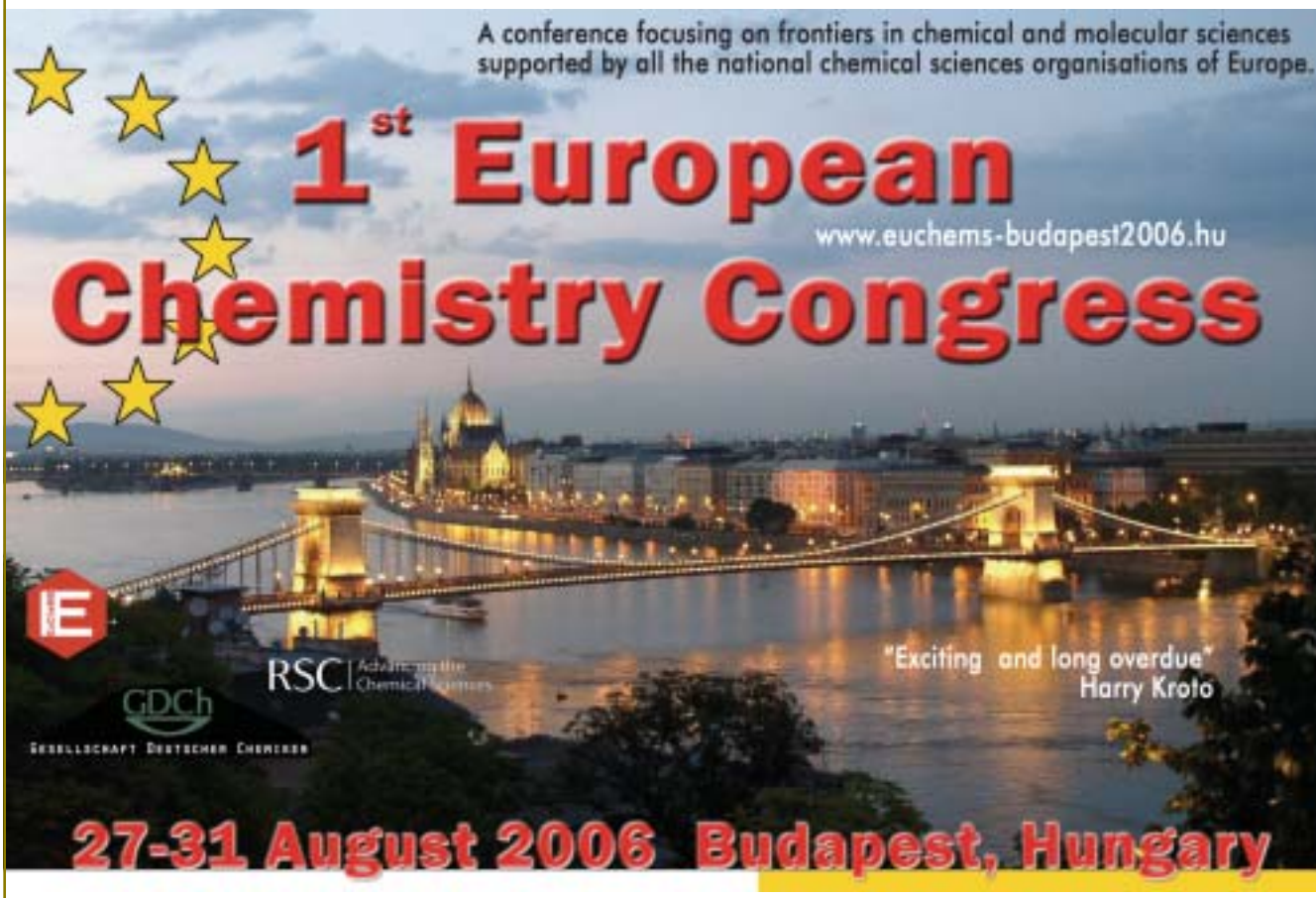
Secretariat: Ms. Evelyn McEwan (Royal Society of Chemistry) , Burlington House, Piccadilly, London W1J 0BA, Tel:+44 20 7440 330, Fax:+44 20 7437 8883, e-mail: mcewane@rsc.org

European Chemistry Congress, to be held 27-31 August 2006 <www.euchems-budapest2006.hu>. At the meeting, which will hopefully be the first in a series of forthcoming continental congresses, participants will convene to discuss major trends in chemistry and related disciplines. Six Nobel Laureates, 10 keynote speakers, and more than 100 invited speakers will discuss interesting hot topics, most of them at the boundary of chemistry and other disciplines. The meeting should help European chemists establish a new identity that more accurately reflects the enterprise in which we are engaged. This might be achieved by enhancing the public image of chemistry with well-established facts and arguments on the one side, but also by raising positive emotions on the other. We hope to spark public interest with, among other things, a special event devoted to "molecules and the senses," which will explore the molecular aspects of vision, taste, and smell through beautiful graphics and lectures on molecular gastronomy and the chemical diversity of odor signals.

The congress logo is intended to illustrate the link between molecules and beauty, or in other words, harmony. Chemists continually produce new molecules and new molecular constructions by gradually understanding more and more about the very nature of chemistry. As a result, chemists take their share from the continuous creation of our world, be this share as tiny as it is. In order to fulfil their duty, chemists require ever more knowledge, but they must acquire knowledge responsibly and for the well being of humankind and the environment.

Gábor Náray-Szabó is past president of EuCheMS; he has been involved in the work of EuCheMS since 1987 when he became joint general secretary. He has been president of the Hungarian Chemical Society and a member of the Executive Council of the World Federation of Engineering Organisations. He is a professor of chemistry at Eötvös University, Budapest.

www.euchems.org



The Tyranny of the Chemist

by Eric Scerri

In a recent book review, Peter Atkins draws attention to my use of the deliberately provocative phrase "the tyranny of the chemist" but immediately dismisses it by saying that readers will want to take issue with this notion.[1] I think my view might not be so abhorrent to chemists, and I would like to take the opportunity to explain it here.

First, a comment about scientific theories and their discoverers: In science, the pioneer of any particular development does not hold the right to dictate the future course of the discovery. For example, once Schrödinger published his second-order differential equation of the electron in the hydrogen atom, others quickly seized upon it to develop what essentially became quantum chemistry. Schrödinger himself was apparently horrified by these developments, which he regarded as highly unimaginative.[2] But his disapproval of what became of his brainchild did not prevent such later developments from taking place and being accepted.

Consider the members of any particular discipline who might make a discovery and wonder whether or not they have the right to pass judgment on what other scientists in other fields might do with their discoveries. Nobody doubts that the periodic system of the elements was discovered by chemists, although the very first recognition of periodicity among the elements seems to have been made by a French geologist, de Chancourtois. The other five discovers, Odling, Hinrichs, Newlands, Lothar Meyer, and, above all, Mendeleev, were all chemists. Does it follow that chemists retain the final say on how the periodic table should be represented or on the question of the placement of vexing elements like hydrogen and helium? Of course not!

And yet contemporary chemists do try to exercise a certain amount of "tyranny" when it comes to alternative forms of the periodic table or alternative placements of these elements. Chemists are perfectly willing to accept support from quantum mechanics when it lends fundamental support to the periodic system, which of course it does. Indeed, there were a number of prior developments in physics, such as the discovery of isotopy and of atomic number, that were readily accepted by chemists because they enriched our understanding of the periodic system rather than threatening it.

Nevertheless, in spite of accepting an explanation of the periodic system in terms of electronic configurations, chemists generally refuse to take any further leaps in accepting to place helium among the alkaline earths, for example, even though it has two outer-shell electrons. In addition, any suggestion that the left-step periodic system presents a more orderly representation of the elements is met with derision. Even more surprisingly, physicists themselves seem to acquiesce to this form of tyranny. Many group theoretical approaches to the periodic system call for a more orderly periodic system with two periods of two elements rather than just one. However, some physicists are willing to go to great lengths to modify their schemes in order to come out in agreement with the chemists' demand for an anomalous first-period length that does not repeat, unlike all subsequent period lengths, which do.[3]

My point is this: If chemists are willing to invite the support of physics because it lends a fundamental underpinning to the periodic system, perhaps they should consider dropping their tyrannical attitude when it is suggested that helium is more appropriately placed among the alkaline earths in spite of its apparent kinship to the noble gases. In the article that Atkins was reviewing, as well as elsewhere, I have given additional reasons as to why such a placement is not as absurd as it may seem at first sight. (This is another story, although one that the reader may wish to pursue.[4]) Needless to say, and as I have written before, I am not suggesting that every reductive step taken by physics should be followed blindly by chemists.[5] My aim here has been to suggest that there are instances when chemists do indeed behave a little like tyrants in believing that they alone can decide on matters relating to the periodic table.

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Defining a Data Standard for Near-Infrared Spectroscopy and Chemometrics

Successful long-term storage and retrieval of analytical data and the more-advanced techniques of data mining and knowledge generation are made possible through the deployment of well-documented, internationally recognized standard data formats.[1] At the end of 2001, a group of scientists with a history of international collaboration met to discuss problems they were encountering in exchanging near-infrared (NIR) spectroscopic data. A more serious problem was the inability to move chemometric data, including raw data and calibration models, among software programs from different vendors and those arising out of various research and development efforts. Also, although the 1988 Joint Committee on Atomic and Molecular Physical data—Data eXchange (JCAMP-DX) standard[2] had been adopted piecemeal by near-infrared instrument manufacturers, there was no data dictionary targeted specifically at the technological needs of the NIR community.

In response to these issues, a task group was formed and began work in 2002 on gathering information about the broader needs of the community. Several members of the task group had worked together on a European food-research project called Quality Established through Spectroscopic Techniques (QUEST). The QUEST team had sought to tackle the problem of a lack of standardization in the fields of NIR and chemometrics by developing their own project standards, providing a good knowledge base on which future efforts could build. This IUPAC project would use this knowledge base as a starting point, but the solutions that it created would need to be of broader scope, covering a wider range of instrumentation types than that deployed in the food and beverage arena.[3,4]

The NIR and Chemometrics Data Exchange Standards group meeting was attended by (from left to right) Rasmus Bro (KVL, Denmark), Mohamed Hanafi (ENITIAA/INRA, France), Douglas Rutledge (INA P-G, France), Tony Davies (Waters Informatics, Germany), Gerard Downey (Teagasc, Ireland), Jeremy Shaver (Eigenvector Research, U.S.) and Ian Cowe (FOSS NIR Systems, Sweden).

Most of the initial IUPAC work progressed slowly and was conducted electronically, but in light of the fact that the members of the group are all very active in industry, academia, and government laboratories, it was eventually concluded that a face-to-face meeting would be beneficial. There were several open issues that needed clarification, and, although the NIR work and the chemometrics work had separate objectives, with distinct timelines, having the entire task group work in both areas simultaneously had been problematic because of the different knowledge required for the two efforts. A meeting was thus called in January 2006 in Dublin, Ireland, with the aim of addressing these issues, getting the project back on track, and exploring the possibility of restructuring the task group into two parallel action groups corresponding to the two separate objectives.

It was particularly important to get the group moving again because the two recommendations it would be generating would be required for inclusion as the standard data dictionaries for Phase 2 and Phase 3 of the work on the new XML Analytical Information Markup Language (AnIML) data standards being conducted jointly with American Society for Testing and Materials (ASTM) International Subcommittee E13.15 <http://animl.sourceforge.net>. The meeting in Dublin brought together a good mix of instrument vendors, end users, third-party software providers, and academics.

Bones of Contention

The meeting began by bringing the participants up to speed on the work being conducted, including a review of the efforts of the ASTM E13.15 Subcommittee, which hadn't been calculated in when the initial project proposal had been drawn up. Extensive constructive debate concerning exactly what information should be addressed by the chemometrics standard cleared up a number of issues that had been slowing progress. One specific issue discussed was the proposed capability of vendor software to export calibration models within the exchange format.

There are major business issues associated with this capability, particularly in the food and agriculture analysis field. The generation and distribution of just these types of calibration models is a major source of revenue for instrument vendors, with thousands of copies of such software sold each year. If the capability to freely distribute these models were built into the instrument software, allowing the models to be exported in an open-standard format, it could undermine, if not eliminate, the essential and profitable development work conducted to produce such models. However, academics developing new chemometric methods wish for exactly this functionality in order to document their activities and compare and contrast them with those of colleagues and the wider scientific audience.

One proposed response to these issues draws on the solution to similar problems faced by vendors of reference spectroscopic databases. In this case, users often want to enhance the software by including and exporting their own reference data. The software packages have this capability and can differentiate between copyrighted vendor databases—which cannot be exported—and user-generated databases—which can. Adopting this solution would mean that vendor-supplied, commercially sensitive chemometrics models would receive the same type of protection, while users would be free to export calibration models that they generated themselves in the new IUPAC/JCAMP-DX chemometrics data file format.

The need to document chemometrics data in a long-term, stable, vendor-neutral format will steadily increase in the future.

Process Analytical Technology

The need to document chemometrics data in a long-term, stable, vendor-neutral format will steadily increase in the future. This is particularly true in light of the wider adoption of process analytical technologies in regulated industries, as highlighted by the U.S. Food and Drug Administration's efforts to actively promote such technologies within the pharmaceutical sector. This risk-based approach to pharmaceutical batch release essentially envisages the software packages using data obtained from the manufacturing plant to make the majority of decisions concerning the release of a particular batch to market.

This is a major departure from the current practice, under which a quality assurance chemist must sign a release certificate following a series of lab tests. It is therefore essential that the models on which the software bases its decisions are available for scrutiny at all times and well into the future, long after a particular product, software package, or installation has been decommissioned. Essentially these models, and the data fed into them to generate a decision, will fall under the same Good Manufacturing Practice predicate rules and 21 CFR Part 11 <www.21cfrpart11.com> electronic-records and electronic-signature rules as do the current analytical results and documentation within the quality assurance environment.

Education and e-Learning

In recent years major steps have been taken to integrate e-learning tools into normal curricula. In the chemometrics field, teachers and trainers have been developing courses with content that includes example calibration data files and the resulting models. The current state of the art is such that e-learning material often needs to be re-worked for each of the various third-party software solutions and instrument-vendor packages. When a standard format finally becomes available, it will greatly ease this burden, allowing trainers to post e-learning materials in the standard format for the trainees to download and install on their own systems, regardless of which chemometrics product they have standardized on.[5]

NIR File Format Standardization

A number of NIR data files in IUPAC/JCAMP-DX format were examined for compliance with the existing standards and found to require only relatively minor changes for compatibility. Participants also discussed what additions need to be made to the data dictionaries already available from prior JCAMP-DX standards. A draft recommendation is now being prepared. A second draft on chemometrics will also include a comprehensive list of the various pre- and post-processing algorithms commonly used in the field. A Web site has also been created to help broaden the discussion <www.jcamp.org>.

An Appeal

As with all such standards-development processes, the task group relies heavily on input from the scientific community and would very much encourage readers to follow the work as it progresses and to con-

tact them with constructive ideas to improve and perhaps speed up the development of these two important recommendations.

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www.iupac.org/projects/2002/2002-020-2-024.html

Analysis and Remediation of Arsenic Contamination in Groundwater

Naturally occurring arsenic contaminates a significant amount of the groundwater in the Asian country of Bangladesh, where thousands of shallow (10-40 m) tube wells sunk in the 1970s were found in the 1980s to be contaminated. Arsenicosis now seriously affects the health of many people in Bangladesh, and probably more than 100 million people worldwide. Arsenic contamination has been found in regional water supplies in Argentina, Australia, Chile, France, Ghana, Hungary, Mexico, Taiwan, the United Kingdom, and the United States.

To review the issues surrounding arsenic contamination, a project sponsored by the Committee on CHEMical Research Applied to World Needs (CHEMRAWN) was initiated, and an International Workshop on Arsenic Contamination and Safe Water was held at the Atomic Energy Centre, Dhaka, Bangladesh, on December 11–13, 2005. The workshop was organized under the joint sponsorship of the Bangladesh Academy of Sciences, the Bangladesh Arsenic Mitigation Water Supply Project, the Arsenic Policy Support Unit, the Bangladesh Chemical Society, the U.S. National Science Foundation, and IUPAC.

The opening session of the workshop included a welcoming address by the local Organizing Committee Chair Mohammed Mosihuzzaman of the University of Dhaka. The working sessions of the three-day workshop covered the following topics:

1. Current Status: Technical Aspects and Mitigation
2. Sources and Mobilization of Arsenic in Groundwater
3. Release Mechanisms and Transport
4. Measurements and Standards
5. Alternative Water-Supply Options
6. Microbial Contamination of Surface Water

Sut Ahuja, workshop chair, described how chemists and chemical engineers worldwide have responded to his appeal for assistance in addressing the problem of arsenic contamination in groundwater. Positive responses from the American Chemical Society's International Activities Committee, various divisions of IUPAC, and the CHEMRAWN committee led to the support for this workshop covering the following objectives:

- develop a better understanding of how arsenic gets into groundwater
- focus on the need to identify one or two optimum remediation techniques that can subsequently be scaled up
- communicate the need to safely dispose of the materials used to remove arsenic

Ahuja also noted a need to develop reliable and economical methods for monitoring arsenic in the laboratory and the field, as well as a need to provide consumers with the means to confirm that any decontamination device they are using is providing potable water.

Participants generally agreed that sedimentary arsenic has been carried downstream by the Ganges-Padma-Megna River system. At the workshop, Farhana Islam (Guelph University, Canada) explained how bacteria can catalyze desorption and dissolution of arsenic in the anaerobic, reducing environment of the subsoil. K.M. Campbell (CalTech, USA) elucidated the effects of reductive mineral dissolution and porewater chemistry on arsenic mobilization. Both Sinha

Ray (Centre for Ground Water studies, India) and D. Chatterjee (Kalyani University, India) discussed the genesis of arsenic in the Ganges delta, with specific reference to West Bengal. A.B.M. Badruzzaman (Bangladesh University of Engineering and Technology [BUET]), discussed his work on the hydrogeological and geochemical causes of arsenic contamination in Bangladesh. K.M. Ahmed (Dhaka University) spoke on arsenic mobilization in Bangladesh groundwater. K.M. Ahmed believes that strategically locating and properly installing arsenic-removal systems into a safe aquifer can provide non-hazardous water to a large number of people.

Feroze Ahmed (BUET) noted that 80 percent of the tube wells in 8,540 villages produce water that contains more than 50 ppb of arsenic. Currently, some 50 million persons in Bangladesh are exposed to high levels of arsenic, exceeding the World Health Organization standard of 10 ppb. Ahmed noted that a National Policy and Implementation Plan for Arsenic Mitigation has been developed, along with protocols for installation of alternative water-supply options, disposal of arsenic-rich sludge, diagnosis of arsenicosis, and water management. However, provision of alternative arsenic-safe water supplies has thus far reached only 4 million citizens, or some 2.9 percent of the population of Bangladesh.

S.M. Ihtishamul Huq (Department of Public Health Engineering [DPHE], Bangladesh) described an arsenic-screening project and subsequent arsenic-mitigation program sponsored by several stakeholder agencies. During the period of July 2002 to June 2005 the program evaluated arsenic-mitigation and -avoidance technologies in 15 regions of Bangladesh. These technologies included a pond sand filter, rainwater harvesting, the use of deep tube wells, dug-well renovation, piped water systems, and in-home arsenic-removal systems.

Several speakers at the workshop compared the cost-effectiveness and efficacy of arsenic-removal technologies applied to groundwater with the risks and benefits of those for purifying surface water, which is plentiful in Bangladesh. The consensus was that all of these technologies are potentially useful, and that the actual choice of which technology to deploy must be based on the specific conditions in each region. Hemda Garelick (Middlesex University, UK) described her IUPAC-sponsored project to employ multi-criteria analysis to assess current options for the mitigation/remediation of arsenic in drinking water.

S.I. Khan (Dhaka University) discussed surface-water microbiology, detection techniques, and quality assessment. Sk. Abu Jafar Shamsuddin (BUET) analyzed the risks arising from bacterial contamination of surface water compared to those associated with tube wells. He concluded that with current technologies, the worst overall public safety risks from bacterial contamination arise from the use of pond sand filters, with risks decreasing in the following order: pond sand filters, dug wells, rainwater harvesting, tube wells. Of these, pond sand filter systems, rainwater harvesting, and deep tube wells were free of arsenic contamination, but not free of bacterial contamination.

While many technologies have been developed to treat arsenic-contaminated water, on scales ranging from individual kitchen filters that sell for less than $40 to industrial-sized treatment plants, none has yet emerged as an optimal solution for the conditions encountered in Bangladesh. In February 2004, the Bangladesh Council of Scientific and Industrial Research identified four home-use systems (designated Alcan, Sidko, READ-F, and SONO) for evaluation. In most cases the materials used are not fully characterized, and the systems sold commercially have not been fully validated. However, while it is relatively easy to remove arsenic by adsorption on supported iron oxides, small point-of-use filters may become clogged after an indeterminate period of time.

Norma Alcantar (University of South Florida, USA) described her research on the use of envi-

ronmentally benign mucilage from a common Mexican cactus. James Navratil (Clemson University, USA) showed how the mineral magnetite can be employed as an adsorbent, isolated using a magnetic field, and cleaned using a regenerating solution.

A.H. Khan (Dhaka University) discussed model calculations on arsenic and other metal species in the groundwater system. He noted that the process of removing arsenic by adsorption on hydrated ferric hydroxide is controlled by first-order kinetics. Furthermore, he outlined standard operating procedures for laboratory analysis of trace metals, as well as quality control protocols. Speciation of arsenic requires separations based on solvent extraction, chromatography, and selective hydride generation. Most of these methods require expensive instrumentation, and the cost of training can also be high. Thus, there is a need to develop more economical and reliable methods of analysis.

Jörg Feldmann (University of Aberdeen, UK) addressed the reliability of field kits for determining the presence of arsenic in water. Much work remains to be done in developing analytical techniques for use in the field and the home. Feldmann also discussed how speciation analysis can help researchers investigate the arsenic uptake of plants, an especially important consideration in areas where phytoremediation might be an option for arsenic removal. P. Visoothiviseth (Mahidol University, Thailand) discussed remediation of arsenic contamination of soil with the help of plants.

Rick Johnson of UNICEF discussed the advantages of alternative water-supply options, including pond sand filters, river sand filters, rainwater harvesting, dug wells, sharing of green tube wells, deep tube wells, and arsenic-removal technologies. He concluded that it will be very important to integrate water hygiene and sanitation programs and that community choice will be very important in selecting the type of water supply utilized locally. He also emphasized the need for continual water-quality testing.

Guy Howard (Arsenic Policy Support Unit) described current progress in monitoring arsenic in water supplies in Bangladesh. He noted that blanket arsenic screening of 4.73 million tube wells revealed 1.29 million wells to be above 50 micrograms/liter. His assessment was that mitigation options have been made available for some 38 percent of the contaminated wells in Bangladesh, and that over the next five years most villages will receive some support. However, the population of Bangladesh is also expected to rise from 140 million to 250 million in the near future. Priority needs for the future include updated strategies, a scaled-up mitigation response, improved cross-ministry coordination, detailed groundwater mapping, studies of the impact of arsenic on agriculture, a better understanding of the epidemiology of arsenicosis, and full-scale clinical trials of antioxidants. A.K.M. Ibrahim (DPHE) described how piped water supplies can be financed through public-private partnerships.

Nicholas Priest (University of Middlesex, UK) outlined data from WHO indicating that there is no "threshold" value for incidence of cancer caused by arsenic. He concluded that there is no safe lower limit for arsenic exposure, since even low-level exposure appears likely to cause some additional incidence of cancer in the population. Moreover, Priest noted that the latency period for the appearance of skin lesions is some 23 years after exposure to arsenic. Priest concluded that authorities should apply the "precautionary principle," taking action to reduce arsenic exposure even before very strong evidence is uncovered.

Recommendations

In a well-attended closing session, the participants offered a large number of recommendations, as follows.

General

- An inventory should be conducted of the current research in arsenic pollution.
- A better communications network should be developed among the research community.
- More research should be conducted on treatment of surface waters.
- Where appropriate, piped water systems with central purification facilities should be installed.
- More research should be conducted on the relationships between arsenic and the incidence of disease.

Geochemistry

- More local information is needed, especially research on hydrology and microbiology.
- Current knowledge of arsenic sources must be expanded to cover the entire region.
- Studies of anaerobic microbial environments must be conducted.
- The aquifer should be mapped.

Analytical

- Economical and reliable analytical methods are needed.
- Additional training, especially of analytical technicians, is needed.
- The number of available service-oriented analytical laboratories is woefully inadequate, and needs to be increased.
- International assistance is needed to develop quality control guidelines.
- More funds are needed for analytical equipment. It is very important that the instrumentation acquired be reliable and accurate, but it does not need to be state-of-the-art.
- An inexpensive method for the detection of arsenic in the field and the home must be developed.
- The aqueous chemistry of arsenic, and especially the environmental effects of speciation, must be further investigated.
- The presence of arsenic in the food chain needs to be analyzed, and its effects elucidated.

Remediation

- The choice of remediation devices should be narrowed down to no more than three to allow better monitoring of these devices and enable scale-up for larger communities.
- The sludge disposal option should be further investigated.

Policies

- Efforts should be made to engage the private sector.
- Better coordination is needed between governmental and NGO operations.
- The policies that have already been promulgated need to be implemented.
- The maximum acceptable level of arsenic in drinking water should be reduced to 10 ppb.

For more information, contact Workshop Chair Sut Ahuja <sutahuja@xaranda.net>, or Task Group Co-Chair and CHEMRAWN Chair John Malin <jmalin023@comcast.net>.

www.iupac.org/projects/2003/2003-050-1-021.html

Herbal Medicine—Development of Methodologies and Protocols for Documentation, Evaluation of Safety and Efficacy, and Standardization

Herbal medicine has long played an important role in the primary healthcare of people around the world, especially those in third-world countries. As herbal medicine gains popularity in developed countries, the safety and efficacy of over-the-counter herbal drugs and other preparations are being scrutinized. The need for documentation and preservation of age-old knowledge of herbal medicine is also a matter of concern. In this context it is considered necessary to establish a Multidisciplinary International Research Center on Herbal Medicine.

As a first step towards this goal, a project has been undertaken to develop appropriate methodologies and protocols for documentation, evaluation of safety and efficacy, and standardization of herbal treatments. These internationally acceptable protocols will form the knowledge base for the establishment of the proposed research center. The documents, once posted on the IUPAC Web site, will be of tremendous value to scientists studying herbal medicine, as well as to producers of herbal preparations. A task group has been created, with members from countries around the globe. This group will work together electronically to develop the necessary protocols and will then meet in Dhaka, Bangladesh, in June 2006. The task group chairman will then take the necessary steps to publish the methodologies and protocols in IUPAC-accepted formats in such a manner as to make them accessible to the largest possible number of people.

For more information and to submit comments, contact Task Group Chairman Mohammed Mosihuzaman <mmosihuzzaman@yahoo.com>.

www.iupac.org/projects/2005/2005-034-1-300.html

Raising Awareness of the Chemical Weapons Convention and the Multiple Uses of Chemicals

At the end of October 2005, Moscow was the setting for the first workshop assessment of educational material produced for the project on the multiple uses of chemicals and professional codes of conduct (see Mar-Apr 2006 *CI*, p. 23). Some 25 academics, high school teachers, and chemistry students gathered at the D. Mendeleyev University of Chemical Technology to consider four papers. Produced over the months following the project start in August 2005, the papers covered the following topics: an introduction to multiple-use issues, background on the Chemical Weapons Convention (CWC), toxicology of selected chemical-warfare agents, and codes of conduct. All of the papers were translated into Russian for the workshop, and readers were asked to judge their suitability as teaching aids.

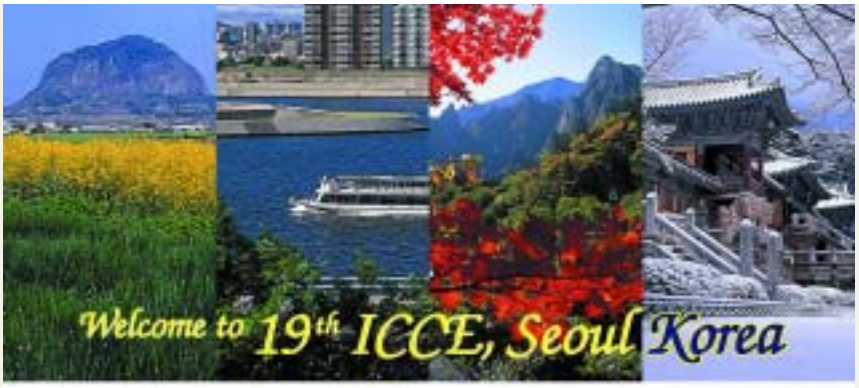
This first workshop was a trial run. The papers were introduced to the audience, who were then asked to break into smaller groups to consider a number of questions. These questions concerned the specific subject matter of the papers, but also extended to consideration of the control of chemicals, the availability of relevant information, and the responsibilities of those who use chemicals. Peter Mahaffy and Alastair Hay led the workshops, with Natalia Tarasova translating. Discussion was enthusiastic, and the feedback sessions equally so. Overall, the participants enjoyed the workshops, finding them lively, dynamic, and democratic. A wide range of opinions was expressed, and the topics clearly generated a great deal of discussion, as intended. As for the working papers, all were determined to be suitable as teaching aids, with some slight modifications required on two. These changes have since been made.

Two presentations on the work covered by this IUPAC project were given by Alastair Hay to the Organisation for the Prohibition of Chemical Weapons (OPCW) in the Hague. The OPCW oversees the CWC internationally. A meeting of national authorities at the OPCW was the venue for the first presentation, on 5 November 2005. These national authorities are responsible in their individual countries for conducting the day-to-day work of collecting data, organizing inspections, and upholding the CWC. The second presentation, on 9 February 2006, was made to the Scientific Advisory Board of the OPCW. Both groups of attendees endorsed the work of the IUPAC project group and offered to help in whatever way they could.

Further workshops are to be held over the next few months in Russia and at the University of Leeds in the United Kingdom to increase the audience reached. The Leeds workshops will test different approaches to using the prepared written material. Feedback from the workshops, together with the working papers in what is hoped will be their final form, will be presented at the 19th International Conference on Chemical Education in Seoul in August 2006.

For more information and to submit comments, contact Task Group Chairman Alastair W. Hay <a.w.m.hay@leeds.ac.uk>.

www.iupac.org/projects/2005/2005-029-1-050.html



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*.

Definitions of Terms Relating to the Structure and Processing of Inorganic and Polymeric Gels and Networks

This document defines terms related to the structure and processing of inorganic, polymeric, and hybrid inorganic-polymeric materials from precursors, through gels, to solid products. The document is divided into four sections—Precursors, Gels, Solids, and Processes—and the terms have been restricted to those most commonly encountered.

For the sake of completeness, in cases in which they are already satisfactorily defined, terms from other IUPAC publications have been used. In all other cases, the terms have been assembled and their definitions developed in consultation with experts in the relevant fields. The definitions are intended to assist the reader who is unfamiliar with sol-gel processing, ceramization, or related technologies and materials, and to serve as a guide to the standard terminology used by researchers in these areas.

Comments by 31 July 2006

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www.iupac.org/reports/provisional/abstract06/jones_310706.html

Explanatory Dictionary of Key Terms in Toxicology

The objective of the *Explanatory Dictionary of Concepts in Toxicology* is to provide full definitions of toxicological terms chosen, based on their importance and complexity, from the point of intersection of chemistry and toxicology. This requires a full description of the underlying concepts of the terms, beyond that provided in a typical dictionary definition. These explanatory definitions should help to overcome the barriers that are often caused by linguistic differences at the international level and between disciplines. The dictionary consists of about 68 terms chosen from the IUPAC Glossary of Terms Used in Toxicokinetics (*Pure Appl. Chem.*, **76**, pp. 1033–1082, 2004), organized under 22 main headings.

Comments by 31 May 2006

See Mar-Apr 2006 *CI*, p. 30, for contact information.

www.iupac.org/reports/provisional/abstract06/nordberg_310506.html

Glossary of Terms Relating to Pesticides

The Glossary of Terms Relating to Pesticides presents definitions of more than 500 terms regularly used in relation to the chemistry, mode of action, and regulation and use of pesticides. A wide range of disciplines are involved in this field, and the glossary was developed to facilitate communication between researchers, government regulatory authorities, and chemists in associated professional areas. The range of terms covers pesticide residue analysis, sampling for analysis, good laboratory practices, metabolism, environmental fate, effects on ecosystems, computer simulation models, toxicology, and risk assessment. The number of important pesticide-related terms has more than doubled since 1996, when the first IUPAC glossary of this type was developed (*Pure Appl. Chem.*, **68**, pp. 1167-1193, 1996), which is an indication of the extent to which this field of study has become integrated with many other scientific and regulatory disciplines.

Comments by 31 May 2006

See Mar-Apr 2006 *CI*, p. 30, for contact information.

www.iupac.org/reports/provisional/abstract06/stephenson_310506.html

The International Harmonized Protocol for the Proficiency Testing of Analytical Chemistry Laboratories (IUPAC Technical Report)

Michael Thompson, Stephen L.R. Ellison, and Roger Wood

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For a laboratory to produce consistently reliable data, it must implement an appropriate program of quality-assurance and performance-monitoring procedures. Proficiency testing is one of these procedures. The usual format for proficiency testing schemes in analytical chemistry is based on the distribution of samples of a test material to the participants. Participating laboratories ("participants") generally know the test material has been sent by a proficiency scheme provider, but occasionally the material may be received "blind" (i.e., it is received from a normal customer of the laboratory). The participants analyze the material without knowledge of the correct result and return the result of the measurement to the scheme provider. The provider converts the results into scores that reflect the performance of the participant laboratory. This alerts the participant to unexpected problems that might be present and spurs the management to take whatever remedial action is necessary.

The ethos of this Harmonized Protocol is that proficiency testing should provide information on the fitness-for-purpose of analytical results provided by participants, to assist them in meeting requirements. This can be achieved when:

- criteria for assessing results take fitness-for-purpose into account, so that scores inform participants when they need to improve their performance to satisfy customer (or stakeholder) needs
- the circumstances of proficiency testing are close to those prevailing during routine analysis, so that the outcome represents "real life"
- the method of scoring should be simple and, where at all possible, consistent over the whole realm of analytical measurement, to ensure ready interpretation by participants and customers

While the first consideration of proficiency testing is to provide a basis for self-help for each participant, it would be disingenuous to ignore the fact that other uses are made of proficiency testing results. Participants commonly use their scores to demonstrate competence to potential customers and accreditation assessors, and this has the unfortunate effect of pressurizing analysts to excel in the proficiency tests rather than simply to assess routine procedures. Participants should make every effort to avoid such a tendency as, for the most part, it is impossible for scheme providers to detect or eliminate it. Participants must also be diligent in avoiding any misinterpretation of accumulated scores.

The international standardizing organizations—International, ISO, and IUPAC—cooperated to produce the International Harmonized Protocol for the Proficiency Testing of (Chemical) Analytical Laboratories. The working group that produced the protocol agreed to revise that protocol in light of recent developments and the experience gained since it was first published in 1993. This revision has been prepared and agreed upon in light of comments received following open consultation.

www.iupac.org/publications/pac/2006/7801/7801x0145.html

Reference Data for the Density and Viscosity of Liquid Aluminum and Liquid Iron

Marc J. Assael, et al.

Journal of Physical and Chemical Reference Data
Vol. 35, No. 1, pp. 285–300 (2006)
doi:10.1063/1.2149380

The available experimental data for the density and viscosity of liquid aluminum and iron have been critically examined with the intention of establishing a density and a viscosity standard. All experimental data have been categorized into primary and secondary data according to the quality of measurement specified by a series of criteria. The proposed standard reference correlations for the density of the aluminum and iron are characterized by standard deviations of 0.65% and 0.77% at the 95% confidence level, respectively. The overall uncertainty in the absolute values of the density is estimated to be one of ±0.7% for aluminum and 0.8% for iron, which is

worse than that of the most optimistic claims but recognizes the unexplained discrepancies between different methods. The standard reference correlations for the viscosity of aluminum and iron are characterized by standard deviations of 13.7% and 5.7% at the 95% confidence level, respectively. The uncertainty in the absolute values of the viscosity of the two metals is thought to be no larger than the scatter between measurements made with different techniques and so can be said to be ±14% in the case of aluminum and ±6% in the case of iron.

The work described in this paper was carried out under the auspices of the International Association for Transport Properties (formerly known as the IUPAC Subcommittee of Transport Properties). Support was provided by IUPAC under project 2003-005-1-100.

www.iupac.org/projects/2003/2003-005-1-100.html

How to Access Structure and Dynamics of Solutions: The Capabilities of Computational Methods (Special Topic Article)

Bernd M. Rode and Thomas S. Hofer

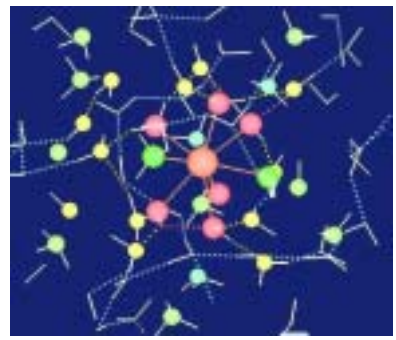
Pure and Applied Chemistry
Vol. 78, No. 3, pp. 525–539 (2006)
doi:10.1351/pac200678030525

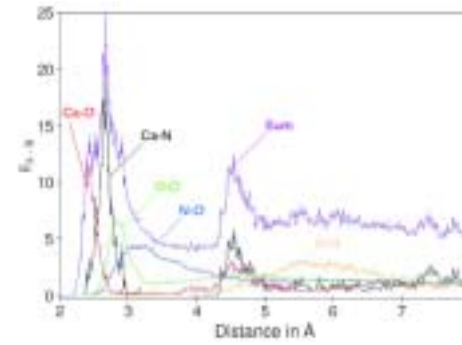
Every experimental result is only as good as the theoretical model employed for its interpretation. Usually there is a complicated way from the actually measured data to the final results; for example, the determination of a structure: A theoretical model has to be defined, to which the measured data are fitted until the "best possible" agreement is achieved, mostly within a few percent of deviation. Though not too error-prone in the case of highly regular solids, this procedure becomes more difficult with gases (with their high mobility of components) and with liquids (where high mobility is combined with a density similar to solids). Any *a priori* postulated models can be much too simplified.

The quality of theoretical models plays a pivotal role in the determination of structural parameters, and even more, when other physicochemical phenomena such as reaction dynamics and mechanisms (where all interpretation of measurements depends on a correct structural model plus corresponding mechanistic models) are evaluated.

In this article, the progress of computational chemistry in the treatment of liquid systems is outlined. Emphasis is on the combination of the statistical methods—Monte Carlo and molecular dynamics—with quantum mechanics as the main foundation of this progress. The difficulties of experimental studies of liquid systems without having obtained sophisticated theoretical models describing the structural entities and the dynamical behavior of these liquids demonstrate that chemistry research is in a transition phase, where theory and high-performance computing have not only become a valuable supplement but an essential and almost indispensable component to secure a correct interpretation of measured data.

www.iupac.org/publications/pac/2006/7803/7803x0525.html





One of the ways in which simulations are superior to experiments is that they offer the possibility of easily evaluating any kind of atom–atom pair distribution. In more complex systems (e.g., mixed solvents and solutions simultaneously containing several solute species), this is an enormous advantage over spectroscopic approaches, where only averaged data (e.g., atom-atom distances) can be "seen." The example shown in this figure illustrates the overlay of various atom–atom radial distribution functions for Ca(II) ion in aqueous ammonia [from A. Tongraar, K. Sagarik, B.M. Rode. Phys.Chem. *4, 628 (2002)].*

XML-Based IUPAC Standard for Experimental, Predicted, and Critically Evaluated Thermodynamic Property Data Storage and Capture (ThermoML) (IUPAC Recommendations 2006)

Michael Frenkel, Robert D. Chiroco, Vladimir Diky, Qian Dong, Kenneth N. Marsh, John H. Dymond, William A. Wakeham, Stephen E. Stein, Erich Königsberger, and Anthony R.H. Goodwin

Pure and Applied Chemistry
Vol. 78, No. 3, pp. 541-612 (2006)
doi:10.1351/pac200678030541

ThermoML is an Extensible Markup Language (XML)-based new IUPAC standard for storage and exchange of experimental, predicted, and critically evaluated thermophysical and thermochemical property data. The basic principles, scope, and description of all structural elements of ThermoML are discussed. ThermoML covers essentially all thermodynamic and transport property data (more than 120 properties) for pure compounds, multicomponent mixtures, and chemical reactions (including change-of-state and equilibrium reactions). Representations of all quantities related to the expression of uncertainty in ThermoML conform to the *Guide to the Expression of Uncertainty in Measurement*. The ThermoMLEquation schema for representation of fitted equations with ThermoML is also described and provided as supporting information together with specific formulations for several equations commonly used in the representation of thermodynamic and thermophysical properties. The role of ThermoML in global data communication processes is discussed. The text of a variety of data files (use cases) illustrating the ThermoML format for pure compounds, mixtures, and chemical reactions, as well as the complete ThermoML schema text, are provided as supporting information.

www.iupac.org/publications/pac/2006/7803/7803x0541.html

Letters in Support of the ThermoML Standard

In a linking agreement between Elsevier and the Thermodynamic Research Center at NIST (USA), the ThermoML standard is used to make freely available thermochemical and physical property data connected to published articles. It concerns articles from *The Journal of Chemical Thermodynamics* (since 2004), *Fluid Phase Equilibria*, and *Thermochimica Acta* (since 2005). Thanks to the ThermoML standard, this data is now available in an as universal-as-possible format, to scientists and engineers in industry and university laboratories. A link to the ThermoML record is available with the journal article on <ScienceDirect.com>, while the respective journal article in which the data was reported can be found following a link on the data record. The editors of the journals and Elsevier consider this a major addition to the published content, and so are our authors who are pleased and eager to submit.

Michiel Thijssen <m.thijssen@elsevier.com>
Publishing Editor,
Elsevier B.V., Amsterdam

ThermoML will continue to have a positive impact on data activities, including scientific publishing (it is already used by five major journals), development of properties databases, and development of tools to correlate or to accurately predict thermodynamic quantities. I would anticipate that the proposed IUPAC standard will have an important role in the sharing of data between research groups as well as the storage and retrieval of such data. In addition, the standard addresses uncertainties of the data in a way that is consistent with the comprehensive reference document *Guide to the Expression of Uncertainty in Measurement* published by the International Organization for Standardization. The power of this concept lies in the fact that a complete knowledge of a physical quantity consists of a numerical value, its units, its uncertainty, and its provenance. This concept can help to create information and knowledge management systems that could carry the field of thermodynamics to the next level of intelligent predictive tools.

Joseph Magee <joe.magee@nist.gov>
National Institute of Standards and Technology, Boulder, Colorado USA

JCAMP-DX for Electron Magnetic Resonance (IUPAC Recommendations 2006)

Richard Cammack, Yang Fann, Robert J. Lancashire, John P. Maher, Peter S. McIntyre, and Reef Morse

Pure and Applied Chemistry
Vol. 78, No. 3, pp. 613–631 (2006)
doi:10.1351/pac200678030613

The Joint Committee on Atomic and Molecular Physical data-Data eXchange (JCAMP-DX) is an evolving, open-ended, machine-independent, self-documenting file format for exchanging and archiving data from computerized laboratory instruments such as spectrometers and diffractometers whose output is commonly represented as spectral (profile) plots, contours, or peak tables. The first JCAMP-DX protocol was designed to meet the need for exchanging infrared spectra between similar instruments of different manufacturers. The present document is the result of ongoing efforts by users and manufacturers to extend JCAMP-DX to other types of instrumental data.

A major objective of JCAMP-DX is to enable routine capture of data at the source to make it available for exchange, archiving, and entry into databases. All data are represented as labeled fields of variable length using printable ASCII characters. A JCAMP-DX file is a text file that can be viewed, corrected, and annotated with ASCII text editors. Use of the name JCAMP-DX in the description of software capability implies the ability to generate and read JCAMP-DX files as defined in the relevant published protocols for a particular datatype.

This version of JCAMP-DX provides for a description of the file structure to be used to accommodate a very wide range of electron magnetic resonance applications. As much as it is very desirable for instrument data systems to be able to read and write files in a standard format directly, instrument vendors are encouraged to develop JCAMP-DX software for the instruments they currently support. This standard of the JCAMP-DX was further extended to cover Y2K-compatible date strings and good laboratory practice, and the next release will cover the information needed for storing n-dimensional data sets.

www.iupac.org/publications/pac/2006/7803/7803x0613.html

Uncertainty Estimation and Figures of Merit for Multivariate Calibration (IUPAC Technical Report)

Alejandro C. Olivieri, Nicolaas (Klaas) M. Faber, Joan Ferré, Ricard Boqué, John H. Kalivas, and Howard Mark

Pure and Applied Chemistry
Vol. 78, No. 3, pp. 633-661 (2006)
doi:10.1351/pac200678030633

This report gives an introduction to multivariate calibration from a chemometrics perspective and reviews the various proposals to generalize the well-established univariate methodology to the multivariate domain. Univariate calibration leads to relatively simple models with a sound statistical underpinning. The associated uncertainty estimation and figures of merit are thoroughly covered in several official documents. However, univariate model predictions for unknown samples are reliable only if the signal is sufficiently selective for the analyte of interest. By contrast, multivariate calibration methods may produce valid predictions also from highly unselective data. A case in point is quantification from near-infrared spectra. With the ever-increasing sophistication of analytical instruments inevitably comes a suite of multivariate calibration methods, each with its own underlying assumptions and statistical properties. As a result, uncertainty estimation and figures of merit for multivariate calibration methods has become a subject of active research, especially in the field of chemometrics.

www.iupac.org/publications/pac/2006/7803/7803x0633.html

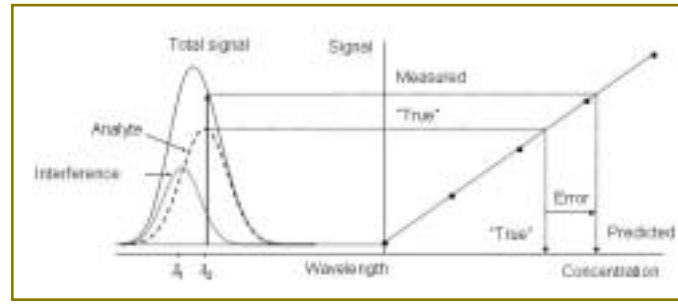


Illustration of how a univariate model will lead to severely biased predictions when unsuspected interferences give a variable contribution to the signal, whereas multiple measurements may permit accurate prediction in such a situation.

Guidelines for NMR Measurements for Determination of High and Low p*K*a Values (IUPAC Technical Report)

Konstantin Popov, Hannu Rönkkömäki, and Lauri H. J. Lajunen

Pure and Applied Chemistry
Vol. 78, No. 3, pp. 663–675 (2006)
doi:10.1351/pac200678030663

Factors affecting the NMR titration procedures for the determination of pK_a values in strongly basic and strongly acidic aqueous solutions (2 > pH > 0 and 14 > pH > 12) are analyzed. Guidelines for experimental procedure and publication protocols are presented in this report. These include:

- calculation of the equilibrium H^+ concentration in a sample
- avoidance of measurement with glass electrode in highly acidic (basic) solutions
- exclusion of D_2O as a solvent
- use of an individual sample isolated from air for each pH value
- use of external reference and lock compounds
- use of a medium of constant ionic strength with clear indication of the supporting electrolyte and of the way the contribution of any ligand to the ionic strength of the medium is accounted for
- use of the NMR technique in a way that eliminates sample heating to facilitate better sample temperature control (e.g., ^{1}H-coupled NMR for nuclei other than protons, GD-mode, CPD-mode, etc.)
- use of Me_4NCl/Me_4NOH or KCl/KOH as a supporting electrolyte in basic solution rather than sodium salts in order to eliminate errors arising from NaOH association
- verification of the independence of the NMR chemical shift from background electrolyte composition and concentration
- use of extrapolation procedures

www.iupac.org/publications/pac/2006/7803/7803x0663.html

Guidelines for Terminology for Microtechnology in Clinical Laboratories (IUPAC Technical Report)

Peter Wilding, Thomas Joos, Larry J. Kricka, and Leming Shi

Pure and Applied Chemistry
Vol. 78, No. 3, pp. 677–684 (2006)
doi:10.1351/pac200678030677

There is no formal terminology used to describe the scope and use of microtechnology in the clinical laboratory. For many laboratory scientists, the word "microchip" is synonymous with high-density microarrays used primarily for investigating gene expression. This document proposes a system of "categories" and "descriptors" that facilitate the classification of a microfabricated device (MFD) in a way that communicates details of its function and analytical role, and describes the analytical principle involved and the methods and materials used for its manufacture. Adoption of this system would enable scientists to employ four descriptors that clearly delineate the function, analytical role, and chemical or physical principle involved in the device.

www.iupac.org/publications/pac/2006/7803/7803x0677.html

NanoChip® Electronic Microarray, Nanogen Corp., San Diego, CA, USA

MFD Categories	A, B, C, D, E
Descriptors	
1. Function	Multi
2. Analytical role	Nucleic acid analysis
3. Chem/Phys principle	Hybridization
4. Device description:	
4.1. Materials	Silicon
4.2. Methods	Lithography
4.3. Physical layout	Digital image
4.4. Peripherals	Cartridge

Agilent 2100 Bioanalyzer®, Agilent Technologies, Palo Alto,CA, USA

MFD Categories	A
Descriptors	
1. Function	Multi
2. Analytical role	DNA sizing
3. Chem/Phys principle	Capillary electrophoresis
4. Device description:	
4.1. Materials	Glass
4.2. Methods	Lithography
4.3. Physical layout	Digital image
4.4. Peripherals	Plastic cartridge

Examples of microfabricated devices (MFD) and descriptions. The MFD categories are: A, microfluidic; B, micro-electronic; C, microarray; D, chemically reactive component-based; E, individually addressable; and F, micro-electromechanical. See full text for details.

Special Topic Articles Featuring the 2005 Winners of the IUPAC Prizes for Young Chemists

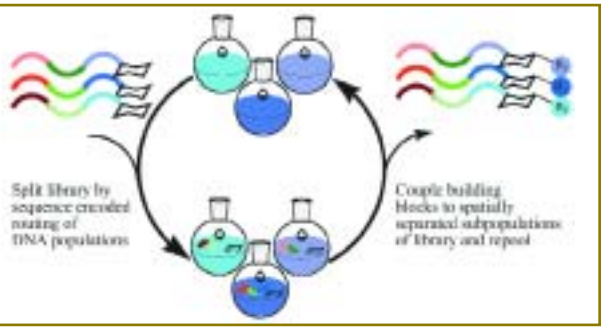
Pure and Applied Chemistry
Vol. 78, No. 1, pp. 1–64, 2006

As an international nongovernmental scientific organization, IUPAC takes great interest in the worldwide achievements of chemists, particularly young chemists. Therefore, IUPAC established the annual prestigious Prizes for Young Chemists. In doing so, we endeavor to encourage research in the chemical sciences and the participation of promising young chemists.

Starting in 2002, prizewinners have been invited to submit manuscripts on aspects of their research topics for consideration as short, critical review articles to be published in *Pure and Applied Chemistry*. Following peer review, the first collection appeared in *PAC* **74**(11), 2021–2081 (2002) and encouraged the view that it offers sufficient readership appeal to become a regular special topic feature of the journal. The second series, covering the works of the 2003 winners was published in *PAC* **76**(2), 263–319 (2004), and the third series in *PAC* **76**(12), 2051–2099 (2004). The most recent series of articles was published in the January 2006 issue of *PAC* and includes the following critical reviews:

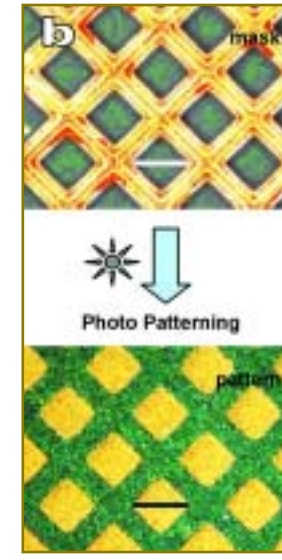
"Evolutionary Approaches for the Discovery of Functional Synthetic Small Molecules," by Zev J. Gartner (pp. 1-14)

Directed evolution is a powerful method for the laboratory discovery of nucleic acids and proteins with desired functional properties. A hallmark of this approach is the iterative translation, selection, amplification, and diversification of genetic information. The potential of evolutionary methods to impact the discovery of synthetic small molecules has recently been explored by a variety of laboratories. Four methods encompassing some or all of the hallmarks of evolution are discussed, including dynamic combinatorial chemistry, genetic algorithms, DNA display, and DNA-templated synthesis.



DNA display: DNA libraries are split into subpopulations according to their sequences. Each subpopulation, having in common a particular DNA codon, is subjected to a particular set of reaction conditions. The reacted subpopulations are re-pooled and subjected to further manipulations. (by Z.J. Gartner)

Flash welding technique can be used to create patterns in nanofiber films. The top optical microscopy image shows a copper grid mask lying on top of a polyaniline nanofiber film. After exposure to a camera flash, the grid pattern is generated on the nanofiber film. The unmasked diamond shaped areas are welded, therefore, reflect more light and look bright under an optical microscope. The previously masked areas still look green (scale bar:100 m). (by J. Huang)



"Syntheses and Applications of Conducting Polymer Polyaniline Nanofibers," by Jiaxing Huang (pp. 15-27)

Nanofibers with diameters of tens of nanometers appear to be an intrinsic morphological unit that was found to "naturally" form in the early stage of the chemical oxidative polymerization of aniline. In conventional polymerization, nanofibers are subject to secondary growth of irregularly shaped particles, which leads to the final granular agglomerates. The key to producing pure nanofibers is to suppress secondary growth. Based on this, two methods—interfacial polymerization and rapidly mixed reactions—have been developed that can readily produce pure nanofibers by slightly modifying the conventional chemical synthesis of polyaniline without the need for any template or structural directing material. With this nanofiber morphology, the dispersibility and processibility of polyaniline are now much improved. The nanofibers show dramatically enhanced performance over conventional polyaniline applications such as in chemical sensors. They can also serve as a template to grow inorganic/polyaniline nanocomposites that lead

to exciting properties such as electrical bistability that can be used for nonvolatile memory devices. Additionally, a novel flash welding technique for the nanofibers has been developed that can be used to make asymmetric polymer membranes, form patterned nanofiber films, and create polymer-based nanocomposites based on an enhanced photothermal effect observed in these highly conjugated polymeric nanofibers.

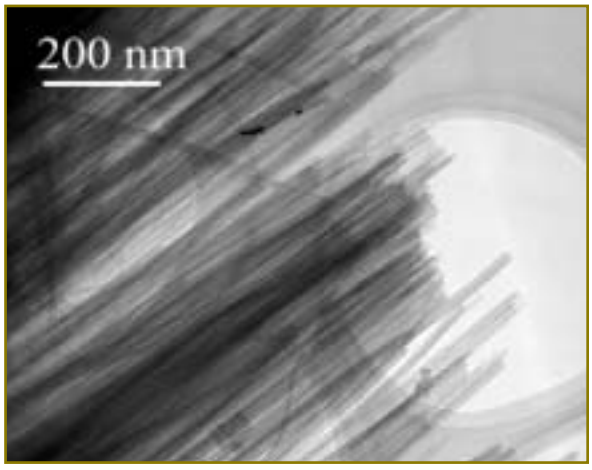
"A Dozen Years of N-Confusion: From Synthesis to Supramolecular Chemistry," by Hiromitsu Maeda and Hiroyuki Furuta (pp. 29-44)

The chemistry of N-confused porphyrin (NCP) and its analogs started in 1994. Since then, considerable progress has been made in understanding the unique properties of NCP and its analogs, which confer characteristic reactivity and metal complex formation. The evolved isomers, multiply NCPs, and expanded N-confused derivatives, have opened up new realms of NCP chemistry. *Cis*- and *trans*-doubly N-confused porphyrin (N_2CP) stabilizes higher oxidation states such as Cu^{III} in square-planar fashion in the core. Confused isomers with five or more pyrrole rings can coordinate several cations owing to their larger cavities compared to tetrapyrrolic system. The peripheral nitrogen(s) of NCP and its analogs can serve as hydrogen-bonding donor and acceptor, and metal coordination site as well. For example, NCP forms versatile dimers with the assistance of metal ions. The square-planar divalent metal complexes of C_6F_5-substituted NCP act as efficient anion-binding receptors. Furthermore, Cu^{III} complexes of N_2CP, possessing both N and NH at the periphery, form self-assembled one-dimensional (1D) hydrogen-bonding networks, whose orientations differ in *cis* (zigzag) and *trans* (straight) isomers.

"Solution-Based Routes to Transition-Metal Oxide One-Dimensional Nanostructures," by Xun Wang and Yadong Li (pp. 45-64)

One-dimensional (1D) nanostructures have drawn continuous research attention because of their unique electrical, optical, and magnetic properties different from that of bulk and nanoparticles, as well as their potential applications in mesoscopic research and nanodevices. The main challenge in this area is how to precisely control the sizes, dimensionalities, compositions, and crystal structures in nanoscale, which may serve as a powerful tool for the tailoring of physical/chemical properties of materials in a controllable way. Here, we review the advances in the solution-based routes to prepare 1D nanostructures. Particularly, three systems of MnO_2, rare-earth compounds, and silicates have been chosen to show the synthetic strategy under hydrothermal conditions. As the main theme, a rolling mechanism has been given special attention to present a relative general understanding of the growth of various transition-metal oxide 1D nanostructures under solution conditions.

www.iupac.org/publications/pac/2006/7801



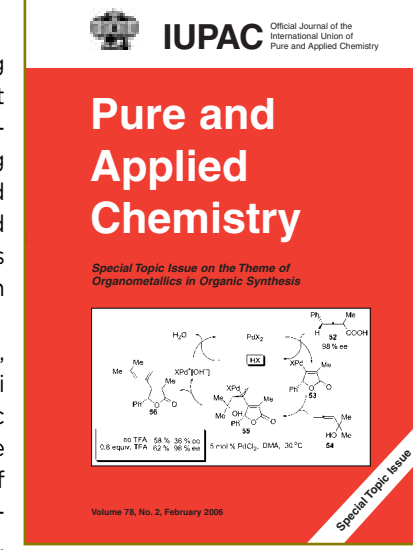
TEM image of δ-MnO_2 nanotubes with α-$NaMnO_2$ as precursors. (Xun Wang)

Evolution of the N-confused porphyrin (NCP) family. (by H. Maeda)

Organometallics in Organic Synthesis

Pure and Applied Chemistry
Vol. 78, No. 2, pp. 197–523 (2006)

*This Special Topic Issue includes reviews and research papers based on lectures presented at the 13th IUPAC International Symposium on Organometallic Chemistry Directed Towards Organic Synthesis (OMCOS-13), Geneva, Switzerland, 17–21 July 2005; Foreward, J.R. Bull (*PAC *Scientific Editor); Preface, A. Alexakis and E.P. Kündig (OMCOS-13 co-chairs).*



The past 25 years have witnessed some quite extraordinary advances in the development and synthetic application of organometallic reagents and catalysts. In 2001, Sharpless, Noyori, and Knowles received the Nobel Prize for their work in this area of chemistry; and the high profile has been maintained by the award of the 2005 Nobel Prize in Chemistry to Chauvin, Grubbs, and Schrock for the development of the metathesis method in organic synthesis. These advances are also reflected in the history of the conference series Organometallic Chemistry Directed Towards Organic Synthesis (OMCOS), which has established itself as a popular and enduring international forum for presentation and discussion of mainstream developments and opportunities in this field.

The series was inaugurated in Fort Collins, Colorado, USA in 1981. Proceedings of the plenary program of that event were published in *PAC* **53**(12), 1981, and the topic has since become a regular feature in the Journal, with the distinction of having recorded some of the seminal advances of the period. Indeed, as the OMCOS series has grown in support and stature over the years, it has played a leading role in a trend toward more in-depth coverage of the scientific proceedings of selected IUPAC-sponsored conferences.

This Special Topic issue is devoted to exclusive coverage of OMCOS-13. No less than 37 papers drawn from invitations to all invited presenters on the main lecture program and a selection of meritorious contributed works feature, and constitute a salute to the centrality of, this theme in modern organic synthesis. It is also a tribute to the exceptional efforts of the organizers and authors, whose energy and cooperation have ensured an expeditious passage to publication of this representative record of an outstanding event.

OMCOS-13 had a record number of nearly 1200 participants from 41 countries, and there was an encouragingly high proportion of young scientists in attendance. Very strong Asian participation at this conference reflected the outstanding level of research and leadership in this field from countries such as Japan, China, South Korea, and Taiwan.

Prof. Shengming Ma, from the Shanghai Institute of Organic Chemistry of the Chinese Academy of Science and the Department of Chemistry, Zhejiang University, China received the OMCOS-13 Award (sponsored by the Yen Chuang Foundation and Springer Verlag). The prize was awarded for his creative research contributions in the field of transition-metal-catalyzed reactions of allenes.

Apart from the OMCOS-13 Award lecture, there were 23 plenary lectures and 20 oral communications that dealt with aspects of reactivity and chemoselectivity of main group and transition metal organometallics. Stereoselectivity issues also figured prominently with a particular emphasis on asymmetric synthesis and catalysis. Mechanistic insights, new reagents for synthesis, new catalyst- and ligand-design and ligand-effects were other important topics. For many of the speakers, total synthesis was the "proving ground" for new or enhanced reactions that demonstrate new levels of selectivity and functional group tolerance. At the other end of the scale, the wealth of practical methods for the flexible synthesis of important building blocks continues to grow. Organometallic methods rest at the heart of the "toolbox" of organic synthesis with the quest for further increases in reactivity, versatility and selectivity.

The quality of the 620 posters that were on display during the entire conference was also outstanding. This extraordinary poster session was highlighted with the Monday evening "poster party" and culminated in the awarding of 37 poster prizes.

The 14th edition of OMCOS will be held in Nara, Japan (2–6 Aug 2007) under the chairmanship of Prof. Koichiro Oshima, Kyoto.

www.iupac.org/publications/pac/2006/7802

Chemical Thermodynamics

by Andrey Ya. Borshchevsky and Svetlana S. Melkhanova

The Russian International Conference on Chemical Thermodynamics (RCCT-2005) was held at Moscow State University from 27 June to 2 July 2005. This international meeting covered new developments in physical chemistry, including general topics of chemical thermodynamics, individual substances, solutions and melts, heterogeneous systems, and complex thermodynamic systems. RCCT-2005 attracted 476 participants from 27 different countries. The meeting was held under the auspices of IUPAC, the Russian Academy of Sciences, and the D.I. Mendeleev Chemical Society. The scientific program embraced all aspects of modern chemical thermodynamics. Among the 15 plenary lectures were the following:

- "Thermodynamic Approaches in Material Chemistry," Y.D. Tretyakov (Moscow State University, Russia)
- "Lattice Vibration and Phase Transition of Quasicrystals and the Related Crystals," A. Inaba (Osaka University, Japan)
- "Thermodynamic Properties and Phase Equilibria of Alloy Systems Relevant for Lead-Free Soldering," H. Ipser, H. Flandorfer (University of Vienna, Austria)
- "The Swelling of Nonionic and Ionic Arcylamide Hydrogels in Aqueous Solutions," G. Maurer (University of Kaiserslautern, Germany)
- "Technical Features and Unique Features of the Modern Heat Flux DSC," J. Schawe, S.V. Averkiev (Mettler Toledo GmbH, Switzerland)
- "Thermodynamic Modeling of Multicomponent Ionic Melts," S.A. Degterev (École Polytechnique de Montréal, Canada)

The head of the thermochemistry lab of Moscow State University, Prof. Lev. N. Sidorov (center), with a group of students who assisted with organizing the conference.

- "A New Field of Modern Thermodynamics—Nonequilibrium Nondissipative Thermodynamics," Ji-Tao Wang (Fudan University, China)
- "Progresses in Polymer Thermodynamics by Scanning Transitiometry," J.P.E. Grolier (Blaise Pascal University)

In addition, 155 oral and 488 poster contributions were presented in five parallel sessions. About 100 participants also took part in two round-tables: "Nanothermodynamics" and "Development of Thermochemistry in M.V. Lomonosov Moscow State University."

During the closing ceremony, doctorate awards, sponsored by Elsevier, were presented by the International Association of Chemical Thermodynamics to Alexey Popov (Lomonosov State University, Moscow, Russia) and Giuseppe Lazzara (University of Palermo, Palermo, Italy).

The conference program was released in the form of a book of abstracts (two volumes) and also on CD. Publications related to the conference will appear in a special issue of the *Russian Journal of Physical Chemistry*. The next conference in this series will be held in July 2007 in Suzdal, an inviting historical town situated about 400 km east of Moscow. Prof. Yuri Tretyakov is chair of the conference. See <www.isc-ras.ru/RCCT2007> for details.

Dr. Andrey Ya. Borshchevsky <borsch@phys.chem.msu.ru>, vice chair of the conference, is a professor in the Chemistry Department of Moscow State University.

Polymers for Advanced Technologies

by György Bertalan, György Marosi, and Andrea Toldy

The 8th International Symposium on Polymers for Advanced Technologies (PAT) 2005, held in Budapest, 13–16 September 2005, was organized by the Budapest University of Technology and Economics, and under the auspices of IUPAC, the European Polymer Federation, Society of Polymer Science Japan, Chemical Society of Japan, Polymer and PMSE Divisions of the American Chemical Society, Budapest University of Technology and Economics, and Hungarian Academy of Sciences.

More than 350 active participants attended the conference, among them experienced researchers and

younger scientists, leading specialists in various domains of the polymer industry, and student representatives of numerous universities.

The scientific program consisted of eight plenary and 44 invited lectures, about 120 oral presentations, and about 140 posters. The presentations covered not only the cutting edge and new trends in contemporary technological methods, but also basic research on new processes. Particularly emphasized were various methods of polymer synthesis that result in special architecture. The oral presentations were organized into four sections, covering the major domains of polymer technology:

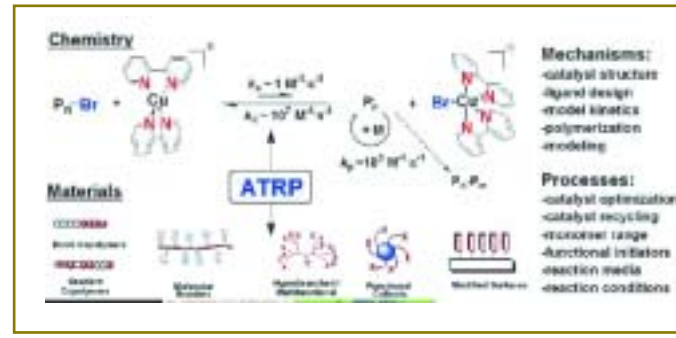
- Section A — Advanced Macromolecular Syntheses/Structures
- Section B — Advanced Multicomponent Systems, Nanocomposites
- Section C — Electro-Optical and Other Advanced Technologies
- Section D — Biomedical Application, Biodegradation

Menachem Lewin (left), the honorary chairman of PAT—founder of the PAT Symposium and the PAT journal—received a ZEMPLÉN award from Prof. György POKOL (Dean of the Faculty of Chemical Engineering of Budapest University of Technology and Economics) for propagation of the results of international and Hungarian science.

The plenary lectures were devoted to cutting-edge and contemporary topics related to a number of advanced polymer technologies, as well as associated basic research. Topics included water purification through plastic optical fibers, nanostructured polymer materials created via atom transfer radical polymerization (ATRP) grafting or inclusion of nanotubes, and the use of photo- and thermally sensitive polymers as templates and surface patterning components. Prof. J. Economy cited a U.S. intelligence report that states that by the year 2015, water—not energy or food—will become the major problem resource in the United States and throughout the world. A number of new systems for trace-contaminant removal were described (e.g., new and improved high-surface-area adsorbent polymer fibers designed to remove trace contaminants to below 1 part per billion). Prof. P. Hodge addressed the theoretical and technological aspects of ring-chain equilibria, including an introduction to entropically-driven ring-opening polymerization (ED-ROP), discussing the useful features of ED-ROPs, the preparation of macrocyclic oligomers, and possible practical applications. Prof. K. Matyjaszewski spoke on recent polymer syntheses using ATRP of acrylates, methacrylates, styrenes, acrylamides, acrylonitrile, and many other vinyl monomers to create polymers with a large range of molecular weights and with low polydispersities.

A discussion of the development of plastic optical fiber materials (POF) was presented by Prof. Y. Okamoto. POF has been increasingly applied to computer LANs. Along with several other advantageous properties, the elastic moduli of POF are typically many times lower than those of silica. Prof. B. Voit gave an especially interesting presentation demonstrating the applicability of photo- and thermally labile polymers for template formation and surface patterning.

Section A of the oral presentations included discussions on a wide range of contemporary synthesis methods. Various basic materials were used for synthesis, including naturally occurring polymers (W.H. Daly), novel block copolymers (R. Faust), functionalized polymers (F. D'Agosto), nanocomposites, nanoparticles, biodegradable polymers, charge-transporting polymers, polymers used for biomacromolecular engineering, smart amphiphilic, and polymer networks.



Chemistry, mechanisms, materials synthesized, and processes arising from ATRP, as presented by Prof. K. Matyjaszewski.

Section B included presentations on a large variety of multicomponent polymer systems, their processing, properties, and applications. Several presentations

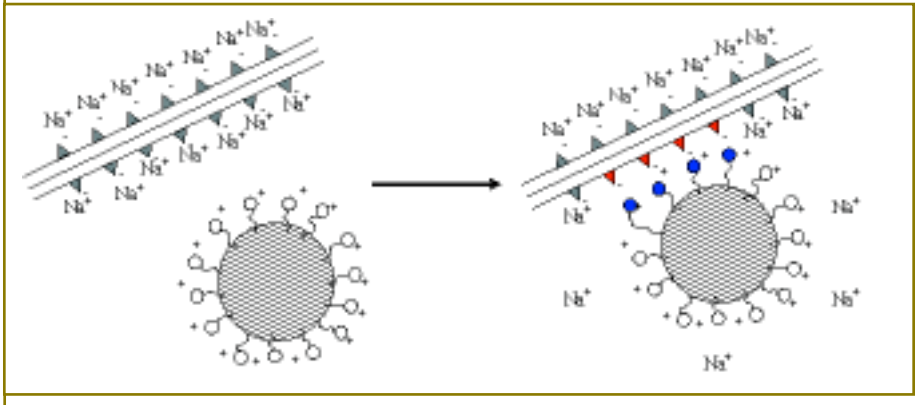
devoted to the structure-properties relationship elucidated not only the functional modification of composites, but also the role of surface and interface modification. Presentations covering the use of nanocomposites as fire retardants represented another significant aspect of Section B. An important phenomenon, the migration of clay and structural changes in nanocomposites occurring upon annealing at elevated temperatures, was discussed by Prof. M. Lewin.

Section C covered a great variety of methods, special materials, and devices, such as sensors, electroluminescents in polymer composites, polymer gels as promising technological smart materials, latex-coated polymer materials as synthetic mimics for micrometeorites, and nanostructure polymer membranes for use in fuel cells. Particular interest was generated by a presentation on polymers as functional components in batteries and fuel cells (G. Wegner).

Section D covered a great number of biodegradable, biocompatible polymers, and their application as carriers for drug delivery and for surface modification, as well as stimuli-responsive and smart polymers. Biodegradable polymers synthesized from fatty acids have been used as injectable carriers for delivery of small drug molecules as well as peptides and proteins (A. Domb). An especially important biomaterial has revolutionized cardiology through the use of metal stents coated with poly (styrene-β-isobutylene-β-styrene) triblock copolymers (SIBS) that release a restenosis-preventing drug. This device has already been implanted in ~1 000 000 patients and reduced the need for invasive coronary bypass surgery by ~85% (J.P. Kennedy). Polymer nanofibers and nanotubes were also discussed as showing promise for medical applications (J.H. Wendorff). The roles of polymer networks, hydrogels, and polymer-based micro- and nanoparticles in controlled drug-delivery systems were also discussed (I. Eros).

The final presentation and closing remarks, made by the chairman of the conference (Gy. Marosi), focused on the convergent trends of advanced technologies. Polymer science and technology was long divided into several branches that developed almost independently. Due to specialization, there was only limited interaction between the research fields of natural and synthetic, hydrophilic and thermoplastic, and linear and cross-linked polymers. This situation is changing, however, as the gap between the different areas of research is gradually narrowing. Convergent concepts can be seen in the areas of advanced polymer systems used as pharmaceuticals, biomaterials, polymer composites, fire retardants, membranes, conductive polymer systems, and polymers used in fuel cells. The widespread use of the ATRP technique, the increasing importance of the controlled synthesis of nanostructures, special interface modifiers allowing the use of in-line controlled reactive processing methods, and advanced surface engineering/analysis are examples of the tendency toward convergence. Examples presented in the last talk of the conference included the use of process control for the synthesis of reactive surfactants and polymer dispersions intercalated with nanolayers, as shown in the figure below.

Such a structure is advantageous both for the controlled release of drugs from solid pharmaceuticals and for activating the protection mechanism in fire-retardant polymer systems. Raman microscopy is a method that is universally applicable in all advanced polymer technologies, and thus also represents a convergence of research areas. Quantitative chemical mapping of complex composites and pharmaceuticals, determination of polymorph structures at interphases of various macromolecular systems, and in-line detection of reactive extrusion of synthetic and biopolymers have been performed using the Raman system. Nanotubes as potential components of composites for drug delivery or in flame-retar-



Intercalated montmorillonite structure formed by emulsion polymerization, presented by Marosi.

dant systems have also been analyzed in this manner. Lastly, the fire retardancy of biodegradable polymers is an excellent example of the convergence of different fields. The tendency toward convergence was clearly evident at the Budapest symposium and will surely continue to increase in Shanghai at PAT 2007.

The abstracts of all presentation are available at <www.bme.hu/pat2005>.

György Marosi <pat@mail.bme.hu>, a professor in the Department of Organic Chemical Technology at the Budapest University of Technology and Economics, served as chairman of the local organizing committee. Bertalan and Toldy were also members of the local organzing committee.

Heterocyclic Chemistry

by Girolamo Cirrincione and Anna Maria Almerico

The 20th International Congress of Heterocyclic Chemistry (20th ICHC) was held in Palermo, Italy, from 31 July to 5 August 2005. ICHCs are major scientific events that have been organized all over the world since 1967, attracting attendees from both industry and academia. These congresses are broad enough in scope to cover the whole range of heterocyclic chemistry, from theory to practical applications. The 2005 congress was organized by Professor Girolamo Cirrincione and Colleagues in the Department Farmacochimico, Tossicologico e Biologico, of the University of Palermo, under the auspices of the International Society of Heterocyclic Chemistry (ISHC) and of the Società Chimica Italiana (SCI).

Heterocyclic chemistry has undergone a noteworthy and scientifically intriguing expansion. In addition to the more traditional subjects of heterocycle synthesis and studies related to heterocyclic natural products, the field has grown to encompass pursuits in areas such as bioorganic and organometallic chemistry, to mention just two. The 20th ICHC was in line with established tradition, offering a scientific program dealing with the latest developments in the following main topics: new methods in heterocyclic chemistry, biologically active heterocycles (pharmaceuticals and agrochemicals), heterocyclic natural products and analogues, and heterocycles in synthesis.

Award lectures were delivered by Larry Overman (University of California, Irvine, U.S.) for the Senior Award in Heterocyclic Chemistry, and by Alois Furstner (Max-Plank-Institut für Kohlenforschung, Mülheim/Ruhr, Germany) for the Katritzky Junior Award in Heterocyclic Chemistry.

The 32 invited speakers—26 from academia and six from industry—were organized into four parallel sessions. There were also 100 oral contributions in four parallel sessions and 282 poster presentations in three sessions. The plenary and invited lectures have been published in part vii of the 2006 volumes of ARKIVOC —the *Free Online Journal of Organic Chemistry* <www.arkat-usa.org/ark/ARKIVOC/arkivoc_articles.asp>.

ICHC organizers and staff with conference chairman Prof. Girolamo Cirincione (held aloft in back row) and ICHC President Prof. Marco A. Ciufolini (seated in center of stage).

During the conference, editor Eric Scriven briefly reviewed the journal's first five years of activity.

The opening ceremony took place at Massimo Theatre, a magnificent example of neoclassic architecture. On the stage, Prof. Girolamo Cirrincione (chairman of the congress), Prof. Domenico Spinelli (representative of SCI), Prof. David St. C. Black (representative of IUPAC), Prof. Marco Ciufolini (president of the ISHC), and Prof. Giuseppe Silvestri (rector of the University of Palermo) welcomed the participants. Since it was the 200th anniversary of the University of Palermo, the rector presented a brief history of the university and of Palazzo Steri, which now hosts the offices of the rectorate.

Two outstanding members of the ISHC were honored during the conference's social banquet, held at the Palazzo Guglielmo, Monreale: past Secretary Prof. Hans Neunhoeffer and past President Prof. Steven Weinreb. Each received a plaque recognizing his enormous contributions to the organization. In addition, Hans Neunhoeffer was named a Fellow of the ISHC. During the banquet, awards were also presented to two young scientists, Dr. Atsuko Ochida from Hokkaido University and Dr. Clara Cena from the University of Torino, for the best poster presentations.

The congress was successful in that it attracted a large number of delegates discussing their latest results, presenting opportunities for suggestions for novel research ideas and for the creation of new relationships.

The main topics, covering the whole range of heterocyclic chemistry, offered an interesting insight into several promising fields of science that have an important role in improving the well-being of humans and their environment. The oral and poster presentations attempted to emphasise the state-of-the-art in key areas of the heterocyclic science as well.

Members of the heterocyclic community are invited to join the next ICHC, to be held in Sydney, Australia, on 15–17 July 2007 <www.chem.unsw.edu.au/research/conferences/ichc2007.html>. On behalf of the organizing committee, the authors would like to wish success to the 21st International Congress and to its chairman, Professor David St. Clair Black.

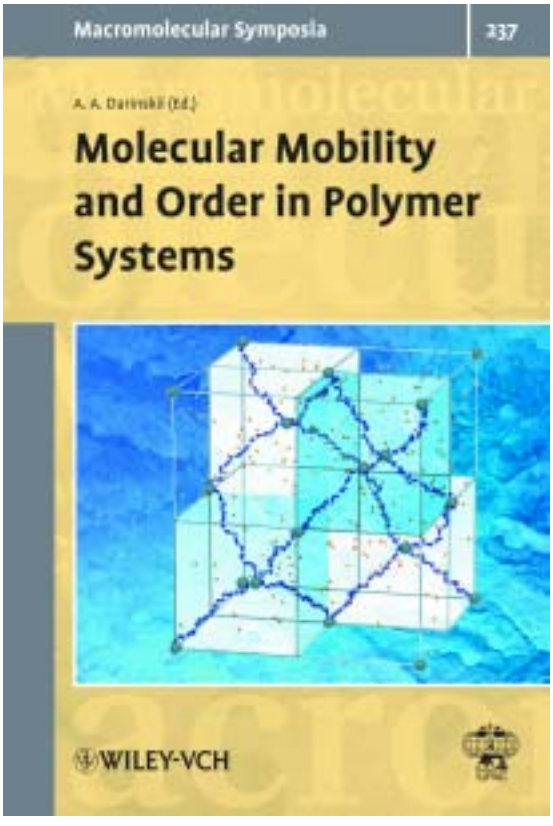
Girolamo Cirrincione <gcirrinc@unipa.it>, a professor at the Università di Palermo, was chairman of the 20th ICHC. Anna Maria Almerico <almerico@unipa.it>, also a professor at the Università di Palermo, served as secretary.

Molecular Mobility and Order in Polymer Systems

by Anatoly Darinskii

The **5th International Symposium on Molecular Mobility and Order in Polymer Systems**, sponsored by IUPAC, was held at the Scientists House (the former Great Duke Vladimir's Palace) in Saint Petersburg, Russia, 20–24 June 2005. The palace is located on the Neva river embankment and is one of the most beautiful in St. Petersburg. The symposium was organized by the Department of Chemistry and Material Science of the Russian Academy of Sciences, the Polymer Council of the Russian Academy of Sciences, and the Institute of Macromolecular Compounds of the Russian Academy of Sciences. The meeting was supported by the Russian Foundation of Basic Research and the St. Petersburg Research Center of the Russian Academy of Sciences.

The symposium was the latest of a series of St. Petersburg meetings on macromolecules, the first of which was held in October 1994. These meetings are



the most important international gatherings of polymer scientists in Russia. They provide a venue in which young scientists and more experienced researchers have the opportunity for close, friendly contact with the leading specialists in the various domains of polymer science.

The symposium included 21 plenary lectures, 60 oral presentations, and more than 210 posters by attendees from 29 countries in Europe, Asia, and the Americas. The primary focus was on the structure and dynamics of polymer systems that combine order and pronounced molecular mobility (i.e., systems with so-called "soft" order). Many such systems arise under certain conditions during the process of self-organization, and many change their structure in reaction to even small changes in these conditions.

Such systems are in the mainstream of modern polymer science and are the reason for the high level of interest in the symposium by both Russian and foreign scientists. Numerous scientists working in theoretical physics and the computer modeling of polymers also traditionally attend these meetings. Many studies presented at the symposium were conducted as collaborative efforts between Russian and Western researchers within the framework of international scientific projects and grants.

In addition, special effort was made to attract young scientists. More than 50 students presented their results at poster sessions. Reduced registration fees for young scientists and for some researchers from less-developed countries promoted their participation in the symposium. Financial sponsorship by IUPAC made it possible to partially cover the expenses of young participants from countries of the former Soviet Union.

Plenary lectures were presented in the White Hall of the palace. Contributed talks were held in two parallel sessions. Two eminent specialists from Russia and abroad chaired each session.

The symposium program covered six broad topics:

- Macromolecules in Solutions, Melts, and Networks Oriented and Stretched in Strong External Fields
- Liquid Crystalline Polymers
- Copolymers and Polymer Blends
- Polymer Layers and Micelles
- Polymer Complexes and Membranes
- Polymer Networks of Different Topologies, Branched and Star Polymers, and Dendrimers

Information from the symposium program can be found online at <www.macro.ru>. A selection of contributions (some plenary lectures and selected oral/poster presentations) appear as full papers in volume 237 (March 2006) of *Macromolecular Symposia* <www.iupac.org/publications/macro/2006/237_preface.html>.

Anatoly Darinskii <adar@imc.macro.ru>, head of the laboratory of the theory and modeling of polymers at the Institute of Macromolecular Compounds, Russia Academy of Sciences (IMC RAS), served as chairman of the symposium.

Chemistry in Kenya—Its Contribution to a Healthy Environment and Socio-Economic Development

by Sidney F.A. Kettle

In July 2005 the Kenyan Government announced a 5-year plan under which, by 2010, 50 percent of all university students will be scientists. This project served as a fitting background for the 5th Annual International Conference organized by the Kenya Chemical Society, which took place at Kenyatta University, Nairobi, on 22–26 August 2005. The author also attended the first of these meetings and was thus able to make a comparison that showed a clear evolution over the last several years.

Funds are most readily available for research relevant to the Kenyan economy, and so it is understandable that a good portion of the papers presented at the conference dealt with local plant products (particularly those with medicinal potential) and local environmental issues (particularly turning waste into useful materials). However, between the two meetings that the author attended, there has clearly been an increase in collaboration between Kenyan scientists and research groups in developed countries. This collaboration enabled, at the most recent meeting, presentations reporting on work entailing the use of

state-of-art techniques. Thus, the structures of some local plant products were described at a level of detail and certainty that was absent 12 years ago. It became clear that Kenya has no shortage of able and aware chemists who can be expected to make an increasing contribution to future chemical research worldwide.

Although there were poster sessions at the conference, virtually all presentations were oral. Although about half of the presentations were made by research students or those who had only recently completed their work, there was no problem with stage fright—one student even offered to answer questions on behalf of her research supervisor, who had to be absent at the time. The general interest in the meeting was reflected in the attendance levels, which were good from start to finish, with no evident falling-off with time. On the final day, in fact, lunch had to be pushed back an hour because of the number of questions.

About a third of the 16 plenaries were presented by Kenyan chemists, and like those presented by scientists invited from abroad, they tended to focus on chemistry topics with local relevance. Topics included the use of clones to gain insights into long-term fertilizer use (Owour), phytochemical studies on popular Kenyan medicinal plants (Midiwo), and, surprising but relevant, the possible use of rice husk ash for low-cost housing (Kamau). Less surprising, but no less relevant, were plenary lectures on the use of indigenous herbs for treating malaria (Chhabra) and tuberculosis (Rajab). There were also presentations that had potential political implications: Wandiga on vulnerability to climate-induced highland malaria, Getenga on pesticide residues, and, clearly, Karanja on the need for a new approach to university research and technological development in Kenya.

Among the lecturers from outside of Kenya, Carles Codina (Barcelona) dealt with natural antioxidants, Keremire (Uganda) reviewed the health benefits of anthocyanins, and Masaaki Kai (Nagasaki) described some very new and sensitive methods of detecting DNA. Chawla (New Delhi) detailed some very simple but effective methods of extending the shelf life of fruit and vegetables without using refrigeration. Liebscher (Berlin) lectured on some novel cyclic peroxides for use as antimalarial compounds. More theoretical were Kruger (Durban), who reported on related preparative and ab initio work on simple acetylation reactions, and Kettle (Norwich), who discussed symmetry and spectroscopy.

There were more than 60 contributed papers, the majority from Kenyans, of course, but also including plenty from authors of other countries: South Africa, Spain, Uganda, Norway, Germany, Madagascar, the Ivory Coast, the United States, Tanzania, Sweden, Botswana, Japan, Belarus, and the United Kingdom. Some of these same countries also appeared on the list of sponsors. The author suspects that world interest in chemistry in Kenya will continue to increase. One plenary commented that the threat of litigation in many developed nations—together with health and safety controls—has severely limited the "hands-on" experience of chemistry students in these countries. No such restrictions exist in Kenya, and, with the backing indicated at the beginning of this article, in the future it will be the most evidently able students who study chemistry. Scientists of more than 12 nationalities, representing about one in 10 participants, attended this meeting, and the author believes that participation in future meetings in this series will increase considerably.

Sidney F.A. Kettle <s.kettle@uea.ac.uk> is professor at the School of Chemical Sciences at the University of East Anglia in Norwich, UK.

The Kenya Chemical Society is an Associate National Adhering Organizations of IUPAC. Prof. Shem O. Wandiga, chairman of the society, can be reached by e-mail at <sowandiga@iconnect.co.ke>.

In September 2006, an IUPAC-sponsored conference on Occupational Health and Safety Management in East Africa will take place in Nairobi—see Where 2B&Y, p. 36

Environmental Best Practices

7–10 August 2006, Olsztyn, Poland

The First International Environmental Best Practices Conference (EBP) will be held 7–10 August 2006 at the University of Warmia and Mazury in Olsztyn, Poland. The EBP conference is organized in collaboration with the Sam Houston University, Huntsville, Texas.

The objective of the conference is to bring together researchers from academic, governmental and industrial institutions to discuss new developments and results in the fields of environmental remediation, wastewater treatment, solid waste management, alternative energy sources and environmental stewardship. It is anticipated that attendees will develop a knowledge and understanding of a broad spectrum of environmental applications and solutions to the challenges facing the world today.

This conference is best suited for individuals working in the fields of Biology, Chemistry, Engineering, Government Regulation and Project Management.

The conference topics will include:

- Environmental Remediation (in situ and ex situ, bioavailability and genotoxicity of compounds, mycotoxins, monitoring of pollutants, modelling contamination)
- Wastewater Treatment (centralized and decentralized systems, sewage sludge processing and disposal)
- Solid Waste Management (strategies, resource recovery and reuse, landfilling, pretreatment)
- Alternative Energy Sources (fuel cell, biofuels, organic solid waste, solar power, liquefied natural and petroleum gas, wind, tidal, geothermal, hydroelectric)
- Environmental Stewardship (agriculture, ecotourism, native flora and fauna, invasive species, water quality and environmental indicators, impact assessment of engineering and biotechnological undertakings)

The social program will include a reception at Olsztyn Castle, a banquet at the lake shore, a post-conference tour to Gdansk and surrounding anti-flood installations. For accompanying persons, there are various tours available, including visits to historical places, museums and leisure centers.

See Mark Your Calendar on page 38 for contact information.

www.uwm.edu.pl/wosir/EBP

Raman Spectroscopy

20–25 August 2006, Yokohama, Japan

The 20th International Conference on Raman Spectroscopy (ICORS 2006) will be held 20–25 August 2006 in the city of Yokohama, Japan, and will be chaired by University of Tokyo Professor Hiro-o Hamaguchi. Seventeen subjects or groups of topics will cover all aspects of basic and applied Raman spectroscopy, including theory; resonance and time-resolved Raman spectroscopy and ultrafast phenomena; vibrational analysis and molecular structure; thin layers, surfaces, and interfaces; and applications to material science, technology, biology, and medicine.

Six satellite meetings will focus on specific subjects related to Raman spectroscopy. These include an International Workshop on X-Ray Raman and Related Phenomena (Okazaki, 17–20 August), Protein Dynamics and Biological Applications of Time-Resolved Spectroscopy (Kobe, 18–19 August), Tsukuba Satellite Symposium on Single Molecule and Tip-Enhanced Raman Scattering (Tsukuba, 17–19 August), International Symposium on Surface-Enhanced Raman Scattering and Spectroscopy (Nishinomiya, 28–29 August), New Horizon of Medical Applications of Spectroscopy (Tokyo, 26–27 August), and Ultrafast Time-Resolved and Time-Domain Vibrational Spectroscopy (Wako, 18–19 August).

About 500 people from more than 25 countries are expected to attend this ICORS meeting—a grand forum for those interested in new Raman spectroscopy.

See Mark Your Calendar on page 39 for contact information.

www.pac.ne.jp/icors2006

Chemical Biology

9-13 September 2006, Antalya, Turkey

The 9th Eurasia Conference on Chemical Sciences (EuAsC_2S-9), "Innovations in Chemical Biology at the Bridge of Eurasia," will be held 9–13 September 2006, in Antalya, Turkey, a beautiful, historic city brimming with culture. This world-class conference will support the scientific research of chemists in developing Eurasian countries through networking with chemists from throughout the world and exchanging information.

The conference program has been divided into 10 sessions covering all areas of chemistry: agrochemistry, analytical chemistry, biodiversity and natural products chemistry, biomolecular chemistry, catalysis and nanotechnology, coordination chemistry, computational chemistry, environmental chemistry, material and theoretical chemistry, and solution chemistry. The conference will include eight plenary lectures and 70 session lectures, oral presentations, and posters. Posters will be highlighted each day and will be a major focus of the conference.

Antalya is home to Aspendos, the best preserved Roman amphitheater in antiquity.

See Mark Your Calendar on page 39 for contact information.

www.eurasia2006.org

Occupational Health and Safety Management

27–29 September 2006, Nairobi, Kenya

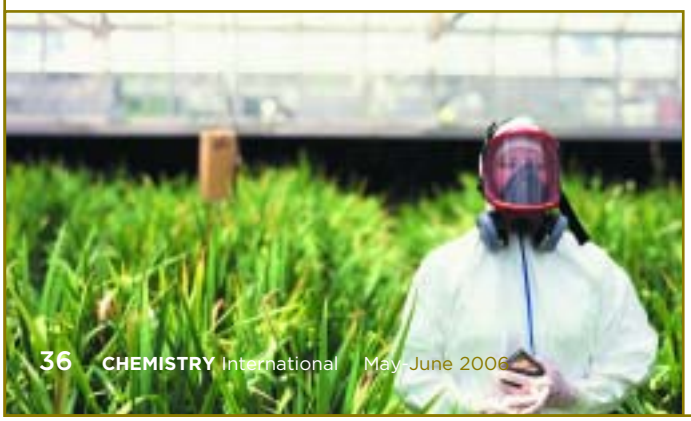
In recent years, public awareness of work-related accidents has driven industries to focus on improving the occupational health and safety status of work environments. Local and national governments are taking a hard look at safety in industry as a whole and the chemical industry in particular, resulting in more government regulation.

A conference on **Occupational Health and Safety Management for East Africa** will be held 27-29 September 2006 in Nairobi, Kenya. This conference for the East African region aims to enable industrialists and other stakeholders to appreciate the purpose of an occupational health and safety (OH&S) management system; explain the legislative framework relevant to such an OH&S management system; and explore the purpose and intent of Occupational Health and Safety Assessment Series (OHSAS) 18001 and 18002. The conference is intended to empower all key health and safety stakeholders to adopt a systematic and comprehensive approach to the management of health and safety issues at the plant level.

Industrialists in developed countries take OH&S issues seriously, but their counterparts in the developing world often do not, largely due to lack of awareness, lack of enforcement of relevant safety laws and regulations, and lack of a systematic structure to guide the establishment of sound OH&S management systems. The result has been an uncoordinated approach to safety issues, exposing workers to high levels of risks and hazards. Chemists and other professionals do the safety work in industry with limited skills and knowledge. Accidents and incidents are not fully investigated, especially where directorates of occupational health and safety are not empowered with adequate tools and safety standards to conduct their duties effectively.

Although hazard elimination is the goal, experience has taught us that guaranteed, failure-free designs and devices have so far eluded mankind, despite astonishing advances in technology. By the end of the conference, participants will be able to:

- Describe the purpose of an OH&S management system in managing health and safety risks resulting from their business operations
- Outline the concept and approaches to OH&S risk



management
- Summarize relevant national and local OH&S legislation in the context of the development of modern OH&S legislation, based on the principles of risk assessment and self-regulation
- Understand and appreciate the purpose of OHSAS 18001 Specification and OHSAS 18002 Guidelines, how they interrelate, and the benefits to organizations that use an OH&S management system specification
- Outline the content of OHSAS 18001 and OHSAS 18002
- Describe with reference to the Plan, Do, Check, Act cycle (the OHSAS 18001 elements of successful OH&S management), the structure and scope of OHSAS 18001
- Explain key OHSAS definitions and terminology
- Determine conformance of a management system to OHSAS 18001

This conference is also sponsored by COCI, the IUPAC Committee on Chemistry and Industry.

See Mark Your Calendar on page 39 for contact information.

www.iupac.org/projects/2005/2005-046-1-022.html

Ionic Polymerization

2–7 September 2007, Bayreuth, Germany

The International Symposium on Ionic Polymerization (IP '07), is the 18th in the series of biannual symposia that began as the International Symposium on Cationic Polymerization in 1976 in Akron, Ohio, in the United States, and which later merged with the Symposia on Anionic Polymerization and on Ring-Opening Polymerization. IP '07 will address contemporary research, both fundamental and applied, in the areas of anionic, cationic, and ring-opening polymerizations. Papers related to other techniques of living/controlled polymerization are welcome in so far as they broaden the scope of ionic polymerizations. The symposium will also incorporate a limited number of contributions on the properties and analysis of materials prepared by techniques of controlled polymerization. The symposium venue is a monastery close to the UNESCO World Heritage city of Bamberg.

See Mark Your Calendar on page 40 for contact information.

Other Upcoming Conferences

Philosophy of Chemistry
6–10 August 2006, Split, Croatia
10th Summer Symposium of the International Society for the Philosophy of Chemistry
E-mail: vancik@irb.hr
<http://ispc.sas.upenn.edu/summer2006.html>

Europe's Younger Chemists
23–26 August 2006, Budapest, Hungary
The 6th Younger European Chemical Researchers' Summer School and Conference will explore "From atoms and molecules in the laboratory to everyday life, processes, and products."
E-mail: ericw@setforeurope.org
<www.setforeurope.org/buda06>

Building the Europe of Knowledge
27–31 August 2006, Budapest, Hungary
The 1st European Chemistry Congress will focus on frontiers in chemical and molecular sciences supported by all the national chemical sciences organizations of Europe.
E-mail: euchems@chemoltravel.hu
<www.euchems-budapest2006.hu>

INTERACT 2006
24–28 September 2006, Perth, Australia
This international conference is being jointly held by three divisions of the Royal Australian Chemical Institute—Analytical Chemistry, Environmental Chemistry, and Electrochemistry—together with the Australasian Society for Ecotoxicology and the Clean Air Society of Australia and New Zealand.
E-mail: promaco@promaco.com.au
<www.promaco.com.au/conference/2006/raci>

Recent Advances in Supramolecular Assemblies with Nucleic Acids
16–17 October 2006, Bordeaux, France
E-mail: barthelemy@bordeaux.inserm.fr

Mark Your Calendar

Upcoming IUPAC-sponsored events
See also www.iupac.org/symposia
for links to specific event Web site

2006 (later than 1 June)

IUPAC poster prizes to be awarded

11–15 June 2006 • Organic Synthesis • Merida, Yucatan, Mexico
16th International Conference on Organic Synthesis (ICOS 16)
Dr. Eusebio Juaristi, Instituto Politecnico Nacional, Departamento de Quimica, Avenida IPN #2508, Esquina Ticoman, Mexico City, DF, 07360, Mexico, Tel: +52 55 50613722, Fax: +52 55 57477113, E-mail: juaristi@relaq.mx

17–18 June 2006 • Neurotoxic Metals • Brescia, Italy
Workshop on Neurotoxic Metals: Lead, Manganese, and Mercury. From Research to Prevention
Dr. Roberto G. Lucchini, Institute of Occupational Health, University of Brescia, Italy, Brescia, Italy, Tel.: +39 0303996080, Fax: +39 0303996080, E-mail: lucchini@med.unibs.it

25–30 June 2006 • Analytical Sciences • Moscow, Russia
International Congress on Analytical Sciences
Prof. Vladimir P. Kolotov, Vernadsky Institute of Geochemistry, Russian Academy of Sciences, 19, Kosygin Str., Moscow B-334 119991 Russia, Tel.: +7 (095) 137 04 86, Fax: +7 (095) 938 20 54, E-mail: kolotov@geokhi.ru

2–7 July 2006 • Polymers and Organic Chemistry • Okasaki, Japan
12th International Conference on Polymers and Organic Chemistry 2006 (POC'06)
Prof. Shinichi Itsuno, Department of Materials Science, University of Technology, Toyohashi, 441-8580, Japan, Tel.: +81 532 44 6813, Fax: +81 532 44 6813, E-mail: itsuno@tutms.tut.ac.jp

9–13 July 2006 • Self-Organized Macromolecular Systems • Prague, Czech Republic
45th Prague Meeting on Macromolecules "Structure and Dynamics of Self-Organized Macromolecular Systems"
Dr. Petr Stepanek, Institute of Macromolecular Chemistry, Heyrovsky Sq. 2, 162 06 Prague 6, Czech Republic, Tel.: +420 296 809 211, Fax: +420 296 809 410, E-mail: stepan@imc.cas.cz

16–21 July 2006 • Macromolecules • Rio de Janeiro, Brazil
41st International Symposium on Macromolecules—IUPAC World Polymer Congress MACRO 2006
Prof. Ailton de Souza Gomes, Caixa Postal 68525, Rio de Janeiro, 21945-970, Brazil, E-mail: asgomes@ima.ufrj.br or macro2006@linkway.com.br

23–28 July 2006 • Biodiversity and Natural Products • Kyoto, Japan
ICOB-5 & ISCNP-25 IUPAC International Conference on Biodiversity and Natural Products
Prof. Michio Murata, Department of Chemistry, Osaka University, Graduate School of Science, 1-16 Machikaneyama, Toyonaka, Osaka, 560-0043, Japan, Tel.: +81 6 6850 5437, Fax: +81 6-6850-5774, E-mail: iscnp25@ch.wani.osaka-u.ac.jp

24–29 July 2006 • Solubility Phenomena • Freiberg, Germany
12th International Symposium on Solubility Phenomena and Related Equilibrium Processes (12th ISSP)
Prof. Wolfgang Voigt, Technische Universitat Bergakademie Freiberg, Institut fur Anorganische Chemie, Leipziger Strasse 29, D-09596 Freiberg (Sachs), Germany, Tel.: +49 3731 39 4338, Fax: +49 3731 39 4058, E-mail: wolfgang.voigt@chemie.tu-freiberg.de

30 July–4 August 2006 • Chemical Thermodynamics • Boulder, Colorado, USA
19th IUPAC Conference on Chemical Thermodynamics
Dr. Michael Frenkel, Physical and Chemical Properties Division, National Institute for Standards and Technology, 325 Broadway, Mail Stop 838.0, Boulder, CO 80305-3328, USA, Tel.: +1 303 497 3952, Fax: +1 303 497 5044, E-mail: frenkel@boulder.nist.gov

6–11 August 2006 • Pesticide Chemistry • Kobe, Japan
11th International Congress of Pesticide Chemistry
Dr. Hisashi Miyagawa, Division Applied Life Sciences, Graduate School of Agriculture, Kyoto University, Kyoto 606-8502, Japan, Tel.: +81 75 753 6118, Fax: +81 75 753 6123, E-mail: miyagawa@kais.kyoto-u.ac.jp

7–10 August 2006 • Environmental Best Practices • Olsztyn, Poland
The First International Environmental Best Practices Conference
Prof. Miroslaw Luczynski, Department of Environmental Biotechnology, University of Warmia and Mazury in Olsztyn, Sloneczna 45G, Olsztyn 10-709, Poland, Tel.: +48 89 5234119, Fax: +48 89 5234119, E-mail: mirekl@uwm.edu.pl

12–17 August 2006 • Chemical Education • Seoul, Korea
19th International Conference on Chemical Education
Prof. Choon H. Do, Sunchon National University, Department of Polymer Science and Engineering, 315 Maegok-dong, Sunchon, Chonnam 540-742, Korea, Tel.: +82 61 750 3565, Fax: +82 61 750 3565, E-mail: choondo@sunchon.ac.kr

13–18 August 2006 • Coordination Chemistry • Cape Town, South Africa
37th International Conference on Coordination Chemistry
Prof. K.R. Koch, Department of Chemistry, Univsersity of Stellenbosch, Private Bage X1 Matieland, Stellenbosch 7602, South Africa, Tel.: +27 21 808 3020, Fax: +27 21 808, E-mail: krk@sun.ac.za

20–25 August 2006 • Physical Organic Chemistry • Warsaw, Poland
XVIII International Conference on Physical Organic Chemistry: New Interactions, New Materials, New Prospects in Physical Organic Chemistry
Prof. Tadeusz Marek Krygowski, Department of Chemistry, University of Warsaw, ul. Pasteura 1, PL-02093 Warsaw, Poland, Tel.: +48 22 822 28 92, Fax: +48 22 822 28 92, E-mail: tmkryg@chem.uw.edu.pl

20–25 August 2006 • Raman Spectroscopy • Yokohama, Japan
20th International Conference on Raman Spectroscopy (ICORS 2006)
Prof. Hiro-o Hamaguchi, Department of Chemistry, University of Tokyo, 7-3-1 Hongo, Bunkyo-ku, Tokyo, 113-0033 Japan, Tel.: +81 3 5841 4327 | Fax: +81 3 3818 4621, E-mail: hhama@chem.s.u-tokyo.ac.jp

3–8 September 2006 • Radical Polymerization • Il Ciocco/Castelvecchio Pascoli, Italy
International Symposium on Radical Polymerization: Kinetics and Mechanism
Prof. Michael Buback, Institut für Physikalische Chemie, Universität of Göttingen, Tammannstrabe 6 D-37077 Göttingen, Germany, Tel.: +49 5-513-931401, Fax: +49 5-513-93144, E-mail: mbuback@gwdg.de

4–8 September 2006 • Nanostructured Composite Films • Warsaw, Poland
E-MRS 2006 Symposium A on Nanostructured Composite Films
Prof. Yves Pauleau, CNRS-LEMD, National Polytechnic Institute of Grenoble, 25 Rue des Martyrs, B.P. 166, F-38042 Grenoble cedex 9, France, Tel.: +33 476 881071, Fax: +33 476 887945, E-mail: yves.pauleau@grenoble.cnrs.fr

9–13 September 2006 • Chemical Biology • Antalya, Turkey
9th Eurasia Conference on Chemical Sciences—Innovations in Chemical Biology at the Bridge of Eurasia
Prof. Bilge Sener, Department of Pharmacognosy, Gazi University, Maltepe, TR-03360 Ankara, Turkey, Tel.: +90 312 212 22 67, Fax: +90 312 213 39 21, E-mail: bilgesen@gazi.edu.tr

10–15 September 2006 • Green Chemistry • Dresden, Germany
First International IUPAC Conference on Green-Sustainable Chemistry
Prof. Pietro Tundo, Dipartimento di Scienze Ambientali, Ca' Foscari, University of Venice, Calle Larga S. Marta, Dorsoduro 2137, I-30123 Venizia, Italy, Tel.: +39 41 2348642, Fax: +39 41 2348620, E-mail: tundop@unive.it

18–22 September 2006 • High Temperature Materials • Vienna, Austria
12th International Conference on High Temperature Materials Chemistry (HTMC XII)
Prof. Dr. Adolf Mikula, Wahringstr. 42, A-1090 Vienna, Austria, Tel.: +43 4277 52606, Fax: +43 4277 52679, E-mail: Adolf.Mikula@univie.ac.at

27–29 September 2006 • Occupational Health and Safety • Nairobi, Kenya
Occupational Health and Safety Management in East Africa
Mr. Kelvin Khisa, Kenya National Cleaner Production Centre, P.O. Box 1360, Nairobi, 00200, Kenya, Tel.: +254 20-604870, Fax: +254 20-604871, E-mail: kkhisa@cpkenya.org

10–13 October 2006 • Advanced Polymers • Busan, Korea
Advanced Polymers for Emerging Technologies
Prof. Sung Chul Kim, Department of Chemical Engineering, Korea Advanced Institute of Sci. & Tech., 373-1 Guseongdong, Yuseong-gu, Daejeon 305-701, Korea, Tel.: +82 42 869 3914, Fax: +82 42 869 8435, E-mail: kimsc@kaist.ac.kr

16–20 October 2006 • Chemistry for Life • Havana City, Cuba
27th Latin American Congress on Chemistry and 6th International Congress of Chemistry and Chemical Eng.
Prof. Alberto J. Núñez Sellés, Center of Pharmaceutical Chemistry, Sociedad Cubana de Quimica, Ave 21 & 200, Rpto. Atabey, Apdo. 16042 Havana, CP 11600, Cuba, Tel.: +53 7 218 178, Fax: +53 7 273 6471, E-mail: alberto.nunez@cqf.sld.cu

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IUPAC poster prizes to be awarded

15–21 April 2007 • Phosphorus Chemistry • Xiamen, China
17th International Conference on Phosphorus Chemistry
Prof. Yufen Zhao, Xiamen University, Department of Chemistry, Xiamen, China 361005, Tel.: +86 5922185610 Fax: +86 5922186292, E-mail: yfzhao@xmu.edu.cn

21–25 May 2007 • Mycotoxins and Phycotoxins • Istanbul, Turkey
XIIth International Symposium on Mycotoxins and Phycotoxins
Dr. Hamide Z. Senyuva, Tubitak-Atal, Konya Yolu No. 67, Besevler, 06530, Ankara, Turkey, Tel.: +90 312 2124620/ext.14, Fax: +90 312 2123749, E-mail: hamide.senyuva@tubitak.gov.tr

26–30 June 2007 • Advanced Materials • Kharkiv, Ukraine
Modern Physical Chemistry for Advanced Materials (MPC'07)
Prof. Yuriy Kholin, Materials Chemistry Department, V.N. Karazin Kharkiv National University, Svobods Square 4, Kharkiv 61077, Ukraine, Tel.: +380 57 707 51 26, Fax: +380 57 705 12 61, E-mail: kholin@univer.kharkov.ua

16–20 July 2007 • Solution Chemistry • Perth, Australia
30th International Conference on Solution Chemistry
Prof. Glenn Hefter, School of Mathematical and Physical Sciences, Murdoch University, Murdoch, WA 6150 Australia, Tel.: +61 8 9360 2226, Fax: +61 8 9360 1711, E-mail: g.hefter@murdoch.edu.au

22–27 July 2007 • Novel Aromatic Compounds • Tsuna-Gun, Japan
12th International Symposium on Novel Aromatic Compounds (ISNA-12)
Prof. Yoshito Tobe, Division of Frontier Materials Science, Osaka University, Toyonaka, Osaka University, Japan, Tel.: +81 6 6850 6225, Fax: +81 6 6850 6229, E-mail: tobe@chem.es.osaka-u.ac.jp

2–6 August 2007 • Organometallic Chemistry • Nara, Japan
14th International Symposium on Organometallic Chemistry Directed Towards Organic Synthesis (OMCOS-14)
Prof. Kazuhiko Takai, Dept. of Applied Chemistry, Okayama University, Faculty of Engineering, Tsushimanaka 3-1-1, Okayama 700-8530, Japan, Tel.: +81 86 251 8097, Fax: +81 86 251 8094, E-mail: ktakai@cc.okayama-u.ac.jp

4–12 August 2007 • IUPAC 44th General Assembly • Torino, Italy
IUPAC Secretariat, Tel.: +1 919 485 8700, Fax: +1 919 485 8706, E-mail: secretariat@iupac.org

5–11 August 2007 • IUPAC 41st Congress • Torino, Italy
Chemistry Protecting Health, Natural Environment, and Cultural Heritage
E-mail: IUPAC.2007@unito.it

2–7 September 2007 • Ionic Polymerization • Bayreuth, Germany
International Symposium on Ionic Polymerization
Prof. Axel Müller, MC II / NW II, Universität Bayreuth, D-95440 Bayreuth, Germany, Tel.: +49-921-553399, Fax: +49-921-553393, E-mail: axel.mueller@uni-bayreuth.de

23–28 September 2007 • Transactinide Elements • Davos, Switzerland
Third International Conference on the Chemistry and Physics of the Transactinide Elements (TAN'07)
Prof. H.W. Gäggeler, Paul Scherrer Institut, Radio- und Umweltchemie, CH-5232 Villigen, Switzerland, Tel.: +41 (0)56 310 24 01, Fax: +41 (0)56 310 44 35, E-mail: heinz.gaeggeler@psi.ch

Visas

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

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Conference organizers are invited to complete an Application for IUPAC Sponsorship (AIS) preferably 2 years and at least 12 months before the Conference. Further information on granting sponsorhsip is included in the AIS and is available upon request from the IUPAC Secretariat or online. <www.iupac.org/symposia/application.html>.

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Mission Statement—IUPAC is a non-governmental organization of member countries that encompass more than 85% of the world's chemical sciences and industries. IUPAC addresses international issues in the chemical sciences utilizing expert volunteers from its member countries. IUPAC provides leadership, facilitation, and encouragement of chemistry and promotes the norms, values, standards, and ethics of science and the free exchange of scientific information. Scientists have unimpeded access to IUPAC activities and reports. In fulfilling this mission, IUPAC effectively contributes to the worldwide understanding and application of the chemical sciences, to the betterment of the human condition.

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Kuwait Chemical Society *(Kuwait)*
Koninklijke Nederlandse Chemische Vereniging *(Netherlands)*
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Norsk Kjemisk Selskap *(Norway)*
Chemical Society of Pakistan *(Pakistan)*
Polska Akademia Nauk *(Poland)*
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Colegio de Químicos de Puerto Rico *(Puerto Rico)*
Russian Academy of Sciences *(Russia)*
Union of Yugoslav Chemical Societies *(Serbia and Montenegro)*
Slovak Chemical Society *(Slovakia)*
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Thieme Publishers and IUPAC in collaboration with the editors of SYNTHESIS, SYNLETT, Science of Synthesis, and Houben–Weyl announce the recipient of the

2006 Thieme–IUPAC Prize in Synthetic Organic Chemistry

David W.C. MacMillan

We are pleased to announce that the 2006 Thieme–IUPAC Prize awardee is David W.C. MacMillan of the California Institute of Technology. The Prize, consisting of 5000 Euros, is awarded every two years on the occasion of the IUPAC International Conference on Organic Synthesis (ICOS) to a scientist under 40 years of age whose research has had a major impact on the field of synthetic organic chemistry. The Prize will be presented to David MacMillan at his Award Lecture on June 13, 2006, at the ICOS-16 Conference in Mérida, Mexico.

David MacMillan was born in 1968 in Bellshill, Scotland. He obtained his undergraduate degree from Glasgow University, and in 1990 moved to the University of California, Irvine, where he obtained his Ph.D. under the direction of Larry E. Overman. Following postdoctoral research with David A. Evans at Harvard University, David began his independent research career at the University of California, Berkeley, in 1998. In 2000, he joined the department of chemistry at Caltech, and was promoted to full professor in 2003.

Through his research contributions, David MacMillan has become a leader in the currently active area of asymmetric organocatalysis. His numerous accomplishments include the design of a series of chiral amines, available from amino acids, to catalyze the enantioselective cycloaddition reactions of dienes or 1,3-dipoles and α,β-unsaturated aldehydes by reversible iminium ion formation.

The approach has been admirably applied to the catalytic asymmetric Friedel–Crafts alkylations of pyrroles, indoles, anilines, and furans, which proceed in excellent yields and with high enantiomeric excess. These are the first examples of this reaction in catalysis; no organometallic catalyst has been devised for these transformations.

In addition, using chiral amine catalysts, David has achieved the first enantioselective cross-aldol condensation of aldehydes, a reaction type which eluded chemists for some time, and could previously only be carried out with the aid of enzymes. This landmark achievement has been improved and extended, and applied to the rapid assembly of natural and nonnatural carbohydrates with enantioselectivities approaching 100%.

Recently, David and his group devised the first enantioselective transfer hydrogenation reaction for alkenes using organocatalysts. He has also introduced a new concept for asymmetric catalysis termed "enantioselective organo-cascade catalysis". This conceptually new strategy relies on David's finding that imidazolidinone catalysts can function as both iminium and enamine activation catalysts (orthogonal activation). By merging these catalytic cycles, it was demonstrated that the biochemical concept of enzymatic catalysis cascades can be emulated in the laboratory using small-molecule catalysts.

David W.C. MacMillan's work has found widespread industrial application, and his generalization, systematic exploration, and brilliant conceptualization has made a major impact in launching enantioselective organocatalysis as a rapidly growing field of research for organic chemists. His success is reflected in the numerous awards he has received from the Royal Society of Chemistry, the American Chemical Society, Tetrahedron, Bristol-Myers Squibb, Pfizer, GlaxoSmith-Kline, Eli Lilly, and Boehringer Ingelheim, among other organizations.

We congratulate David MacMillan and look forward to hearing the latest exciting developments from his laboratories, an *Account* of which will be published in *SYNLETT*, at his Award Lecture in Mérida, Mexico.

David W.C. MacMillan

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