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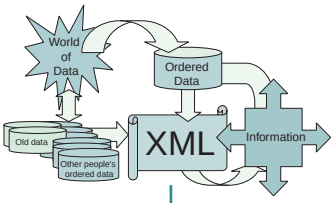

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Cover: A Bayer scientist handles multi-wall sheets made of Makrolon.® Courtesy of Bayer MaterialScience AG.

Past President's Column

IUPAC's Recognition of Chemists

by Piet Steyn

Self-actualization is the strong drive of humans to achieve success; professional recognition directly contributes to that. In the case of chemistry, the highest accolade is undoubtedly the award for the Nobel Prize in Chemistry. Most national or regional chemical societies, national academies, or other professional bodies give recognition through, for example, the awarding of medals, endowed lectureships, invitations to present plenary lectures at conferences or symposia, invitations to contribute to scholarly works, and the election to positions of leadership in such professional bodies. *Chemistry International* (Jan-Feb 2004) recently reported that the FECS (Federation of European Chemical Societies and Professional Institutions) Award was given to Leiv Sydnes, the IUPAC president, for his significant contribution to European cooperation in chemistry and the public understanding of chemistry.

In IUPAC, we offer three prizes that recognize achievements in chemistry: the Thieme-IUPAC Prize in Synthetic Organic Chemistry, the Franzosini Award, and the recently established IUPAC Prize for Young Chemists.

The prestigious Thieme-IUPAC Prize in Synthetic Organic Chemistry is awarded to a scientist less than 40 years of age whose research has had a major impact in synthetic organic chemistry. The most recent recipient (announced in May-June 2004 *CI*) is Professor John F. Hartwig from Yale University. He will be awarded the prize at the Award Lecture on 3 August 2004 at the 15th International Conference on Organic Synthesis (ICOS-15), in Nagoya, Japan.

The Franzosini Award is given to promising young contributors to the Solubility Data Project so that they may attend, in even years, the International Symposium on Solubility Phenomena (ISSP), or, in odd years, the annual meetings of the Subcommittee on Solubility and Equilibrium Data. In 2003, at the second annual meeting of the subcommittee, the Franzosini Award went to Dr. Pirketta Scharlin in appreciation of her continuous scientific and administrative contributions to the Solubility Data Project (Nov-Dec 2003 *CI*). This year, the deadline for nominating candidates for the 2004 Franzosini Award was 1 June 2004, and the awardee will be announced at the forthcoming 11th International Symposium on Solubility Phenomena, in Aveiro, Portugal, to be held from 25–29 July 2004.

The IUPAC Prize for Young Chemists is intended to encourage promising young research scientists at the outset of their careers. The prize is given for the most outstanding Ph.D. thesis in the general area of the chemical sciences, as described in a 1000-word essay. The first IUPAC Prizes for Young Chemists were awarded in Brisbane, Australia, in 2001. The most recent group of prize winners (2002 and 2003) was recognized at a grand occasion during the opening of the IUPAC Congress in Ottawa, Canada.

This year, we received 44 applications for the 2004 IUPAC Prize for Young Chemists. We must express our appreciation to each of the young chemists who submitted essays, based on their Ph.D. theses, and also to their supervisors who provided guidance during their advanced studies. The essays were of a very high standard and the adjudication process, conducted by senior members of IUPAC, was not easy.

Recipients of the 2004 IUPAC Prize for Young Chemists are as follows:

- Parag Acharya (Uppsala University, Sweden; supervisor: Jyoti Chattopadhyaya)
- Yu Huang (Harvard University, USA; supervisor: Charles M. Lieber)
- Zhipan Liu (Queen's University of Belfast, UK; supervisor: Peijun Hu)
- S.G. Srivatsan (Indian Institute of Technology, Kanpur, India; supervisor: Sandeep Verma)

See page 20 for more information on the award winners.

Congratulations to the 2004 winners of the IUPAC Prize for Young Chemists. They will be invited to participate in the forthcoming IUPAC Congress in Beijing, China, in 2005. They will also be invited to submit topic articles to *Pure and Applied Chemistry* (*PAC*), the flagship publication of IUPAC. The February 2004 issue of *PAC* contained the contributions from 2003 prize winners, namely Gonzola Coza, Martin Lemaire, Kaihsu Tai, and Roman Boulatov. What an honorable way to launch a successful career in the chemical sciences!

Pieter S. Steyn <psst@sun.ac.za> is the IUPAC past president and chairman of the Committee adjudicating the Prize for Young Chemists; he has been involved with the Union since 1973 and is currently senior director of research development of Stellenbosch University in South Africa.

When Ideas Become Deeds

Chemical Education and Sustainable Development in Russia

by Natalia P. Tarasova

After the United Nations "Earth Summit"—held in June 1992 in Rio de Janerio, Brazil—the phrase "education for sustainable development" became known to the general public for the first time. A major reason for this was chapter 36, "Promoting Education, Public Awareness, and Training," of *Agenda 21*, a pathbreaking document that was adopted by more than 178 governments at the conference. *Agenda 21* is a comprehensive plan of action to be taken globally, nationally, and locally by organizations of the U.N. system, governments, and major groups in every area in which humans impact on the environment.[1] As chapter 36 states, education is indispensable for achieving sustainable development.

Following the adoption of *Agenda 21*, contributions to increasing education, public awareness, and training in sustainable development were made by the U.N. Commission on Sustainable Development (CSD) at its sessions, by the U.N. General Assembly at its Special Sessions (1997), and at the World Summit on Sustainable Development (WSSD) (Johannesburg, 2002).

In 1996, the CSD adopted an International Work Program on Education, Public Awareness, and Training for Sustainability in order to give added impetus and visibility to this theme. The Work Program encouraged the identification and sharing of best practices and the forging of linkages with the Work Program on Changing Production and Consumption Patterns. This lead to a call for the review of national education policies and the integration of education and awareness into national strategies and plans for sustainable development. These were the events that inspired the D. Mendeleyev University of Chemical Technology of Russia to organize the first international conference on Chemical Education and Sustainable Development, in Moscow in October 2000.

The objective of the conference was to discuss experiences with education for sustainable development in the field of chemical education. Specifically, the conference reviewed the implementation of recommendations from *Agenda 21* and discussed how to develop innovative methods of chemical education and how to increase the involvement of educators in sustainable development. It was stressed that chemical education can be effectively used for this purpose because chemistry is a fundamental science and provides a scientific basis for a variety of technologies in different branches of industry.

The conference was supported by IUPAC, UNESCO, the Ministry of Education of the Russian Federation, the Russian Academy of Sciences, and the Russian Chemical Society. More than 250 participants from 10 countries discussed the following themes at 4 symposia and 2 plenary meetings: chemical education and technical progress, chemical education and environmental problems, chemical education and human health, and chemical education and food problems.

One output of these discussions was the recognition that chemical sciences should play a very positive role in sustainable development, contributing to improvements in quality of life for present and future generations. At the same time, conference participants agreed that without proper control, human-made chemicals have the potential for enormous negative impacts. So, enlightened management of the chemical sciences is necessary to ensure that as the field advances, the effects are beneficial to humanity as well.

An analysis of the history of Russian engineering education provides some compelling lessons. At the beginning of the twenty-first century, Russia celebrated 300 years of engineering education, its foundations having been laid by Peter the Great, who issued the order to organize the School of Mathematics and Navigation Sciences. This school trained not only military engineers, but also the civil engineers needed for the transformation of feudal Russia into an industrial country. Scientists from

1. www.un.org/esa/sustdev/documents/agenda21/index.htm

When Ideas Become Deeds

Europe, mainly from Germany, were invited to help establish the Russian educational system. So, it is easy to understand why for quite a long time Russian engineering was modeled on German higher technical schools.

During the former Soviet Union's periods of industrialization and construction of the centrally planned economy, higher engineering education was subject to quite strict state control as far as the content and the performance of teaching were concerned. The state maintained strict control over the content of curricula and the structure of education in general. The in-depth specialization of graduates and their placement in jobs was the responsibility of the state ministries and the higher institutions themselves. Such an approach resulted from the fast growth of industry and the beginning of the Cold War. The goal was "victory at any price."

In today's modern world, it is quite obvious that such an approach cannot be put into action and would lead nowhere. The strategy of sustainable development is the only alternative. The new techniques and technologies in all branches of material goods production make it evident that the role of

engineers is becoming even more important.

The problems of the rational use of natural resources, energy conservation, protection of the environment, prevention of technological accidents, and risk management all require the active participation of engineers, with their particular knowledge and skills. So the goal of education must be to train specialists within a holistic life paradigm, so that they can be responsible citizens. The special role of engineer-

Chemistry Clearing House

Last year, a Chemistry Clearing House (CCH) was established at the Mendeleyev University of Chemical Technology of Russia (see Sep-Oct 2003 *CI*, p. 19). The project and its underlying ideas are starting to render tangible outcomes.

The project goals include the adaptation and dissemination of educational materials and pedagogical practices recommended by IUPAC, to teachers in Russia and countries of the Commonwealth of Independent States (CIS). Since chemical education problems are mostly regional and differ significantly depending on country and territory, IUPAC is expected to mostly supplement the efforts of national chemical societies and to facilitate the coordination of information exchange. The CCH hopes to provide schools and universities with information on new trends in chemistry education and how to adapt these ideas locally.

In the context of this IUPAC project, the Task Group Chairman Elena S. Gryzlova attended the Mendeleyev Congress, held in September 2003 in Kazan. Dr. Gryzlova made an oral presentation describing the project, and displayed a poster titled "Realization of Scientific Education Ideas in Chemistry Education." Around the same time, a seminar for teachers was organized on micro-chemical experiments. The seminar was taught by Prof. John Bradley on the premises of the Chemical Technology University. Bradley's presentation was translated into Russian and a more practical Q&A session was held on how to conduct microchemistry in the school classroom and laboratory. During the event, teachers were asked to fill out a questionnaire regarding their specific needs and their interest in foreign methods of teaching chemistry.

An important impetus for this project is the educational reform that is taking place in Russia. Of particular relevance are two programs: one called Development of Unified Educational Informational Media (2001-2005) and another called Integration of Science and High Education in Russia for 2002-2006. CCH can provide significant help meeting the goals of these programs by accomplishing the following:

- documenting the educational programs of Russia and other countries, from primary schools up through universities
- disseminating foreign methodological literature to teachers who have no easy access to the information available in most

chemists should be mentioned, because environmentally friendly technologies and green chemistry could provide real help in the transition to sustainability. While today this is well understood in Russia, the idea gained further momentum when representatives of industry and university professors at the conference formulated these goals into a specific recommendation of the international conference.

After the disintegration of the former USSR, two-thirds of the Soviet Union's technical universities, which educate 2.8 million students, remained part of the Russian Federation. Of the approximately 220 000 pedagogic staff, 13 700 were Doctors of Science and 115 000 were Candidates of Science. Practically all the leading engineering schools remained in Russia, including chemical engineering schools.

U.N. Division for Sustainable Development.

During the 1990s, the Russian government took steps to improve the system of educational management. Several laws have been adopted for this purpose, including the *Law on Education* (1992, amended in 1996) and the *Federal Law of the Russian Federation on Higher and Post-Higher Professional Education* (1996). Thus, a legislative base was created for the functioning of higher education. Later, the concept of federal educational standards was developed and adopted. This set of standards describes the minimum knowledge compulsory for graduates to obtain the state diploma of higher education. A system of licensing of educational activities, attestation, and state accreditation of institutions of higher education was put into effect. The attempt to copy the Western system of public attestation and accreditation failed.

These measures led to the development of university autonomy and to an increase in the academic mobility of students. The multi-level system of education (Master of Science and Bachelor of Science) started to develop alongside the traditional training of engineers. With academic freedom, higher institutions may choose the form of training most suited to their regional conditions. Not all of them have chosen the European system of Master of Science and Bachelor of Science degrees. Nevertheless, in the second edition of the Federal Educational Standards (adopted in the 2000) one can find sets of specializations for Bachelor

"university" cities, such as Moscow, Sankt-Petersburg, or Kazan
- advocating chemical scientific education at every level and educational strategy coordination between Russia and CIS
- supporting the development and dissemination of new educational technologies, including distance education

While the Internet is still not widely accessible in some Russian schools, the CCH initiated the development of a Web site designed to make translations and other relevant materials more easily available. The first documents will include publications from the Ministry of Education of the Russian Federation regarding chemical education and integration of science and education, the translation of the most recent IUPAC Committee on Chemistry Education (CCE) chairman's report to the IUPAC Council (Ottawa, August 2003), other information concerning CCE and its subcommittees, and translation of selected articles from *Chemical Education International*, such as "Systemic Approach to Teaching and Learning Chemistry," by A. F. M. Fahmy and J. J. Lagowski.

Among others, contacts have been formalized with the Department of General Education of Ministry of Education of RF (Russian Federation), the Department of International Cooperation of Ministry of Education of RF, the Research Institute of Russian Academy of Education, the Scientific Research Institutes of Russian Academy of Sciences.

Several publications papers related to this project have been submitted for publication or will soon be published in *Khimiya: Metodika Prepodavaniya* (Chemistry: Methods of Teaching Chemistry), *Khimiya v Shkole* (Chemistry in School), and *Chemical Education International*. An abstract has been submitted for a presentation at the Sixth International Symposium "TECHNOMAT & INFOTEL," to be held in Bulgaria, in September 2004. A proposal titled "Organization of Consulting Methodological Center on Chemistry Education" has been submitted to a contest on innovative ideas, concepts, projects, programs, and technologies, sponsored by the Russian Educational Forum.

For more information, contact Elena S. Gryzlova <ncrc@geokhi.ru>. The task group expresses continued interest in obtaining from chemistry teachers all over the world, descriptions of methodological and pedagogical experiences that could serve teachers in Russia and the CIS.

www.iupac.org/projects/2001/2001-003-5-050.html

of Science and Masters of Science degrees as well as for "diplomated engineers."

Through these types of degrees, the idea of widening the profile of training has been realized. All engineering and technological specialties are grouped under the umbrella of "Techniques and Technologies." For example, instead of 37 specialties in chemical technology, as there used to be in the late 1970s, now there are only 5 branches. Technical specialties in environmental protection are grouped under "Protection of the Environment," with the qualification "engineer-ecologist" on the diploma. According to the recommendations of the international conference, "Environmental Chemistry" is a compulsory course for the engineer-ecologists. Since 2000, several summer schools have been organized at D. Mendeleyev University to teach young university teachers the innovative methods of teaching.

The educational community of Russia is quite optimistic about the idea of lifelong education for sustainable development . . .

In 1995, D. Mendeleyev University of Chemical Technology became the first school in Russia to organize a Department for the Problems of Sustainable Development. Later, following the recommendations of the international conference, D. Mendeleyev University created the Institute of Chemistry and the Problems of Sustainable Development (2000), which now includes the College for Rational Use of Natural Resources, the Department of Sociology, Department of Risk Assessment and Risk Management, and the Department for the Protection of the Producers' Rights (dealing with legislation of chemicals, the chemical industry, and environmental regulation).

Research is a compulsory component of contemporary higher education in Russia. So, a number of research universities have recently been organized to collaborate with research institutes of the Russian Academy of Sciences. As an example, Higher Chemical College of Russian Academy of Sciences is a part of D. Mendeleyev University. Through these arrangements, students start working in the laboratories of research institutes during their first year at college. By the time of graduation they normally have several publications in national or international scientific journals. Some of the results of the students' research have found practical application in Russia and abroad. Of course, those who are admitted to this college are gifted students, winners of Chemistry Olympiads or graduates of the Moscow Chemistry Lyceum. As recommended by the international conference, special courses have been offered to these students, as well as to other students from advanced colleges, on the problems of sustainable development and environmental risk assessment and management.

The technological approach to the training of engineers-chemists cannot prevail given current societal conditions. Higher school in Russia is in a state of transition to the new educational paradigm—training specialists in a holistic way of thinking. Engineers trained in a holistic manner could give momentum to the practical implementation of the concept of sustainable development. The leading universities of Russia are successfully moving in this direction. The educational community of Russia is quite optimistic about the idea of lifelong education for sustainable development, the momentum having been given by the first international conference on Chemical Education and Sustainable Development four years ago.

Following WSSD recommendations, the U.N. General Assembly, at its 57th Session (2002), decided to adopt a decade of education for sustainable development, starting in 2005. To define the goals and the strategies for the decade, D. Mendeleyev University decided to hold the Second International Conference on "Chemical Education and Sustainable Development" in November 2004. Chemists from all over the globe who are interested in the contribution of chemistry to the future of humankind should contact the organizers; conference details may be found at on the D. Mendeleyev University Web site at <www.muctr.edu.ru>.

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www.iupac.org/projects/1999/1999-035-1-025.html
www.muctr.edu.ru

Collaborative Trial Tests for Method Validation: Lessons to be Learned

This article describes the lessons that were learned in the course of a project entitled "Collaborative trial study for the determination of aflatoxin B1 in ground products of peanuts and corn by immuno-affinity clean-up and thin-layer chromatography," which was co-funded by IUPAC's Division on Chemistry and the Environment (#1999-010-1-600). The project, which was carried out between 2000 and 2003, aimed to obtain a robust and simple validated method capable of quantifying aflatoxin B1 in corn and peanuts at levels of 1-10 ng/g using thin-layer chromatography (TLC). The project did not achieve its objective, but it did provide some valuable lessons that the authors felt were important to share with the IUPAC community. The article describes the background and results of the collaborative study, as well as lessons learned and conclusions.

by E. Anklam and J. Stroka

Mycotoxins are food contaminants that are frequently found in a variety of different food products. Among these toxins, the aflatoxins are the most well known. Aflatoxins were identified in food and feed contaminants in the 1960s and can occur in many valuable products derived from plant origin, such as peanuts, pistachios, figs, paprika, and corn, to name the most relevant. One aspect that all these products have in common is that they are produced mainly in regions with warmer climates. Very often, countries in these regions (e.g., Africa, South America and Asia) are also economically disadvantaged and a large fraction of the produce is grown for export to industrial states.

Importing countries, among which are the Member States of the European Union, have legislative limits for some of these contaminants in order to protect the health of consumers and animals. In EU countries, these limits follow the ALARA principle (As Low As Reasonably Achievable) in order to ensure high-quality imports. Currently, the most effective approach to keeping mycotoxins from entering the food market is the regular monitoring of them at all stages of production. As a result, reliable and validated analytical methods must be available to ensure that the producer can trace any contamination prior to shipping or processing. In the worst cases, such contamination can result in the rejection of goods at the point of entry into another market.

In general, the analysis of mycotoxins, and in particular the analysis of aflatoxins, is a challenging task, as a suitable method should be easy to perform, robust in its application, and reliable in its results. Furthermore, all parties should agree on the analytical results obtained from such a method. This has been recognized by the European Commission, which has set performance criteria in EU Directives for analytical methods, rather than so called "reference methods."

The validation of a method for the analysis of aflatoxin B1 at a level around 2 ng/g has recently been successfully carried out using high-performance liquid chromatography (HPLC) in combination with a very powerful clean-up and concentration step involving immuno-affinity.[1] This well-established clean-up procedure was expanded in order to encompass successfully the determination of aflatoxin M1 in milk by thin layer chromatography (TLC).[2] TLC is a relatively simple but powerful chromatographic method that is still widely used in control laboratories, but has been replaced in the food sector to a certain extent by HPLC. However, HPLC requires more expensive, high-quality solvents and requires advanced instrument support and reliable electrical power because short power shutdowns or voltage fluctuations will result in analysis failure. With TLC, standard solvents can be used in most cases and electricity or maintenance problems play only a marginal role. As a result, and because this technique is much cheaper, TLC is still commonly used in economically disadvantaged areas.

Robust and reliable analytical methods are necessary to control compliance with legislative limits. For aflatoxins, the limits have been set at relatively low levels in Europe. As many food commodities at risk of contamination with aflatoxins are produced in developing countries, the limits have to control the food prior to export. Due to the fact that TLC is widely

applied in many countries, this IUPAC project aimed to validate a TLC method involving mainly developing countries. The method and in-house validation results have been successfully tested with simple and economic alternatives to commercial densitometers developed in our laboratory, and as described in the literature.[3-4]

Collaborative Study Design

A total of 27 laboratories from 16 countries participated in the collaborative trial study for the determination of aflatoxin B1 in peanut and corn by TLC. The countries of origin of the participating laboratories were Argentina, Australia, Brazil, Bulgaria, Cuba, Egypt, France, Hungary, Indonesia, Iran, Latvia, Malaysia, Philippines, Switzerland, Thailand, and Uruguay. The final collaborative trial was performed in 2002.

A multi-media show, to be used in combination with the method description, was produced on CD-ROM and sent to study participants to show them the important and critical steps. Homogenous test materials of corn and peanuts were produced by the coordinator in 50 g units. Each matrix consisted of blind duplicate samples for blank and naturally contaminated materials of aflatoxin B1 ranging from 1 ng/g to 10 ng/g. The number of samples and the conduct of the trial were in compliance with the IUPAC Harmonized Protocol.[5] Each participating laboratory received all coded samples and the necessary consumables (e.g., immuno-affinity columns, standards) and some specific glassware.

Results of the Collaborative Trial

The collaborative trial study was finalized at the beginning of 2003. A total of 17 laboratories, out of the 27 that received the materials, submitted results. One laboratory was not able to detect any aflatoxin in the samples and those results were therefore excluded from further data evaluation. This resulted in 16 laboratories submitting analytical data. The analysts were asked to comment on several questions concerning the procedure.

Based on the submitted results it can be concluded that the participants could identify different levels of aflatoxin B1 in the samples. However, the statistical analysis of the results from the collaborative trial and the comments made by the participants led to the conclusion that the method may not be "fit for purpose" at this stage when compared with the requirements given by European legislation. However, it must be stressed that most of the results were obtained by individual visual detection (not using densitometric scanners). Figures of repeatability and reproducibility are listed in the following table, showing clearly that there are problems with the analysis of aflatoxin B1 at these low levels.

	Target Level		
Performance	**1 ng/g**	**5 ng/g**	**10 ng/g**
RSD_r for corn	127 %	119 %	60 %
RSD_r for peanut	136 %	76 %	33 %
RSD_R for corn	139 %	125 %	80 %
RSD_R for peanut	145 %	91 %	81 %

Relative Standard Deviation (RSD) of repeatability (r) or reproducibility (R) obtained from the collections of results.

Although communication was frequent between participants and the coordinator of the collaborative trial, and considerable effort has been put into this project from all sides, it appears that at this stage the proposed TLC approach is not applicable in all laboratories.

Several critical issues have been identified during this trial, which are mainly due to logistics. For example, problems occurred due to the late arrival of parcels in some cases, but also due to communication problems, as some participants did not respond after parcels arrived (as asked by the coordinator). This also concerns those laboratories of the 27 that did not submit results at all. In fact, it appeared that the majority of participants who had been involved previously in international projects and for whom personal contacts (face to face) existed were the first ones to supply results and to successfully perform the analysis.

Most problems were caused by the participants' lack of familiarity with the method and the calculations used. Since most of the participants analyzed the samples by visual inspection, there was, unfortunately, too little data available to evaluate the method by densitometry, as was originally envisaged. This explains to a certain extent why the method proved unsatisfactory in the lower contamination ranges. To conclude, visual inspection at these low levels is not to be recommended, although it is thought that instrumental quantification might be the solution for the determination of aflatoxin B1 by TLC at these levels.

Because commercially available densitometers may

not always be affordable for laboratories in economically deprived areas, the coordinators also aimed to supply a solution for this by designing cheap alternative instruments that show similar performance.[4] However, these instruments are still at the prototype stage at this time, but are being further developed and will be used in a future validation study, it is envisaged, using the same TLC method.

Lessons Learned—Recommendations for Future Collaborative Trial Studies

Some of the comments from and results of communication with selected laboratories led to recommendations for future collaborative studies of this kind:

- An appropriate selection of laboratories must be made. This is more significant the greater the geographical distance of all involved parties. On the one hand, it is helpful to collaborate with known partners, while it is also critical to exclude laboratories that are new to the field.
- A training workshop involving "hands-on" training—held either at the beginning of the project or after a pre-trial, so that results could be discussed—would certainly have facilitated communication regarding problems. However, it must be considered that, although this is the most appropriate strategy in such cases, the additional costs are high. Unfortunately "long-distance communication" by email and phone alone do not allow any "hands-on" problem-solving solutions (e.g., training on use of the method).
- After such a workshop the participants should implement the method at their own laboratories. Furthermore, it is crucial that participants have a clear understanding of the "philosophy" behind each step of the method right from the beginning. This holds especially true when the method includes relatively new principles such as immunoaffinity clean up or other new techniques. In addition, the pit-falls and critical steps could be discussed and demonstrated. This can be accomplished by drafting an "extended" method description, as is usually done for a collaborative trial.
- A questionnaire on problems faced by the laboratories should be sent out for the trial and pre-trial in order to learn about the laboratories' experiences with a particular method. This is very important, as participants must be familiar with the method in order to participate in a collaborative trial.
- A formal agreement with the official heads of laboratories of unknown partners might help to stress the importance of such method validation projects.
- In order to keep the workload for participants low, only one matrix should be handled at one time. Unlike previous collaborative trials that were successfully carried out using HPLC, the effort of the TLC method must not be underestimated, as laboratories using HPLC often have sophisticated laboratory infrastructure that might not be available in all cases. Even though this would mean a greater logistical and organizational workload for the coordinator, it would likely optimize the outcome.

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www.iupac.org/projects/1999/1999-010-1-600.html

IUPAC and Commercial Polymers

IUPAC Working Party on Structure and Properties of Commercial Polymers—History, Output, and Future Prospects

by D.R. Moore and H.M. Laun

It is nearly an axiom that working groups within organizations of almost all sorts come and go with need, interest, and fashion. Thus, the continuous existence of a Working Party (WP) within IUPAC for over 40 years is, to say the least, unusual. Nevertheless, since 1963 academic and industrial scientists with similar interests have contributed to the distinguished history of the Working Party on Structure and Properties of Commercial Polymers. Today the WP functions as a formal Subcommittee of the Macromolecular Division.

The WP has a robust current membership of 66 scientists from 17 countries, representing industry, universities, and institutions. It has held 70 meetings and published more than 80 scientific papers in its 40 years; it is largely self-governing and elects its own executive officers.

As so often is the case, its beginnings were humble. At the first meeting of the WP in 1963 there were only 7 scientists in attendance. However, the numbers of participating scientists, companies, and institutions grew quickly. The first publication, *The Relationship of Performance Characteristics to Basic Parameters of Polymers. I: A Collaborative Study of Polystyrene Using Torsion Pendulum and Impact Methods*, was published in 1968. Six laboratories contributed to this publication: BASF, DOW, Monsanto, Solvay, TNO, and Technická Prague.

The first publication on the collaborative study of polystyrene and polyethylene melts was published by J. L. S. Wales in 1969. Contributing laboratories were Monsanto, Péchiney-Saint-Gobain, Solvay, and TNO. Polyvinyl chloride (PVC) was an early focus, especially its mechanical and capillary-flow properties. Initially most participating scientists were from U.S. and European plastics industries, but they were increasingly supplemented by scientists from academia worldwide, including the then Soviet Union. In addition to the early work on polyolefins, PVC, and polystyrene, there were also excursions into polypropylene film.

In its first 10 years, the WP was particularly concerned with how to relate mechanical and rheological measurements to the practical world of plastics processing and performance. In one project, the rheological properties of three low-density polyethylene samples were related to their tubular-film-blowing characteristics. From this work, the importance of extensional-flow testing became obvious and motivated further efforts in the development of extensional rheometers.

In the period between 1963 and 1980, the WP held 37 meetings, all of them in Western Europe. However, there was a strong presence from the USA in the membership of the group and the WP finally held its first meeting in the USA in 1981. In addition, two regional subgroups were established in the early 1980s, one in Japan with members from Japan, China, and Korea, and another in eastern Europe, with members from Czechoslovakia, Hungary, Poland, and the USSR. The motivation for the formation of these subgroups was to expand membership on a global basis and to ease travel restricted by cost or political conditions. These subgroups established their own projects and reported to the main WP.

The early 1980s was a time of expansion for the WP. There were projects on the impact behavior of injection moldings led by C. B. Bucknall, and feasibility studies for understanding polymer blends in terms of processing-structure-property relationships. In particular, in projects led by H. M. Laun and P. Hope, the WP looked at suitably selected model systems for miscible and immiscible blends based on technical polymers. In East Asia there were also projects relating to structure-property relationships for polybutadiene-rubber blends.

A significant development involved establishing projects on contemporary polymeric materials and systems. Polymeric fiber-reinforced composites were fast emerging and the WP was well placed to contribute to this area. Studies were started by D. R. Moore and J. C. Seferis on continuous carbon-fiber reinforced semi-crystalline polymers, followed by projects led by A. Cervenka and P. S. Allan on discontinuous fiber-reinforced polymeric systems.

The traditional interest that the WP has had in linking rheological properties to processing continued. In two projects, J. L. White explored a link between rheological properties and unstable melt-spinning for linear and branched poly(ethylene terephthalates), and examined the stability of extrusion, melt spinning and tubular film extrusion for some high-density, low-density, and linear-low-density polyethylene samples.

The final decade of the 20th century was a time of considerable achievement; it was also what can be

described as a political period. IUPAC was undergoing considerable restructuring; this naturally had a profound influence on the organizational aspects of the WP, though almost none on its activities.

The emergence of *détente* and political freedom within continental Europe provided new ease of access and communication between scientists in the East and West. The WP held meetings in Czechoslovakia (just before it became the Czech and Slovakia Republics) and in Poland in 1992 and 1993, respectively. The WP closed the East-Europe subgroup after these meetings and integrated the scientists involved into the main group.

The integration of the East Asian subgroup was more difficult because there were more substantial cost barriers to meetings at a single location. An arrangement was established whereby the members of the subgroup became members of the WP, but could hold a research meeting in their area once a year. This was consolidated with a full meeting of the WP in Korea in 1996. Ten of the 28 participants were members from Europe, USA, and Canada.

Polymeric fiber-reinforced composites became of significant interest in the 1990s; in particular, composites with a potential for use in primary aerospace structures. A project led by D.R. Moore and J.C. Seferis studied two materials systems of continuous carbon-fiber reinforced thermoplastics. A key feature in the overall study was to find a way of accommodating the massive anisotropy in these fiber-reinforced composites whilst retaining an ability to measure some conventional but important properties.

A second fiber-reinforced composites study was led by P. S. Allan and A. Cervenka and became the largest single project undertaken by the WP, with 21 participating laboratories and 7 published papers. The project was concerned with the processing and properties of injection-molded discontinuous fiber-reinforced thermoplastic composites, with the aim of providing characterization of the processing-property-structure relationships that characterize this complexity.

A third composites project led by D. R. Moore and A. Cervenka focused on future requirements for the characterization of continuous-fiber-reinforced composites. In this study, contributing scientists reviewed some of the history of processing and properties of these composite materials and tried to identify factors that would be important in the future. This was the first WP project with a philosophical rather than an experimental output.

Meanwhile a major strategic thrust was being developed on immiscible and miscible blends. The first blends project, coordinated by A. P. Plochocki, was a joint study of the effect of mixing and processing conditions on the phase morphology and rheology of polystyrene/low-density polyethylene (PS/LDPE) blends. A second study, led by P.S. Hope and J.E. Curry, focused on the reactive blending of immiscible blend components.

A project on miscible blends was co-ordinated by H. M. Laun, J. Lyngaae-Jorgensen, and V. Alstädt. It focused on the preparation of blends of various morphologies, but with the same composition of the constituents and the study of the effects of morphology

Participants at the Working Party IV.2.1 research meeting in Ludwigshafen (2003), hosted by H.M. Laun at BASF. Front row from left: S. Monsheimer (Degussa), U. Handge (ETH Zürich), H. M. Laun (BASF), A. Machado (Guimares), Ch. Chai (BP chemicals), W. Gleissle (Karlsruhe), G. Ourieva (Exxon Mobile), J. Lyngaae-Jörgenson (Lyngby). Middle rows: P. Pelz (Freudenberg), M. Rüllmann (BASF), D. Stocks (ICI), R. S. Bailey (ICI), D. Dijkstra (Bayer), J. Meissner (ETH Zürich), R. Koopmans (DOW), V. Rouyer (BP Solvay), T. Inoue (Kyoto), G. Biebaut (Shell), H. Steininger (BASF),V. Altstädt (Bayreuth). Back rows: R. Brummer (Beiersdorf), F. Ramsteiner (BASF), W. Zoetelief (DSM), B. Hochstein (Karlsruhe), I. Fortelny (Prague), C. Gabriel (Basell), U. Göschel (Stuttgart), E. Piorkowska-Galeska (Lodz), C.B. Bucknall (Cranfield), T. Tagigawa (Kyoto), K. Nitta (JAIST), A. Galeski (Lodz), F. Langouche (Solvay), E. Wassner (Elastogran), B. Ouriev (Bühler AG).

on rheological and mechanical properties. The constituents were very similar in their viscoelastic behavior. The shift of the regime of miscibility by simple shear flow was investigated, and the observed morphology changes in oscillatory shear were compared with available theories for droplet/matrix and cocontinuous structures. The composition and temperature dependence of the interaction parameter χ was quantified by means of neutron diffraction and cloud-point studies for blends of PαMSAN with PMMA and with poly(methylacrylate-*co*-methylmethacrylate). Finally, the effects of morphology on the mechanical properties of the blends were investigated.

C. B. Bucknall and M. Kozlowski undertook another large project on blends. In this work, the addition of "core-shell" rubber particles to thermoplastic matrix materials was studied for enhancement of toughness with an aim of understanding the mechanisms involved in the toughening process. Two rubber-particle systems were selected having quite different glass-rubber transition temperatures. These were blended with four different thermoplastic matrix materials at the same volume concentration of the rubber. Mechanical and rheological properties of these systems were investigated, and structural and deformational mechanisms were discussed for tensile impact behavior, dart-drop and notched bending test, and fatigue behavior. A transmission-electron-microscopic investigation of *in situ* deformation was published.

Following the IUPAC Strategy Development and Implemention Committee recommendations of 1998, the Macromolecular Division moved to a project-driven system. As a direct consequence, starting in 2000 the WP no longer held official status within IUPAC and became an ad-hoc working group. In the reorganized division, the chairman of the WP became one of the characterization coordinators within the division, while both the secretary of the WP and the chairman of the East Asian Research Meeting acted as task group chairmen of projects.

R. B. Bailey (Secretary) became task group chairman of a five-year project on "Quantifying scratch resistance of commercial polymers." The goal is to consider the range of scratching, abrasion, and erosion techniques used in the plastics industry and to apply a more fundamental understanding of the issues that contribute towards scratch resistance. In stage 1 of the project, key links between bulk and coating mechanical properties and scratch and abrasion resistance are to be identified using generic techniques to manufacture materials with a "scratch-resistant" surface on acrylic and polycarbonate polymers. Stage 2 will focus on emerging and novel scratch-resistant coatings.

S. C. Kim became task group chairman of a three-year project on "Structure and properties of cyclic olefin copolymers (COC)." Here, the focus is on relating the chemical structure of commercially available COCs to rheological and processing properties as well as to optical and mechanical properties in the solid state.

In 2002, a former feasibility study of the East Asia members became a three-year project on "Structure and properties of polyester elastomers composed of poly(butyleneterephthalate) and poly(ε-caprolactone)," with T. Tagigawa as task group chairman. Subtopics of the joint study are molecular structure, rheological properties, rubber elasticity, aggregate structure and deformation mechanism, and blends with other polymers.

The WP amended its rules to require that all communications be conducted via e-mail. A WP homepage <www.launweb.de/iupac> was set up to keep the documentation on projects, reports, people, and actions continuously updated. It contains a public sector open to anyone and a private sector for members only.

Under new IUPAC guidelines, projects are to last about three years. Based on WP experience, this is often not enough time for voluntary and unfunded joint experimental work. Therefore, proposals for new projects within the WP are converted into feasibility studies in which the outline and goal of the work, the suppliers of the material, and contributors and coordinators are defined. Only then is the project application submitted to IUPAC via the Macromolecular Division.

In 2003, the WP again became an official part of the IUPAC Macromolecular Division and was recognized as the Subcommittee on Structure and Properties of Commercial Polymers, a most welcome change of status for the 40th anniversary of the group. Studies that will occupy the group over the next few years include the following:

- structure and properties of linear and crosslinked, structural PVC foams
- flow properties of ceramic and metal injection-molding feed stocks
- recommendations for data presentation applicable to mechanical and rheological measurements of polymers
- critical check of capillary-flow predictions using viscoelastic finite-element simulation and low-density polyethylene literature data
- the role of stress-induced cavitation in mechanical

performance of semi-crystalline polymers
- rheological characterization of polyamides
- future developments of new materials based on commodity polymers by physical structure and morphology alteration
- investigation of morphology parameters governing the properties of melt-processable filled polymers

The direction of the WP was set in its early days. It was broad ranging and flexible, and it has not changed significantly over the years. The group existed within the IUPAC organizational structure, which monitored but did not define its activities. The group's project base was self-defined and the consequences of this are extremely important.

First, the WP has consistently initiated projects that it knew were of relevance to industry, academia, and the world at large. Also, in a general sense, the work had to be convincing to the paymasters, namely, industrial managers or academic supervisors. It was, therefore, crucial that the appropriate skills be present and active in the WP.

Second, the members of the WP find great value in working with like-minded scientists on a global basis; it offers contacts and networks that would be difficult to establish by any other means. In addition, there is considerable value in scientific projects in which an individual (or his or her organization) is funding only a fraction of the cost.

Third, the definition of a project by its task group members ensures that the project is of contemporary value and importance. Common themes that are important to several industrial scientists can be turned into a useful, but non-competitive project. Further, seeking academic involvement often provides useful input from leading experts. Despite moves within the broader IUPAC organization to generate and define projects on a top-down basis, it will be vital to retain some projects that come from the bottom-up approach of the WP.

The driving force behind the WP has always been the motivation to obtain value (to them and their businesses) from participation in the group. If value is obtained, participation is funded. This principle has guided the WP for 40 years through changing economic climates; there is no reason to assume it won't work for another 40 years.

The international network of scientists making up the WP will continue to pursue projects that have contemporary value and that lead to publications. The types of materials and the approaches used will no doubt change, but there will always remain issues relating to polymeric systems or particular properties that will need to be characterized and understood.

There is likely to be demand for shorter projects in the future, as impatience for returns on investment is always present. In a recent trial of a possible approach, a philosophical document on the future requirements for the characterization of composites was written. This type of approach is based solely on an existing knowledge base, eliminating the need for conducting new measurements. The decline in major corporate organizations in the chemical industry suggests that the need for such an approach could be larger than we might predict.

Some completed projects have provided comprehensive data on commercial polymers that are still available and may be used for further research outside of the WP. Recent examples are poly(α-methylstyrene-*co*-acrylonitrile) (PαMSAN) and poly(ethyl methacrylate) (PMMA) and their blends. Besides a rheological and mechanical characterization of the constituents and their blends, there is valuable information available on the interfacial tension as well as the interaction parameter χ as a function of temperature and composition. Further studies on this system are specifically encouraged.

There are also educational values that the WP could satisfy. A new recruit could serve a few years on the WP in order to become acquainted with the network of activities and people or merely to learn a different approach to conducting research or a project.

It is obvious that the future lies with the people involved and their commitment to the broader aims of the WP. It will depend on whether they involve others in the activities of the group because they see and appreciate its benefits. Finally, it will depend on whether they communicate the values and virtues of the WP and ensure that their organizations support their continued involvement.

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D. Royston Moore <r.moore@imperial.ac.uk> has been involved with the WP for more than 10 years and is now an IUPAC Fellow; he is now at the Mechanical Engineering Department of the Imperial College in London, U.K.; H. Martin Laun <martin.laun@basf-ag.de> works at the Polymer Research Division of BASF Aktiengesellschaft in Ludwigshafen/Rhein, Germany.

John Pople

by Balazs Hargittai and István Hargittai

"We are perhaps not far removed from the time when we shall be able to submit the bulk of chemical phenomena to calculation, wrote J. L. Gay-Lussac in 1888." Although chemistry will always remain primarily an experimental science, John A. Pople did perhaps more than anybody else to make Gay-Lussac's prophecy true. Pople (b. 1925 in Burnham-on-Sea, Somerset, England—d. 2004 in Evanston, Illinois) revolutionized chemistry by pushing it into the computer era. He was awarded the 1998 Nobel Prize in Chemistry "for his development of computational methods in quantum chemistry." He shared the prize with Walter Kohn (b. 1923) who received it "for his development of the density-functional theory."

Pople's father was a local businessman and his mother came from a farming family. However, little John was told early enough that he was expected to do more than run a small business in a small town. His road to education was not without hurdles. The local preparatory school, which was of good quality, was not open to children of retail tradesmen, so John was sent to study in Bristol. Some of his school years coincided with the Second World War, yet he managed to get a good education. His intense interest in mathematics started at the age of 12. In 1943, Cambridge University awarded his excellence in this subject by accepting him.

Photo by I. Hargittai

Walter Kohn (left) and John Pople in Stockholm, 2001, during the Nobel Prize Centennial celebrations.

When the war ended, discharged servicemen flooded the university and Pople sought industrial employment for a while. In a couple of years, however, he was able to resume his education at Cambridge. He took many courses, especially in theoretical subjects, and felt an attraction to scientific research. However, he also felt that challenging the likes of Einstein and Dirac would be over ambitious and opted for less crowded fields. At one point he became a research student of John Lennard-Jones, who taught theoretical chemistry at Cambridge, lectured about molecular orbital theory, and was interested in electronic structures. This was a decisive influence in Pople's career.

John Pople became a research fellow at Trinity College of Cambridge University in 1951, and lecturer on the mathematical faculty in 1954. However, by 1958, he became dissatisfied with his position in Cambridge and wanted to find a new job with more scientific activity. The first attempt was not very successful in that the position he took in a national physics laboratory was burdened by administrative duties. The breakthrough was the result of a sabbatical leave at Carnegie Institute of Technology in Pittsburgh, from 1961 to 1962. This led the Pople family to relocate to Pittsburgh in 1964. He joined the Mellon Institute, which had excellent computational facilities. The Mellon Institute and the Carnegie Institute merged in 1967.

Pople viewed the relationship between experimental and computational work as complementary.

The Poples moved from Pittsburgh to Evanston in 1981 to be closer to their daughter, but he remained affiliated with Carnegie-Mellon. In 1993, his relocation became complete as he joined Northwestern University where he worked, until his recent death, at the Chemistry Department as Board of Trustees professor.

Pople received many awards and other distinctions in addition to the Nobel Prize. He became Fellow of the Royal Society (London) in 1961 and he was knighted in 2003. So, during his last months he lived as Sir John Pople. In 2002, the Royal Society bestowed upon him its most prestigious award, the Copley Medal. He also won the von Humboldt Award in Germany and the Wolf Prize in Israel.

Pople defined computational chemistry as the implementation of existing theory to studying chemical problems by means of computer programs. He preferred not to draw a distinction between computational chemistry and the underlying theory. The the-

ory preexisted, and the computers just enabled it to be implemented much more broadly than was possible before. His approach was to apply theory to the whole of chemistry. His practical approach made him sensitive to considering the "experimental errors" in computational work, something that many computational chemists ignore.

The way he liked to do this was to set up a theoretical model and apply it to all molecules. By applying one approximation to all molecules, he obtained an entire chemistry corresponding to that approximation. This was not real chemistry, but approached it well if the model was good. He used the model to calculate a large number of facts that had also been obtained experimentally. Then he applied statistics and could state that this theory reproduced the experimental facts with certain accuracy. This approach built some level of confidence into that particular level of theory. Therefore, the theory could be applied to a situation where experiment might have not yet existed.

Pople viewed the relationship between experimental and computational work as complementary. He thought that even experimentalists should augment their work with calculations, but he noted that the older generation of chemists was suspicious of theory. He did not think that computational chemistry should be a separate discipline and he advocated for it to be in the general curriculum. He thought that the computer program should be considered a black box, just like a complicated spectrometer, and chemists should learn how to use these programs, and to use them in a critical manner, to understand the limitations of what they find, just like any other technique.

Pople was always more interested in making the computational approach available for application to a large number of people than in going for the highest level of sophistication for some selected systems. He formulated his research strategy back in 1952, when he was still a postdoctoral fellow in Cambridge. This strategy was that one level of theory implies an entire chemistry. He charted this strategy at a time when nothing was yet possible in terms of computational facilities; so he had tremendous foresight. The first theory in this category was the so-called PPP theory, Pariser-Parr-Pople. It handled essentially only one electron per atom and was used for the π-electrons of aromatic hydrocarbons. It became very popular and successful in the 1950s. It was a simplified theory, which was possible to apply even without computers in those days.

Compliments of Rudy Pariser

Pariser, Parr, and Pople (L to R) in Chapel Hill, North Carolina, in November 1998 at the occasion of a symposium on Quantum Chemistry in honor of Robert G. (Bob) Parr."

Pople's general objective, however, was always to produce theories and the associated computational techniques that would be extensively applicable and illuminate as many chemical properties as possible. This has proved to be enormously successful and was greatly helped by the huge advances in electronic computation. Pople anticipated this technical progress, although not its extent and speed. It might seem that computational technology has advanced so far that there are no longer any limits to computational chemistry, but this was not how Pople viewed advancement. He considered his objectives as such that it will always be necessary to push for more progress.

When Pople was awarded the Nobel Prize, there was universal satisfaction among chemists although he was not a chemist by training. Everybody thought that the 1998 chemistry prize corresponded to the letter as well as to the spirit of Alfred Nobel's will, which stated that in terms of the prize money, "one part [should go] to the person who shall have made the most important chemical discovery or improvement." Even if there had been a Nobel prize for mathematics, Pople should have earned the chemistry prize. It does happen from time to time that physicists or even biologists earn chemistry prizes, but it is rare that mathematicians receive them.

John Pople will have a long-lasting impact on how modern chemistry is conducted and where it goes.

In this article, we used extensively materials from the interview John Pople gave one of us in 1995 [I. Hargittai, *Candid Science: Conversations with Famous Chemists*, Imperial College Press, London, 2000, pp. 178–189].

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XML in Chemical Education

The IUPAC Committee on Printed and Electronic Publication is concerned with good practice in information and data exchanges at all levels and is supporting the eXtensible Markup Language (XML)-based standard in some areas. The committee believes that the following article is a helpful contribution to the subject. The views are the author's own and are not a part of IUPAC's strategy.

by Daniel Tofan

In the July 2002 issue of *Chemistry International*, Jonathan Goodman raised the question of "How well are we using XML in chemistry?" He also stated that "from an academic and educational viewpoint, one could say, unfortunately, not too well right now." This is absolutely true, and indeed unfortunate, but may change in the very near future.

In a conversation I had at the recent American Chemical Society (ACS) meeting with Peter Murray-Rust, the developer of the Chemical Markup Language (CML), he noted that most chemistry journals do not require or even encourage authors to submit chemical data using CML. This is unfortunate, since CML has been specifically designed to facilitate the exchange of chemistry data in a format that is easy to use and understand, yet powerful enough to allow the interchange of such data among applications, web browsers, and text processors. For example, rather than having an "experimental" section in a chemistry paper, that describes the preparation of various compounds and solutions as a narrative, it would be more useful to submit such details in CML, so that the experimental details can then be imported into other programs automatically. Such XML-aware programs would know how to convert the information from CML to a variety of other formats for display or use somewhere else. As another example, crystallographic data that are currently submitted as crystallographic information files (CIFs) should probably be encoded in CML instead, considering the flexibility that the latter offers and its validation capabilities.

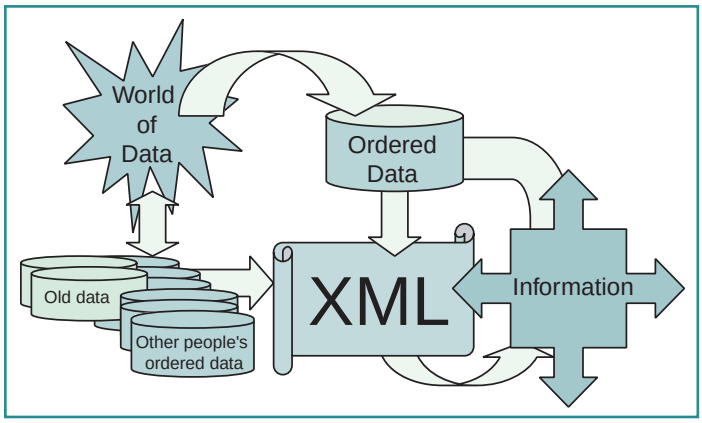
The field of chemical education, seems likely to benefit the most from the existence of a markup language . . .

The field of chemical education, on the other hand, seems likely to benefit the most from the existence of a markup language designed specifically to exchange assessments, question banks, data on student performance, and so on. With the widespread use of course management systems such as Blackboard or WebCT, there is the need to exchange items and assessments among users at various institutions. The Instructional Management System (IMS)—the global learning consortium dedicated to developing specifications for distributed learning—has developed XML specifications for the interoperability of such items and assessments, among others. While these specifications provide for basic response types such as strings, numbers, multiple choice, simple drag and drop, and more, they offer no support for chemistry types. Anybody who wants to write chemistry questions that can be used in a course management system must limit themselves to those basic types of responses. But what if we want to ask and grade a question such as "Predict the products and balance the net ionic chemical reaction between copper sulfate and ammonium hydroxide?" How do we provide the correct answer, which consists of a balanced chemical reaction that contains states and charges, into the XML format proposed by IMS?

Currently, I can see two ways of doing that. One is to use a multiple choice format and to offer several options that include the correct answer, so the students can choose among them. The other way is to use a string response, and somehow decide on a format that the students can use to enter chemical formulae with states and charges (for example HTML fragments with <sub> and <sup> tags). The challenge would be to enforce that format among users and to provide a parsing algorithm in the implementing software that can figure out whether a submitted response is the correct one. I find none of these approaches even close to satisfactory. Not only would I want students to enter a response on their own rather then pick one from a list of presented possible options, but I would also want them to actually enter a chemical reaction with formulas that contain indexes, states and charges as superscripts and subscripts. I would also like to have a software tool that knows what to look for and how to analyze and grade such a response. So what is the solution, then?

The answer, in my view, is that there should be some XML format that can be used to encode a response that consists, for example, of a complete chemical reaction (or any other kind of chemistry specific information) and to place that XML into the

response analysis section of an IMS-compliant item. Thus, by having a defined ontology (set of XML tags) that encode basic chemistry entities and concepts such as reactions, electron configurations, Lewis structures, and so on, chemistry teachers will be able to write questions that contain chemical information and that require responses with chemical content from the students. Authoring tools will then be able to generate this XML when the questions and test items are written to files for export, and other systems will be able to import such items and use them in chemistry activities and tests. While it is not too difficult to generate XML, as Peter Murray-Rust also noted, it is more challenging to read in XML and to make use of it in a real-world course management system, or any other application for that matter.



"How Well Are We Using XML in Chemistry?" by J. Goodman, reprinted from Jul-Aug 2002 CI, *p.7.*

Another reason why XML is necessary in chemical education becomes apparent when considering the ongoing development of digital libraries. One example is the National Science Digital Library initiative, funded by the National Science Foundation. Such collections have a need to store, among other things, question banks and data that pertain to chemical education. It seems that a text-based format that is easy to understand and use, yet powerful and flexible, is needed for this purpose. XML provides all these characteristics, and in the absence of an existing standard, a tag set needs to be invented to provide the vocabulary that allows chemical education data to be included in digital libraries.

Having stated the reasons why XML is needed in chemical education, the only remaining problem is to actually define the set of XML tags that potential users can agree upon, adopt, and implement. This task seems to be a rather laborious one, and the result is likely to be debated by various groups that can argue over what elements and attributes should or should not be included, and even what their names should be. Community consensus on this subject is absolutely critical. I thought, however, that a step forward can be taken by actually proposing a specification and making it known to the academic community, therefore inviting constructive criticism and support so that useful chemistry markup can eventually be developed.

One other issue to address is interoperability with other chemistry markup languages that are currently available or under development. Examples include ThermoML for thermophysical and thermochemical property data, AnIML, GAML and SpectroML for analytical chemistry data, NDML and UnitML for encoding units of measurement, and expML for experimental data interchange in science and engineering. These are generally industry-strength formats, many of which are being developed by, or in collaboration with, the National Institute for Standards and Technology. There are also XML initiatives from the *Journal of Chemical Education*, which is developing a digital library for chemical education and needs an XML vocabulary for storing question and test items, as well as other digital libraries such as ASDL for analytical chemistry. Some of the XML elements and/or attributes present in the specifications for these markups may be similar. While from an educational point of view it may be more difficult to see why simple concepts such as balanced chemical reactions would need to be encoded in other markups as well, it is nonetheless a possibility that should be taken into account. Having many ways of representing things like chemical formulas unavoidably leads to the "multiplicity of formats" problem that has been identified by the chemistry XML community. It is therefore important that some consensus exist when developing these various chemistry XML formats, so that standardization is possible. After all, this is what the IUPAC is aiming for.

The specification that I propose is what I call the Chemical Education Markup Language, or ChEdML. Whether this will be a full-blown markup language remains to be seen, but it is a start and I think the name is representative of its purpose. ChEdML is currently intended to be an XML namespace for educational chemistry. By defining a namespace rather than

a standalone markup language, ChEdML fragments can be included into larger XML files, such as items and assessments that comply with the IMS specifications. IMS itself encourages the development of extensions for their current response types. It is quite evident that chemistry provides a lot of room for extending the IMS markup to cover many new types of responses that are specific to chemistry. It just needs a mechanism to do this, and ChEdML will provide that mechanism.

As far as its integration with other XML types is concerned, ChEdML is looking at both the past and the future. It seems natural that encoding of molecular structure or spectral information should be done by using CML elements, as they already exist and have been developed for just this purpose. Mathematical equations, which are always present in educational chemistry material, can be coded using MathML. Units can be coded in UnitML, laboratory experimental data can be submitted in expML and so on. By combining together fragments from various XML namespaces and specifications, truly powerful, structured XML documents can be produced. The development of software tools that can handle this XML should be just a matter of time.

By combining together fragments from various XML namespaces and specifications, truly powerful, structured XML documents can be produced.

At present, ChEdML is a project under development, and only a few tags have been invented to code concepts such as isotopic symbols, molecular formulas, chemical reactions, electronic configurations, Lewis structures, electrochemical cell notations, and other subjects taught and assessed in general chemistry. ChEdML also has provisions for the formatting of chemical symbolism for display in Web browsers and other specialized tools, and also for the inclusion of numeric parameters and units into quantitative problems. It should also extend to cover other areas besides introductory and general chemistry, but right now it is mostly GenChemML (which can be very useful, although limited in scope).

A Web site is being maintained at <www.chedml.org> to bring awareness to the project and inform the community about the progress being made. Currently, the information available online is rather limited—a few examples are up to show what can be done, and future directions are proposed. It seemed prudent not to develop a full specification before gaining the support of the academic community, especially in the absence of external funding. However, feedback received at the recent ACS meeting has been very positive, which indicates that perhaps ChEdML will be useful. New ideas and real contributions to the markup from interested parties are kindly invited and criticism is also welcome. The Web site provides a way to submit comments and feedback.

It should be possible to make ChEdML a truly useful tool for chemical education. With time, perhaps other sciences will develop their own markup languages. Mathematics already has MathML. Physics could be next, and a general purpose Science Education Markup Language (ScEdML) might be able to incorporate these formats into a larger one. One thing seems certain—the academic community does need XML.

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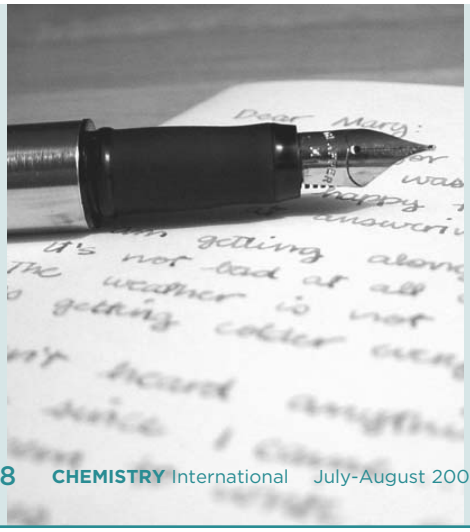
www.chedml.org



News Items Wanted

***CI* is currently seeking articles for the IUPAC Wire section.**

Please note that articles should be submitted no later than two months before the issue date. Contact the editor for more information at edit.ci@iupac.org

Executive Committee Looks at IUPAC's Role in the World

IUPAC's Executive Committee (EC), which oversees the proper functioning of the Union, meets once a year to discuss a range of issues. At the EC meeting held 3-4 April 2004 in Bangalore, India, a number of "big-picture" issues were discussed. In the following report, Secretary General David StC. Black comments on some of these issues, which will be of general interest to the IUPAC community.

The EC comprises the IUPAC officers, namely the president, vice president, past president, secretary general, treasurer, and three elected members, currently Chunli Bai, Oleg Nefedov, and Ed Przybylowicz. IUPAC Executive Director John Jost acts as secretary of the EC. The meeting was hosted by our colleagues at the Indian Institute of Sciences in Bangalore, and offered an opportunity to witness first hand the thriving chemical scene there.

IUPAC's EC members in Bangalore, April 2004: front, from left: past president Pieter S. Steyn, president Leiv K. Sydnes, secretary general David StC. Black; rear, from left: Chunli Bai, Edwin P. Przybylowicz, vice president Bryan R. Henry, executive director John W. Jost, and Oleg M. Nefedov.

by David StC. Black

Interaction with Industry

There was considerable discussion at the meeting about IUPAC's interaction with industry. It was felt that we should be emphasizing the role of IUPAC as an international, independent non-governmental organization. We are already addressing industrial issues through the Committee on Chemistry and Industry (COCI) and the CHEMRAWN (CHEMical Research Applied to World Needs) conferences, and some innovative approaches are being prepared. There are indications that IUPAC projects can help industry considerably, whether by creating specific databases or by generating positive publicity. Clearly, industry is interested in the big chemical issues, and this is certainly consistent with IUPAC goals. For example, industry is concerned about non-tariff trade barriers, and it might be possible for IUPAC to play a role in mediation.

It was felt that we should be emphasizing the role of IUPAC as an international, independent non-governmental organization.

There was much discussion about the value of the Company Associates program, which appears not to be well understood, and is certainly not widely adopted. The scheme will be publicized more vigorously in terms of its value to National Adhering Organizations, to the companies themselves, and also to IUPAC. COCI is already working on this matter.

Union Advisory Committee Matters

Membership in the Union Advisory Committee (UAC) is almost complete, and the EC has identified several issues on which to seek advice. While members serve in a personal capacity, they would also need to communicate with their local chemical community. The first item for the UAC to consider is the project Chemistry's Contributions to Humanity—A Feasibility Study, otherwise known as the "Value of Chemistry" project, which is being carried out by a task group led by Ed Przybylowicz. A great deal of information has been gathered for this project from publications, Web sites, special events, and other sources, and a Web site is being created. UAC members are being asked to review the accumulated material and consult chemical contacts within their respective countries to identify any additional sources of information (see project update, p. 24).

The second item concerns a resolution arising from the Ottawa Council to investigate how to encourage young people to pursue careers in chemistry. This is particularly important for the future health of the chemical industry. The resolution can be paraphrased as follows: (i) to encourage and facilitate the coordination of the variety of initiatives to enhance chemical education at all levels, and to utilize younger chemists to promote the subject and its achieve-

ments; and (ii) to collaborate with industry, trade associations, learned societies, and academe to discuss how best to achieve these aims and, if considered appropriate, to solicit new financial resources to achieve them.

It was decided to survey UAC members about efforts in their own countries to promote careers in chemistry. As it is clear that national chemical societies and chemical interests in individual countries already have robust projects underway, the exchange of information and coordination of activities could be very useful. It was further noted that while fewer young people are pursuing chemistry in most, if not all, Western countries, this is not true in Asia. In Bangalore, EC members had first-hand experience of a country with strong interest from students in chemistry, and also a booming chemical industry. The work of the suggested "Propagation of Chemistry" task force and the "Value of Chemistry" task group is not entirely unrelated, and both groups of responses will be coordinated, and hopefully lead to a valuable project proposal.

One other issue for the UAC to consider is possible changes suggested by the Governance Structure Committee. These were discussed in Ottawa, and it was felt that more time was needed for their consideration. A timetable will be set in place to allow for full discussion and consequent resolutions.

IUPAC Poster Prizes

It is quite common for poster prizes to be awarded at conferences, and it is acknowledged that this is an excellent way to encourage young chemists. Some IUPAC poster prizes have been awarded in an ad hoc way at several conferences, but it was resolved at the EC meeting to develop a more general and widespread program of prizes. Conference organizers will be therefore asked to take advantage of this opportunity. The following guidelines were approved:

- Prizes will be awarded at all IUPAC Congresses and Division-sponsored meetings where poster sessions are held.
- Prizes will be awarded at national meetings if requested. Not more than one meeting per country a year should apply, and that meeting should be selected by the relevant NAO.
- Except for IUPAC Congresses, normally there will be two, with a maximum of three, prizes awarded per conference.
- Selection of prizewinners is in the control of the conference organizers.
- Each prize will consist of a certificate signed by the IUPAC president, a copy of the Gold Book, and two years' subscription to *Chemistry International*.

The minutes of the EC meeting are available online at <www.iupac.org/news>, under Minutes of Meetings: Executive Committee.

Please address questions/comments to the Secretary General David StC. Black <d.black@unsw.edu.au>.

www.iupac.org/news/archives/2004/131_ec.html

2004 Winners of the IUPAC Prize for Young Chemists

On 1 June 2004, IUPAC announced the winners of the IUPAC Prize for Young Chemists, which is an award for the best Ph.D. thesis in the chemical sciences as described in a 1000-word essay. The winners are as follows:

- Parag Acharya, Uppsala University, Sweden
- Yu Huang, Harvard University, Cambridge, MA, USA
- Zhipan Liu, Queen's University of Belfast, UK
- S. G. Srivatsan, Indian Institute of Technology, Kanpur, India

The winners will each receive a cash prize of USD 1000 and a free trip to the IUPAC Congress, 14-19 August 2005, Beijing, China. Each prize winner will be invited to present a poster at the IUPAC Congress describing his/her award winning work and to submit a short critical review on aspects of their research topics to be published in *Pure and Applied Chemistry*. The awards to the four winners of the 2004 prize and those of 2005 will be made during the Opening Ceremony of the Congress. The essays describing the winners' theses, which can be found on the IUPAC Web site, cover a wide range of subject matter:

- Dr. Acharya, "Studies on the Non-covalent Interactions (Stereoelectronics, Stacking and Hydrogen Bonding) in the Self-assembly of DNA and RNA"
- Dr. Huang, "Integrated Nanoscale Electronics and Optoelectronics: Exploring Nanoscale Science and Technology through Semiconductor Nanowires"
- Dr. Liu, "Insight into Chemical Reactions: From Heterogeneous to Enzymatic reactions"

- Dr. Srivatsan, "Modeling Prebiotic Catalysis with Adenylated Polymeric Templates: Kinetic Characterization of Assisted Phosphate Ester Cleavage and Oxygen Insertion Reactions"

There were 44 applicants from 23 countries. The Prize Selection Committee was comprised of members of the IUPAC Bureau with a wide range of expertise in chemistry. The committee was chaired by Prof. Pieter S. Steyn, IUPAC past president.

In view of the quality of many applications, the Committee decided also to give four Honorable Mention Awards:

- Orlando Acevedo, Duquesne University, Pittsburgh, PA, USA
- Neel Sarovar Bhavesh, Mumbai University, Mumbai, India
- Anand Mahadeo Gole, University of Pune, India
- Jennifer J. Sokol, University of California, Berkeley, CA, USA

The Honorable Mention Award winners will receive a cash prize of USD 100 and a copy of the *Compendium of Chemical Terminology*, the IUPAC "Gold Book."

Applications for the 2005 Prize are now being solicited, as described at the Web address listed below.

www.iupac.org/news/prize.html

Up for Discussion

A forum for members and member organizations to share ideas and concerns.
Send your comments by e-mail to <edit.ci@iupac.org>.

Questionable Stereoformulas of Diastereomers

The comments below have been received in response to the ideas of using "thick" and "hatched" bonds to represent relative configurations expressed by G. Kaupp and M. Reza Naimi-Jamal in their article in the Jan-Feb 2004 Chemistry International*, p. 15. These comments add to the debate and will be considered in the course of the recently initiated IUPAC project on Graphical Representation Standards for Chemical Structure Diagrams, chaired by William Town—see project announcement on page 23.*

by H.D. Flack

Kaupp and Naimi-Jamal's comments and suggestions are to be taken very seriously for the reporting of crystal and molecular structures determined by X-ray diffraction. We take this opportunity to express our point of view on some matters that relate directly to this subject.

No matter what graphical representation is finally agreed upon for molecular diagrams, we consider it essential that these must be usable by a human chemist or crystallographer and allow for a high degree of automatic checking by a computer.

Editors, co-editors, and editorial staff do not have the time to go around checking the stereochemistry and labelling of every diagram in every paper. Automation provides a very cost-effective aid in the process of verifying scientific communications. The molecular diagram must be machine-interpretable. Molecular diagrams, molecular identifiers, and molecular names must be designed so that they are in one-to-one correspondence with one another. Moreover, any caption labelling of a molecular diagram must be compatible with the presented molecular diagram.

In terms of the reporting of molecular structures from crystal-structure determinations, we distinguish three distinct cases: enantiopure compound of known absolute configuration, enantiopure compound of unknown absolute configuration, or racemate.

The "Basic Terminology of Stereochemistry," (1996) *Pure Appl. Chem.* **68**, 2193–2222, gives the terminology for attributing distinct names to the compounds in these three classes. However Kaupp and Naimi-Jamal's suggestions for molecular diagrams do not produce graphical representations of enantiopure compound of unknown absolute configuration distinct from racemate, and conversely. However the physical state of these two classes is very different and such properties as the melting point, optical

activity, and CD spectrum would be different.

Although we have noted elsewhere [H.D. Flack (2003), *Helv. Chem. Acta* **86**, 905–921] that the IUPAC naming of racemates may readily be extended to take account of enantiomeric mixtures in rational proportions other than 1:1, it is completely unclear to us how molecular diagrams should be presented in such cases.

The late André Collet brought to our attention that the definition of absolute configuration as given in the "Basic Terminology of Stereochemistry" (1996) is inadequate in one important respect. Essentially, his argument is that it is useless to specify a stereo-configuration by a molecular diagram or molecular name unless it is accompanied by an appropriate physical characterization of the bulk compound. [see H. D. Flack and G. Bernardinelli (1999) *Acta Cryst.* **A55**, 908–915 for a full and open-access discussion.]

H.D. Flack <crystal@flack.ch> is professor at the Laboratoire de Cristallographie, at the University of Geneva, Switzerland. <www.flack.ch/howard/cristallo/Howard.Flack.html>

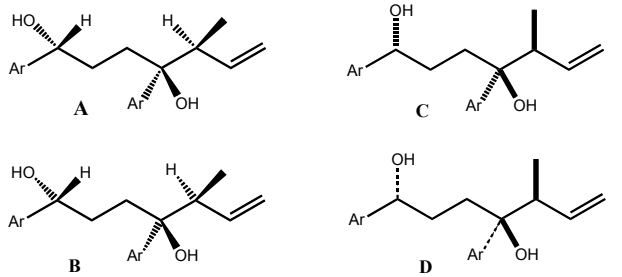


Figure reprinted from Jan-Feb 2004 CI*, p. 16. According to Kaupp and Naimi-Jamal, formula A, or even more distinct formula B (traditionally with exactly the same meaning), will then rightfully look like formula C (alternatively like formula D), if it is not the (1R,4S,5S)-enantiomer, but the racemate of this diastereomer.*

by Michinori Oki

As someone interested in conformation, I cannot agree with Kaupp and Naimi-Jamal's suggestion because it is quite different from common practice.

Their paper states that **"**wedged chemical formula should be used only for indication of absolute configuration.**"** We had known that IUPAC wanted to indicate stereochemistry by using solid or hatched lines as shown in the figure below. But this is very inconvenient in discussing conformations.

We therefore have used wedges to indicate that the bond in question is directed to the rear of the paper and the solid wedge directed toward the eye. Incidentally, normal lines or solid or hatched lines, if they do not change in width, mean that these are in the plane of the paper. Therefore, the formula C below does not provide any information about conformation. However, if one use wedges, it is easy to recognize that a bond in question is is antiperiplanar (ap) or synclinal (sc) to a given bond that is attached to the neighboring carbon. I hope that IUPAC does not adopt Kraupp's proposal, unless the usage of formula C is confined to indication of configurations. Rather, wedges should be recommended for indication of the direction of a bond in question.

Michinori Oki <michinori.oki@jcom.home.ne.jp> is an IUPAC Fellow who recently retired from the Okayama University of Science, Japan.

Link to Kaupp and Naimi-Jamal's original article:

www.iupac.org/publications/ci/2004/2601/ud1.html

Graphical Representation Standards for Chemical Structure Diagrams

Although some existing IUPAC nomenclature recommendations already discuss some aspects of chemical structure diagrams, they do so only tangentially. Even if they were to be collected in one location, these existing recommendations on chemical structure diagrams are incomplete, and do not discuss many basic issues. As a result, many organizations have formulated their own guidelines for creating chemical structure diagrams; however, none of those guidelines is comprehensive. Provision of a single, comprehensive set of guidelines for creating chemical structure diagrams would be a significant benefit to the chemistry community and the aim of this project is to provide such a set of guidelines for creating chemical structure diagrams in printed and in electronic media.

An IUPAC project titled "Graphical Representation Standards for Chemical Structure Diagrams" has recently begun with a "scoping exercise" in which some 20 members of the chemistry community were invited to discuss those aspects of creating chemical structure diagrams that are amenable to standardization through IUPAC recommendations. Some draft recommendations were created during the course of that scoping exercise, and these will serve as a useful starting point. The participants also identified several areas that are likely to be contentious or otherwise were incompletely specified; those areas will receive specific attention during the course of the project. Polymer representations are excluded for now but will be addressed later; one or more polymer nomenclature experts will than be added to the task group.

With the ever-increasing importance of electronic publication, this project will consider issues related to the production of chemical structure diagrams both in printed and in electronic media. Where possible, every effort will be made to ensure identical recommendations in all media. The recommendations for the production of chemical structure diagrams will aid in the correct recognition of structural information by the IUPAC/NIST Chemical Identifier algorithm.

In some cases, the current state of chemistry software may preclude the use of the most-preferred styles for chemical structure diagrams. When necessary, this project will also provide practical advice for the production of electronic chemical structure diagrams according to the current state of the art of chemistry software. It is likely that this project will also produce a set of recommendations for enhancing chemistry software.

For more information, contact the Task Group Chairman William G. Town <bill.town@kilmorie.com>.

www.iupac.org/projects/2003/2003-045-3-800.html

Explanatory Dictionary of Concepts in Toxicokinetics

IUPAC is the world authority on chemical nomenclature and terminology and sets standards for the critical evaluation of data. In order to encourage and facilitate the interaction of chemistry and toxicology, a project was initiated to create a glossary of terms used in toxicokinetics (project #2000-034-2-700). This glossary is now accepted as an IUPAC Recommendation (May 2004 *PAC*, in press). During the preparation of this glossary, the Working Party realized that while some of the definitions are adequate in themselves, it might be useful to provide explanations of the underlying and related concepts and related, practical scientific considerations. Thus, the objective of this "Explanatory Dictionary of Concepts in Toxicokinetics" is to select terms from the original glossary of toxicokinetics and provide a full explanation of the subtleties that may affect their use and thus the meaning of related scientific papers, reviews, or other documents.

The "Explanatory Dictionary of Concepts in Toxicokinetics" is one of a number of projects addressing toxicology and chemistry under the Chemistry and Human Health Division (VII) and should be a valuable educational resource in its own right. It is envisaged that by facilitating communication among chemists, toxicologists, and risk assessment specialists, the "Explanatory Dictionary" will play an important role in helping chemists meet the increased requirement from society and government for risk assessment of chemicals. Better risk assessment will help to ensure that the practice of chemistry remains safe and continues to benefit human health. Thus, the project will support IUPAC objectives and help to improve the image of chemistry in society. In doing so, it will serve the needs of chemists worldwide.

The task group for the Glossary is chaired by Monica Nordberg, and the current members are John H. Duffus and Douglas M. Templeton. Scientists active in the

fields of chemistry, toxicology, medicinal chemistry, pharmacology, and biostatistics will be consulted. The time period for the project is from 2003 to 2006.

For more information contact the Task Group Chairperson Monica Nordberg <monica.nordberg@imm.ki.se>.

www.iupac.org/projects/2003/2003-001-2-700.html

Chemistry's Contributions to Humanity—A Feasibility Study

Initiated in July 2003, the objective of this project, titled "Chemistry's Contributions to Humanity—A Feasibility Study," is "to evaluate the feasibility of developing a Web site that chronicles historical innovations in chemistry that have contributed to the improvement of human life."

The first task in this project was to assess what information on this topic was available to the general public through publications, Web sites, and special events. As part of this process, the task group sent letters to over 40 organizations world wide to solicit input.

At this time the task group has identified and compiled a first list of books, pamphlets, and Web sites that contain information on the theme of chemical contributions to society. This listing is by no means complete; the task group is soliciting help from all members and the community at large to augment this list or critique it from the standpoint of what is included. See Web address below for list of documents.

For more information, contact the Task Group Chairman Edwin P. Przybylowicz <eprzy@rochester.rr.com>.

www.iupac.org/projects/2003/2003-022-1-020.html

Bio-Physical Chemistry of Fractal Structures and Processes in Environmental Systems

The objective of the project "Bio-Physical Chemistry of Fractal Structures and Processes in Environmental Systems" is to produce a book that will provide a novel and valuable approach—based on fractal geometry concepts—to the chemistry, biochemistry, physical-chemistry, and analytical chemistry of structures, properties, and processes in environmental systems. This project should provide a fundamental knowledge base for facing and solving practical environmental problems. The project is expected to be instrumental in enhancing education and increasing availability and dissemination of novel information and awareness of environmental issues.

The book will contain nine chapters, each authored by a different task group member possibly in collaboration with selected coauthors. The book is intended to provide a novel approach in these sciences, but should be regarded as integrative and additional and not substitutive to the classical approaches. The intended audience for the book will be mainly graduate students, scientists, and scholars. It should also be of interest to professionals involved in fundamental and applied studies in environmental sciences. The project will also promote integration of IUPAC activities in various fields of chemistry and collaboration with other environmental sciences.

For more information contact the Task Group Chairman Nicola Senesi <senesi@agr.uniba.it>.

www.iupac.org/projects/2003/2003-014-2-600.html

Quantifying the Effects of Compound Combinations

As ever more combination therapies are applied in various areas of medicine, there is a growing need for quantitative descriptions of combination effects. While most of the scientific community has agreed on a basic standard for synergy, there is no consensus on quantifying the degree to which a combination may deviate from synergy, and no predictive models are accepted to serve as benchmarks.

This project will convene a working group, involving leading experts on combination effects, to (1) endorse the synergy criterion recommended at a recent meeting in Finland, (2) adopt standard measures of combination effect to quantify deviations from synergy, and (3) explore predictive combination-effect models for multiply-inhibited biological interaction networks.

For more information contact the Task Group Chairman Joseph Lehár <jlehar@combinatorx.com>.

www.iupac.org/projects/2003/2003-059-1-700.html

XML in Chemistry and Chemical Identifiers

by Antony (Tony) N. Davies

Steve Stein of the National Institute of Standards and Technology (NIST) in Gaithersburg, Maryland, USA, and Alan McNaught of the Royal Society of Chemistry, Cambridge, UK, jointly hosted a three-day meeting to discuss IUPAC projects on **XML in Chemistry and the Chemical Identifier Project**. The meeting was held at NIST from 12–14 November 2003.

The meeting was exceptionally well attended with over 50 attendees from governmental and regulatory bodies, research and academic institutes, and industry. A wide range of experts in the field were brought together for a lively exchange of views on many of the topics covered.

XML in Chemistry

Numerous speakers related tales of XML initiatives involving chemistry in their respective organizations, including the European Patent Office, the International Union of Crystallography, and the U.S. Food and Drug Administration's Center for Drug Evaluation and Research. Various projects within NIST itself were also discussed, such as UnitsML for scientific units and ThermoML for thermodynamic properties. ToxML was described for toxicology data. Despite the range of speakers' views on the issue of XML in chemistry, one thing became clear. The decision of IUPAC to take a leading role to avoid multiplication of effort was clearly correct.

Some very detailed technical discussions were held on the mechanisms surrounding the generation of controlled ontologies or data dictionaries that highlighted the speed at which the field is moving. The number of XML initiatives that have been born, flourished briefly, and then vanished into obscurity was also discussed.

These arguments underlined the essential nature of the problem, which is that the research effort ought to be better placed in producing novel ways to handle information to enhance productivity and produce better more advanced tools for data mining rather than repeatedly discussing how best to move the data from A to B. With luck, the IUPAC initiative will bring a certain degree of stability to the information technology base in chemistry and allow teams working in this area to concentrate on their core business without having to worry whether their underlying technology is about to be made obsolete!

IUPAC/NIST Chemical Identifiers (INChI)

Alan McNaught introduced the project, the aim of which is to produce a public Chemical Identifier to uniquely identify compounds. The current version is available for testing and has been expanded to cover organic, inorganic, and organometallic chemistry. It should be noted that the project acronym IChI (for IUPAC Chemical Identifiers) has been changed to INChI, where N stands for NIST. This change was made to recognize the immense contribution of NIST to the project.

But how does INChI work? Well, INChI starts off by looking at the chemistry of the structure to be assigned an "Identifier." The structure is normalized and a number of chemical rules applied. Next, some mathematics "canonoicalises" the structure (labels atoms) with equivalent atoms receiving the same numbers. Finally, the labelled structure is "serialized" and the output is a character string. Sound simple? Well, as they say in Germany, the devil hides in the details!

The normalization of the structure involves a series of layers for the raw chemical substance, the molecular formula, and a connectivity layer followed where necessary by a stereochemistry and isotopic layer. The connectivity layer consists of four "sub layers," with increasing amounts of detail, generated as follows:

1. disconnect all H and meta atoms to create a "skeleton"
2. reconnect fixed hydrogen atoms to reveal tautomers
3. optionally reconnect all mobile hydrogen atoms
4. optionally reconnect all metal atoms

As you would expect this very simple approach came in for some heavy discussion, but "the proof of the pudding is in the eating," as they say. So far, with some very large structural databases being analyzed in this way, no insurmountable problems have arisen. The developers are looking for beta testers so please get in touch through the IUPAC Web site if you are interested!

Antony N. Davies <tony.davies@creonlabcontrol.com> works at Creon Lab Control AG, in Frechen, Germany. He is secretary of the IUPAC Committee on Printed and Electronic Publications and chairman of the Subcommittee on Spectroscopic Data Standards; he is JCAMP-DX external professor at the University of Glamorgan, Wales, United Kingdom.

www.iupac.org/projects/2002/2002-022-1-024.html
www.iupac.org/projects/2000/2000-025-1-800.html

XML-Based IUPAC Standard for Experimental and Critically Evaluated Thermodynamic Property Data Storage and Capture

One of the activities of IUPAC's Committee on Printed and Electronic Publication is a project to develop an XML-based standard for thermodynamic data communications. On 29 January 2004, this project task group—lead by Michael Frenkel (National Institute of Standards and Technology, Boulder, USA)—met at the ESDU International plc, London, U.K.

Of the 10 attendees, about half represented the data-supplying side of the thermodynamic data delivery process (in particular, major journals in the field, data books, and various data compilation documents), while the other half represented the data-receiving side (databases and chemical engineering software applications). The data-supplying side was represented by Prof. Kenneth Marsh (editor in chief of the *Journal of Chemical and Engineering Data*), Dr. J.W. Magee (associate editor of the *Journal of Chemical and Engineering Data*), Dr. A.R.H. Goodwin (editor of the *Journal of Chemical Thermodynamics*), Dr. D. Lide (editor in chief of the *CRC Handbook Chemistry and Physics*), and Dr. R. Craven (coordinator of various data evaluation projects within ESDU). Drs. M. Satyro, N.I. Johns, and M. Schmidt—who are responsible in their respective organizations for the development of major chemical engineering software and database products—represented the data-receiving side.

Task group meeting participants: front, from left: Prof. W.A. Wakeham, Dr. A.R.H. Goodwin, Dr. A.I. Johns; rear, from left: Dr. M. Satyro, Dr. D. Lide, Dr. M. Frenkel, Dr. M. Schmidt, Prof. K.N. Marsh, Dr. J.W. Magee, and Dr. J.H. Dymond.

Dr. Frenkel emphasized the need for an international standard for thermochemical and thermophysical data storage and exchange (Jan-Feb 2004 *CI*, p. 17), and gave a description of ThermoML, an XML-based structure, which was being developed to provide a practical solution to this problem. ThermoML includes essentially all experimentally determined thermodynamic and transport property data—a total of more than 120 properties—for pure compounds, multicomponent mixtures, and chemical reactions. The framework of ThermoML has been published in *J. Chem. Eng. Data*, **48**, 2-11 (2003). It has been validated using the NIST/TRC SOURCE data archival system for 9000 data sets from 7500 publications. The extension of ThermoML for description of various measures of uncertainties and precision of thermodynamic data was also published (see *J. Chem. Eng. Data*, **48**, 1344–1359 [2003]). The next stage, which is in progress, involves incorporation of predicted data, critically evaluated data, and fitting equations.

ThermoML has already been established for global data communication through guided data capture of thermophysical and thermochemical data from papers accepted for publication in scientific journals, or in publications from bodies such as IUPAC, or from measurements in industry. These data can then be read, using the appropriate software, by data-user groups such as industrial chemical engineers or academic researchers.

The *Journal of Chemical and Engineering Data* was the first journal to agree upon ThermoML as the format for the exchange and storage of thermophysical property data. When letters of acceptance are sent to authors, they are invited to submit data files to TRC (Thermodynamics Research Center) at NIST (National Institute for Standards and Technology). The process has been in place for one year, during which time the compliance of authors has risen from 3% to 92%. The data are available to authors at <www.trc.nist.gov>. The *Journal of Chemical Thermodynamics* is the second journal to take advantage of this data archival and electronic dissemination scheme (see *J. Chem. Thermodyn.*, **36** iv [2004]). It is expected that *Fluid Phase Equilibria*, the *International Journal of Thermophysics*, and *Thermochimica Acta* will follow shortly.

Prof. K.N. Marsh said that in order to establish a commonly accepted protocol for meta- and numerical data submission by authors of original publications, there had to be the following:

- an agreed-upon standard format for particular property data
- a mechanism, and an incentive, for data producers

to submit their data
- a body to accept and verify the data
- the means for authors to access their own and other authors' data
- an access for other researchers and engineers to the archived data

Marsh firmly believes that the NIST/TRC scheme met all these objectives and that was why it had been implemented with his journal. The process was described in an editorial (*J. Chem. Eng. Data*, 48, 1 [2003]), and authors were sent a note on electronic data submission if their data were suitable for guided data capture (GDC). Once a manuscript is accepted, the authors are asked to download the GDC software, enter the data, and submit the file to NIST/TRC. The data are then checked, the authors are told of any inconsistencies, and they then have the opportunity to correct the data prior to publication. This has led to an improvement in the quality of the publications.

Dr. M. Satyro said that small and medium-sized companies had no access to experts in thermodynamics, and so used commercial process simulators. The problem with this was that process simulation orientated databases had often been developed piecemeal, and there was an artificial separation of pure component and mixture property data. Furthermore, the data had not been evaluated for uncertainties. As a result, it was impossible to quantify the quality of the simulator results, and simulated flash engine behavior was often poorly documented. Satyro gave some examples of serious differences between simulated results and actual behavior. He asserted that to test the quality of different thermodynamic models, reliable thermodynamic data are necessary, and these data need to be readily available in a form that can be integrated into a user's program. The ultimate aim is to have reliable estimates of the uncertainties in data so that full error propagation can be carried out.

Satyro said that having a standard format for thermophysical property data would greatly simplify the input of verified data, with uncertainty estimates, to simulation packages. This would result in significant savings in process plant costs, by eliminating the need for overdesign on the current scale. He informed attendees that Virtual Material Group has developed a ThermoML file-reader-software populating the database feeding a simulation engine directly from the Web-based ThermoML file-dissemination system supported by the NIST/TRC.

Current and Future Work

The task group members *accepted* the developed framework of the proposed XML-based IUPAC standard and the dictionary developed to describe uncertainties. They also *approved* the proposal that the "ThermoML" namespace be reserved on the IUPAC Web site for the standard being developed within the project (subsequently, this has been implemented, see <www.iupac.org/namespaces/ThermoML/>. Finally, they *agreed* to the following items:
- inclusion of predicted data, critically evaluated data, and coverage of fitting equations in ThermoML
- inclusion of the IUPAC Chemical Identifier (see description of the IUPAC project at <www.iupac.org/projects/2000/2000-025-1-800.html>)
- expansion of ThermoML to include electrolytes and molten salts, with possible extension to polymers
- continued collaboration with authors, editors, and publishers, in particular with participating journals, *J. Chem. Eng. Data* and *J. Chem. Thermodyn.*, extension to include *Fluid Phase Equilib.*, *Thermochim. Acta*, and *Int. J. Thermophys.*, and exploration of links to *J. Phys. Chem. J. Chem. Phys.* and *J. Solution Chem.*
- continued collaboration with user groups, including the chemical process design community

Publications

Members approved the following publication plans:
- ThermoML coverage of predicted and critically-evaluated data and fitting equations
- a description of thermochemical data communication
- a recommendation of ThermoML as the XML-based IUPAC standard for experimental and critically evaluated thermodynamic property data storage and capture

The next task group meeting will take place 17–21 August 2004 during the IUPAC Conference on Chemical Thermodynamics in Beijing, China. A final meeting (venue to be arranged) will be held in December 2004.

For more information, contact the Task Group Chairman Michael Frenkel <frenkel@boulder.nist.gov>.

www.iupac.org/projects/2002/2002-055-3-024.html

Provisional Recommendations

IUPAC Seeks Your Comments

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

Name and Symbol of the Element with Atomic Number 111

A joint IUPAC-IUPAP Working Party has confirmed the discovery of element number 111 by the collaboration of Hofmann et al. from the Gesellschaft für Schwerionenforschung mbH (GSI) in Darmstadt, Germany. In accord with IUPAC procedures, the discoverers have proposed a name and symbol for the element. The Inorganic Chemistry Division Committee now recommends this proposal for acceptance. The proposed name is roentgenium with symbol Rg.

This proposal lies within the long established tradition of naming elements to honor famous scientists. Wilhelm Conrad Roentgen discovered X-rays in 1895.

Comments by 31 October 2004

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www.iupac.org/reports/provisional/abstract04/corish_311004.html

Numbering of Fullerenes

Rules for numbering $(C_{60}\text{-}I_h)$[5,6]fullerene and $(C_{70}\text{-}D_{5h(6)})$[5,6]fullerene were codified in a publication "Nomenclature for the $(C_{60}\text{-}I_h)$[5,6] and $(C_{70}\text{-}D_{5h(6)})$[5,6]fullerenes" published in *Pure and Applied Chemistry*, **74**(4), 629-695, 2002.

The current publication contains recommendations for numbering a wide variety of fullerenes of different sizes, and of various point group symmetries, including low symmetries such as C_s, C_i, and C_1, as well as many fullerenes that have been isolated and structurally well characterized. These recommendations are based on the principles established in the earlier publication, and aim to identify well-defined, and preferably contiguous helical pathway for numbering.

Comments by 31 August 2004

Dr. Warren H. Powell, 1436 Havencrest Court, Columbus, Ohio 43220-3841, USA,
Tel.: +1 614 451 1830, E-mail: wpowell2@juno.com

www.iupac.org/reports/provisional/abstract04/powell_310804.html

Nomenclature of Inorganic Chemistry

Since the publication of IUPAC's *Nomenclature of Inorganic Chemistry—Recommendations 1990* (the "Red Book"), inorganic chemistry has continued to expand and flourish, bringing with it the need to adapt and develop associated nomenclature. A revision of the Red Book was therefore initiated in 1998. This revised Red Book will supersede not only the 1990 Red Book but also, where appropriate, *Nomenclature of Inorganic Chemistry II—Recommendations 2000* (Red Book II). One of the main changes from the old Red Book is the different organization of material, adopted to improve clarity. Overall, the emphasis on additive nomenclature (generalized from the classical nomenclature of coordination compounds) which was already apparent in the 1990 Red Book, is reinforced. Examples are even included of organic compounds, from the borderline between inorganic and organic chemistry, which may be conveniently named using additive nomenclature.

The reader facing the problem of how to name a given compound or species may find help in several ways. A flowchart is provided that will in most cases guide the user to a section or chapter where rules can be found for generating at least one possible name. A more detailed subject index is also provided, as well as an extended guide to possible alternative names of a wide range of simple inorganic compounds.

Comments by 31 August 2004

Prof. Neil G. Connelly, University of Bristol, School of Chemistry, Cantock's Close, Bristol, BS8 1TS, UK,
Tel: +44 117 928 8162, Fax: +44 117 929 0509,
E-mail: neil.connelly@bristol.ac.uk

www.iupac.org/reports/provisional/abstract04/connelly_310804.html

Internet Connection

Providing brief overviews of helpful chemistry resources on the Web

Kids and Science

Kids and Science (KaS) is about helping kids see, understand, and enjoy the science around them in everyday life. It is also about encouraging kids to make things better, even make inventions, because they are kids and they think like kids. Our challenge to kids is "Look around you, at all the things in your normal life, and think about ways to make something better."

The main feature of the KaS Web site is a Virtual Science City that provides kids with a choice of seven themes, presented as subway systems, on which the kids can travel and explore. Everything that kids see and know in their everyday lives can be found in one or more of these subway systems. There are a total of 71 stops along the subway system where kids can get off and look more closely at a particular issue in their lives. In the Forum section, they can start to ask questions, begin discussions with other kids, and also write their own articles about the way they see things happening around them.

KaS also provides kids a place to come together with the Science Village. Here, they can participate in hands-on workshops as young scientists. The Web site has pictures of the Science Village held in Austria in 2003. At these events, real scientists take kids on a journey into science. During these "summer camps," kids can spend a fabulous week conducting experiments, carrying out research, and satisfying their curiosity. Of course the leisure time is packed with a lot of fun and many games, so the kids certainly don't get bored!

KaS was made possible by funding from the European Commission (2003). Now the plans are to make KaS an international project, attracting kids from all over the world. The Web site is now in English and German, but soon more languages will be added. In the Forum section, kids can use whatever language they like. The important thing is for kids to have a place to talk to other kids and to write about things that really matter to them.

A new activity of KaS involves school projects in which kids come up with ideas for a better world, and then work with companies to develop their ideas into a prototype that they can test. Perhaps it is a new sort of sports shoe or a completely new soft drink? Whatever it is, kids can couple their science from school with their amazing energy and creativity. KaS is very happy to have contact with teachers around the world to set up these projects. We provide the platform where the kids can report on their projects. KaS is for all kids, anywhere.

For more information, contact Dick Wife (KaS coordinator) <dickwife@compuserve.com>.

www.kidsandscience.org

Bio-Based Polymers

by Stanislaw Penczek

The **1st IUPAC International Conference on Bio-based Polymers** (ICBP 2003) took place from 12–14 November 2003 at the Suzuki Umetaro Hall at the RIKEN Institute in Saitama (actually, within the Tokyo area). The conference was attended by 226 participants, with about two-thirds from Japan and one-third from 24 different other countries. The scientific program featured 47 main lectures and 90 posters. The conference was chaired by Prof. Yoshiharu Doi, director of the Polymer Institute, and Prof. Tadahisa Iwata, both from The Institute of Physical and Chemical Research (RIKEN Institute). It was sponsored by Japan Science and Technology Agency and the Biodegradable Plastics Society.

The conference was organized around the following major themes:

- bio-based polymers synthesis
- biodegradable polymers
- commercial products of bio-based polymers
- microbial poly(hydroxyalkanoates)
- poly(amino acid)s
- polyesters, composites, and monomer synthesis

The following lecture titles provide a sense of how these themes were addressed during the conference:

1. "Unspecific Polymerases for Biosynthesis of Novel Biopolymers," A. Steinbüchel (University of Münster, Germany)
2. "Structure Analysis of P(3HB) Films and Fibers by Synchrotron Radiation," T. Iwata (RIKEN Institute, Japan)
3. "Mater-Bi products: Present Status and Future Perspectives," C. Bastioli (Novamont, Italy)
4. "Fibrous Protein Assembly and Cellular Interactions," D.L. Kaplan (Tufts University, USA)
5. "Fermentation Production of Chemicals that Can be Used for the Polymer Synthesis," S. Y. Lee (KAIST, Korea)
6. "Lactic Acid-Based Polymers via Copolymerization and Chemical Modification," M. Vert (University of Montpellier, France)
7. "A Comparative Overview of LCA Studies for Bio-Based Polymers," M. Patel (Utrecht University, Netherlands)
8. "Industrial Biodegradable Plastics as Bio-Based Materials in Japan," K. Ohshima (BPS, Japan)

Numerous and vivid discussions after the lectures and during the intermissions clearly indicated the importance of this field and its future trends. It is thought that in the not-too-distant future, bio-based polymers will be an important alternative to petroleum-based polymers. Several new achievements were very well documented, indicating that particularly polyesters based on the microbial poly(hydroxyalkanoates) and polymers of lactic acid are quickly becoming more common as industrial polymers. The expected commercial impact of bio-based polymers is also related to the biodegradability of macromolecules derived from natural products.

The meeting also encompassed a large number of high-level research papers, describing synthetic and mechanical features of biosynthesis of poly(hydroxyalkanoates) (A. Steinbüchel, Germany; T. Iwata, Japan), novel lactic acid polymers and copolymers (M. Vert, France), to cite just a few of the over 20 in this particular area of research. Biomedical application and biological functions of some polypeptides and proteins were discussed by L. Kaplan (USA). The bio-based polymers are the most natural candidates for medical applications, since the studies till now have shown their perfect biocompatibility.

The meeting was held in the RIKEN institute, which is surrounded by a beautiful landscape. Accompanying persons enjoyed seeing the sights of Tokyo, including the Kabuki theatre, one of the most impressive in the world.

Highlights from the conference have been published recently as a special issue of *Macromolecular Bioscience* (Vol. 4, No. 3, pp. 133–367, March 2004)

Stanislaw Penczek <spenczek@bilbo.cbmm.lodz.pl> is a professor at the Centre of Molecular and Macromolecular Studies of the Polish Academy of Sciences in Łódz, Poland. He has been a member of the IUPAC Macromolecular Division since 1994.

www3.interscience.wiley.com/cgi-bin/jissue/107632675

Advanced Materials

by Michael Hess

POLYCHAR 12, World Forum on Advanced Materials, was held 6–9 January 2004 at the Univerity of Minho in Guimarães, Portugal. This conference was the first of the 12 in the series to be held somewhere other than its "place of birth," the University of North Texas in Denton, Texas, USA. After Portugal, the World Forum will now start its way around the world.

The conference was organized by Antonio M. Cunha, Joao F. Mano, and Júlio C. Viana, all of whom are at the Department of Polymer Engineering at the University of Minho. Besides the location and the weather, the conference appeared not much different than other years. The conference program was divided into the following sessions:

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

All sessions consisted of oral presentations and posters. There were 2 plenary lectures and 16 invited speakers. There was a total of about 51 lectures and more than 80 poster contributions. The 100 participants and 28 students came from 28 different countries—from the United Kingdom to the Fiji Islands and from Venezuela to South Korea, literally from all parts of the world.

It is impossible to mention all the important contributions, but most of them will be published in e-polymers <www.e-polymers.org>. Following are a few highlighted lectures that are representative of the quality of material presented at the conference:

- Christine Ortiz, MIT, Cambridge, USA, "Ultrastructure and Nanomechanics of Biological Tissues"
- Moonhor Ree, Pohang University of Science and Technology, South Korea, "Synchrotron X-Ray Scattering Studies on Nanoporous Organosilicate Thin Films Revealing Ultralow Dielectrical Constant"
- Witold Brostow, University of North Texas, Denton, USA, "Multiscratching as a Measure of Polymer Wear and Effects of Irradiation on Wear"
- Graham Williams, University of Wales, Swansea, UK, "Dielectric Spectroscopy and Molecular Dynamics of Polymeric Materials"
- B. W. R. Chowdari, National University of Singapore, "Polymer Electrolytes for Lithium Ion Batteries"
- Arnon Siegmann, Technion, Haifa, Israel, "Hybrid Carbon Black and Carbon Fiber Polymer Composites: Effect of Structure on Electrical Behaviour"
- Ram Prakash Singh, Indian Institute of Technology, Kharagpur, India, "Novel Applications of Drag Reducing Polymers in Agriculture"
- Timothy Lodge, University of Minnesota, Minneapolis, USA "Characterization of Intra- and Intermicellar Structure in Block Copolymer Solutions"
- Karel Dusek, Academy of Sciences of the Czech Republic, Praha, Czech Republic, "Recent Developments in Polymer Networks and Gels"
- Dusan Berek, Polymer Institute of the Slovak Academy of Sciences, Bratislava, Slovakia, "Enthalpic Partition Assisted Size Exclusion Chromatography"

This year's Paul Flory Polymer Research Prize was shared by Timothy P. Lodge, University of Minnesota, and Karel Dusek, Academy of Sciences of the Czech Republic. There were also two winners of the Bruce-Hartmann Award for Young Scientists: Allison Saiter, University of Rouen, France, and Alexander Bismarck, Imperial College, London, UK. The Carl Klason Award for the best student was shared this year between Julien Ibarretxe Urigen, Catholic University of Leuven, Heverlee, Belgium, and Dimitre Tchalamov, University of Minho, Guimarães, Portugal. The Second Prize for a student presentation was partitioned among Michaela Avedanei, Petru Poni Institute of Macromolecular Chemistry, Iasi, Romania; Ljerka Kratofil, University of Zagreb, Zagreb, Croatia; and Youngseok Song, Seoul National University, Seoul, South Korea.

Guimarães, Portugal, at night.

Finally, it can be stated that POLYCHAR 12 was

another very fruitful meeting for all participants, in particular the young scientists and the students who found a world forum to present and discuss their results, meet scientists from other countries, exchange experiences, and socialize with scientists from all fields of polymer science. Many of these contacts have led to new cooperations and exchanges among students and young and senior scientists.

Two winners of the Karl Klason Best Student Presentation Award: Julien Ibarretxe Urigen (left) and Michaela Avedanei.

The short course, which was held the day before the conference, consisted of the following sections:

- "Microscopic Techniques," S. Henning, Halle, Germany
- "X-ray Diffraction Techniques," Denchev, Guimarães, Portugal
- "Spectroscopic Techniques," Hess, Duisburg, Germany
- "Mechanical Characterization," Mano, Guimarães
- "Tribology and Volumetric Properties," Brostow, Denton, Texas, USA
- "Thermal Analysis, Gomez-Ribelles," Valencia, Spain
- "Dielectrical Relaxation," Williams, Swansea, UK
- "Transient and Quasi-Transient Dielectric Techniques," Vassilikou-Dova, Athens, Greece

Moving the conference to a different location after 12 years in Texas has made it easier for many people from other parts of the world to attend. Although it had become a tradition to hold the conference in Texas, our Portuguese friends at the University of Minho have impressively shown that hospitality, friendship, and cooperation among scientists is a world-wide phenomenon.

POLYCHAR 13 is planned for 3–8 July 2005 in Singapore; POLYCHAR 14 for April 2006 in Nara, Japan; POLYCHAR 15 for January 2007 in Rio De Janeiro; and POLYCHAR 16 for January 2008 in Vigyan Bgavan-New Delhi.

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Where 2B&Y

Announcements of conferences, symposia, workshops, meetings, and other upcoming activities.

Biological Polyesters

22–28 August 2004, Beijing, China

China is now the second largest oil consuming country in the world. Sustainable development based on renewable resources is now the only realistic choice for China, but also for the rest of the world. Increasingly, renewable resources are attracting the attention of researchers and governments around the world. The growing field of biological polyesters is showing great promise in developing renewable materials that are not made from petroleum. In recent years, companies have invested heavily in this type of research and there is now a good deal of accumulated knowledge about the production and marketing of biological materials.

The **International Symposium on Biological Polyesters**, to be held 22–28 August 2004 in Beijing, China, will send a strong message to governments and societies around the world: biological polyesters could have a major positive impact on the environment and stimulate a bio-industrial revolution in materials science. Participants of ISBP2004 can and will contribute to the understanding of this interesting material. They can also contribute to the "Green Olympics and High-Tech Olympics" concept of the 2008 Beijing Summer Olympic Games.

See calendar on page 36 for contact information

http://microbes.biosci.tsinghua.edu.cn/ISBP/

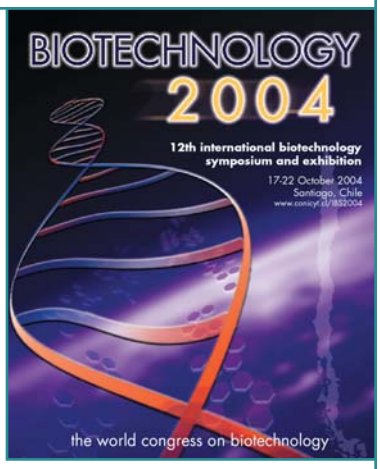
Biotechnology

17–22 October 2004, Santiago, Chile

The 12th International Biotechnology Symposium will be held 17–22 October 2004 in Santiago, Chile. This well-known event is held every four years on a different continent. It is the main international meeting in the rapidly expanding field of biotechnology. This will be the first time this conference will be held in Latin America.

The scientific program of the 12th IBS will include many of the newer areas in the field. In keeping with previous symposia, the program is arranged in a number of sections, with all presented papers being by invitation. Each section is chaired by two or three internationally recognized leaders in the field. In addition, key international figures have been invited to give eight plenary lectures. Finally, a very large number of posters will be available, representing the latest scientific activities throughout the world.

The symposium will be held in the heart of Santiago at the Casapiedra Convention Center. This is a custom-designed location that allows for the concurrent sessions, trade show, and poster area to be in the same building.



See calendar on page 36 for contact information

www.conicyt.cl/IBS2004

Liquid Chromatography/Mass Spectrometry

10–12 November 2004, Montreux, Switzerland

The International Association of Environmental Analytical Chemistry will hold the **21st Annual Meeting on Liquid Chromatography/Mass Spectrometry (LC/MS)** in Montreux, Switzerland, 10–12 November 2004. A short course will be held 8–9 November. Following the continuous growth in LC/MS, nearly 700 scientists are expected, including research and development managers, technicians and LC/MS operators, and company representatives, particularly vendors from the mass spectrometry and separation science area.

The Montreux LC/MS conference is the world's premier conference on LC/MS and all related hyphenated technologies including important aspects of sample pretreatment, separation technologies, and novel software/bioinformatics approaches. Novel instrumentation will be a key focus of the meeting. New developments in the field will allow for maximum

interaction between the participants. Introductory courses will stimulate newcomers to enter the exciting world of LC/MS.

Important trends like miniaturization and automation will be included in the program, as will highlights from strategic industrial developments impacting on the LC/MS field (for example, within the pharmaceutical industry). Novel approaches in drug discovery and development will be discussed, such as proteomics, metabolomics, systems biology, target and biomarker discovery, novel bioanalytical methodology, and impurity screening. In addition, developments in agriculture, chemical biotech, and environmental areas will be well covered.

www.iaeac.ch/lcms-montreux.htm

Chemistry for Agriculture

30 November–3 December 2004, Jesenik, Czech Republic

The **30th International Conference on Chemistry for Agriculture** will present scientific research achievements obtained in various interdisciplinary projects, from pollution control in agriculture and chemical industry to agriculture practices. The conference, which will be held 30 November–3 December in Jesenik, Czech Republic, is a unique forum in which new concepts of technological innovations evolve.

The conference sessions will focus on the following themes:

- chemical technology—mineral fertilizers, feed phosphates and other additives
- agricultural chemistry—fertilizer nutrient's changes in the soil, nutrient availability
- phosphorus and nitrogen problem in the environment
- ecotoxicology—selected problems
- new production technologies of chemical agents for agriculture
- new methods of chemical products application in agriculture
- impact of chemical products on plant and animal production
- harmful substances in agriculture and the environment

The meeting will also provide a chance to look into research programs and projects that focus on the use of chemicals in accordance with European directives: nitrate and urban waste directives, the Code of the Best Agricultural Practices, and the Best Available Technology in the fertilizer industry.

www.conference.republika.pl/introduction.htm

Young Chemists

25–29 August 2004, Torino, Italy

A central aim of the **2004 Younger European Chemist's Conference** is to bring together younger European chemical researchers for novel networking and interaction. The conference, which will be held 25–29 August 2004, in Torino, Italy, is intended for chemists who are around 21 to 35.

The event will bridge European research, discovery, and invention across the entire spectrum of the chemical sciences—from fundamental, molecular-level chemistry to large-scale chemical processing technology. The conference program will also delve into biology, nanotechnology, materials science, medicine, and more. Full details of the program can be found on the Web site below.

This event is unique because it allows early-stage researchers a non-threatening and informal opportunity to present a poster and give a short talk at an international conference. Participants also compete for the prestigious 2004 Europa Medal and 1,000 Prize and the Runner-Up Awards.

The keynote speakers will be Nobel Laureate Richard R. Ernst and IUPAC President Leiv K. Sydnes.

www.setforeurope.org

Mark Your Calendar

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

2004

4–9 July 2004 • Phosphorus Chemistry • Birmingham, United Kingdom
16th International Conference on Phosphorus Chemistry (ICPC 16)
Prof. Pascal Metivier, Rhodia, R&D for Phosphorous and Performance Derivatives, Oak House, reeds Crescent, Watford, WD24 4QP, UK, Tel.: +44 1923 485609, E-mail: pascal.metivier@eu.rhodia.com

4–9 July 2004 • Macromolecules • Paris, France
40th International Symposium on Macromolecules—IUPAC World Polymer Congress (MACRO 2004)
Prof. Jean-Pierre Vairon, Université Pierre et Marie Curie, Laboratoire de Chimie des Polymères, Case 185, 4 Place Jussieu, F-75252 Paris Cédex 05, France, Tel: +33 1 44 27 50 45, Fax: +33 1 44 27 70 89, E-mail: macro04@ccr.jussieu.fr

11–15 July 2004 • Polymer Biomaterials • Prague, Czech Republic
43rd PMM Microsymposium: Polymer Biomaterials: Biomimetic and Bioanalogous Systems
Drahomir Vyprachticky, Institute of Macromolecular Chemistry, Heyrovskeho nam. 2, CZ-162 06 Praha 6, Czech Republic, Tel.: +420 296 809 332, Fax: +420 296 809 410, E-mail: sympo@imc.cas.cz

17–22 July 2004 • Photochemistry • Granada, Spain
20th IUPAC Symposium on Photochemistry
Prof. Dr. Miguel A. Miranda, Departamento de Química/Instituto de Tecnologia Química UPV-CSIC, Universidad Politecnica de Valencia, Avenida de los Naranjos, s/n, E-46022 Valencia, Spain, Tel: + 34 963877807, Fax: + 34 963877809, E-mail: mmiranda@qim.upv.es

18–21 July 2004 • Chemical Sciences in Changing Times • Belgrade, Serbia and Montenegro
4th International Conference of the Chemical Societies of the South-Eastern European Countries
Prof. Ivanka Popovic, Belgrade University, Faculty of Technology and Metallurgy, Karnegijeva 4, 11000 Belgrade, Serbia and Montenegro, Tel.: +381 11 337 0478, Fax: +381 11 337 0473, E-mail: icosecs@elab.tmf.bg.ac.yu

18–23 July 2004 • Coordination Chemistry • Merida, Yucatan, Mexico
36th International Conference on Coordination Chemistry
Prof. Norah Barba-Behrens, Dept. de Química Inorgánica, Universidad Nacional Autónoma de México, Ciudad Universitaria, Coyoacán, México, D. F., 04510, México, Tel./Fax: +52(55)5622-3810, E-mail: norah@servidor.unam.mx

18–23 July 2004 • Polymers and Organic Chemistry • Prague, Czech Republic
11th International Conference on Polymers and Organic Chemistry 2004 (POC '04)
Dr. Karel Jerabek, Institute of Chemical Process Fundamentals, Rozvojova 135, 165 02 Prague 6, Czech Republic, Tel.: +420 220 390 332, Fax: + 420 220 920 661, E-mail: kjer@icpf.cas.cz

23–27 July 2004 • Carbohydrates • Glasgow, United Kingdom
22nd International Carbohydrate Symposium
Prof. E. Hounsell, School of Biological and Chemical Sciences, Birkbeck University of London, Malet St., London WC1E7HX, UK, Tel.: + 44 207 631 6238, E-mail: e.hounsell@bbk.ac.uk

25–29 July 2004 • Solubility Phenomena • Aveiro, Portugal
11th International Symposium on Solubility Phenomena, Including Related Equilibrium Processes (11th ISSP)
Prof. Clara Magalhaes, Department of Chemistry, University of Aveiro, P-3810-193 Aveiro, Portugal, Tel.: +351 234 401518, Fax: +351 234 370084, E-mail: issp@dq.ua.pt

25–30 July 2004 • Organometallic Chemistry • Vancouver, Canada
21st International Conference on Organometallic Chemistry (ICOMC)
21st ICOMC Secretariat, Conferences & Accomodation at UBC, 5961 Student Union Boulevard, Vancouver, BC, Canada V6T 2C9, Tel.: +1 604 822-1050, Fax: +1 604 822-1069, E-mail: registration@housing.ubc.ca

1–6 August 2004 • Organic Synthesis • Nagoya, Japan
15th International Conference on Organic Synthesis (ICOS-15) (see poster on inside back cover)
Prof. Minoru Isobe, ICOS15 Secretariat, c/o International Communications Specialists, Inc., Sabo Kaikan-bekkan, 2-7-4 Hirakawa-cho, Chiyoda-ku, Tokyo 102-8646 Japan, Tel: +81 3 3263 6474, Fax: +81 3 3263 7537, E-mail: icos@ics-inc.co.jp

2–7 August 2004 • Chemistry in Africa • Arusha, Tanzania
9th International Chemistry Conference in Africa—Chemistry Towards Disease and Poverty Eradication
Dr. G. S. Mhinzi, University of Dar es Salaam, Chemistry Department, PO Box 35061, Dar es Salaam, Tanzania, Tel./Fax: +255 22 2410038, E-mail: mhinzi@chem.udsm.ac.tz

Mark Your Calendar

3–8 August 2004 • Chemical Education • Istanbul, Turkey
18th International Conference on Chemical Education (18th ICCE)
Prof. Dr. Mustafa L. Berkem, Chairman, Marmara University, Ataturk Faculty of Education, TR- 81040 Goztepe-Istanbul, Turkey, Tel: +90 2163459090/231, Fax: +90 2163388060, E-mail: icce2004@marmara.edu.tr

15–19 August 2004 • Polymers • Bethesda, Maryland, USA
Polymer Networks 2004
Dr. F. Horkay, Section on Tissue Biophysics and Biomimetics, National Institutes of Health, Bldg. 13, Room 3W16E, 13 South Drive, Bethesda, MD 20892, USA, Tel: +1 301 435 7229, Fax: +1 301 435 5035, E-mail: horkay@helix.nih.gov

15–20 August 2004 • Physical Organic Chemistry • Shanghai, China
17th IUPAC Conference on Physical Organic Chemistry (ICPOC-17)
Prof. Guo-Zhen Ji, Shanghai Institute of Organic Chemistry, Chinese Academy of Sciences, 354 Fenglin Road, Shanghai 200032, China, Tel: +86 21-64163300, Fax: +86 21-64166128, E-mail: jigz@pub.sioc.ac.cn

17–21 August 2004 • Chemical Thermodynamics • Beijing, China
18th IUPAC Conference on Chemical Thermodynamics
Prof. Haike Yan, Chairman, 18th ICCT c/o Chinese Chemical Society, PO Box 2709, Beijing, 100080, China, Tel.: +86 10 62568157, +86 10 62564020, Fax: +86 10 62568157, E-mail: qiuxb@infoc3.icas.ac.cn

20–25 August 2004 • Heteroatom Chemistry • Shanghai, China
7th International Conference on Heteroatom Chemistry (ICHAC-7)
Prof. Lin-xin Dai, ICHAC-7, c/o Shanghai Institute of Organic Chemistry, Chinese Academy of Sciences, 354 Fenglin Road, Shanghai 200032, China, Tel: +86 21 64163300- 3405, Fax: +86 21 64166128, E-mail: ICHAC@pub.sioc.ac.cn

22–28 August 2004 • Biological Polyesters • Beijing, China
International Symposium on Biological Polyesters (ISBP 2004)
Prof. George Guo-Qiang Chen, Department of Biological Sciences & Biotechnology, Tsinghua University, 100084 Beijing, China, Tel.: +86 10 62794217, Fax: +86 10 62794217, E-mail: chengq@mail.tsinghua.edu.cn

3–5 September 2004 • Chemistry of Vanadium • Szeged, Hungary
4th International Symposium on Chemistry and Biological Chemistry of Vanadium
Prof. Tamas Kiss, University of Szeged, Department of Inorganic and Analytical Chemistry, PO Box 440, H-6701 Szeged, Hungary, Tel.: +36 62 544337, Fax: +36 62 420505, E-mail: tkiss@chem.u-szeged.hu

5–10 September 2004 • Analytical Chemistry • Salamanca, Spain
European Conference on Analytical Chemistry—Euroanalysis XIII
Prof. J. Hernández Méndez, Departamento de Química Analítica Nutrición y Bromatología, Universidad de Salamanca, E-37008 Salamanca, Spain, Tel./Fax: +34 923 294483, E-mail: jhm@usal.es

12–15 September 2004 • Heterocyclic Chemistry • Sopron, Hungary
XXI European Colloquium on Heterocyclic Chemistry
Prof. György Hajos, Chemical Research Center, Institute of Chemistry, H-1025 Budapest Pusztaszeri ut, Hungary, Tel.: +36 1 3257550, Fax: +36 1 3257863, E-mail: ghajos@chemres.hu

20–23 September 2004 • Soil Science • Wuhan, China
Environmental Significance of Mineral-Organic Component-Microorganism Interactions in Terrestrial Systems
Dr. P. M. Huang, Department of Soil Science, University of Saskatchewan, 51 Campus Drive, Saskatoon SK S7N 5A8 Canada, Tel.: +1 306 966 6838, Fax: +1 306 966 6881, E-mail: huangp@sask.usask.ca

7–8 October 2004 • Trace Elements in Food • Brussels, Belgium
2nd International Symposium on Trace Elements in Food (TEF 2)
Dr. Michael Bickel, European Commission—Joint Research Centre, Institute for Reference Materials and Measurements, B-2440 Geel, Belgium, Tel.: +32 14 57 17 34, Fax: +32 14 57 17 87, E-mail: michael.bickel@cec.eu.int

17–22 October 2004 • Biotechnology • Santiago, Chile
12th International Biotechnology Symposium
Prof. Juan A. Asenjo, Centre for Biochemical Engineering and Biotechnology, University of Chile, Beauchef 861, Santiago, Chile, Tel.: +56 2 6784288, Fax: +56 2 6991084, E-mail: IBS2004@conicyt.cl

18–22 October 2004 • Chemical Engineering • Havana, Cuba
Vth International Congress on Chemistry and Chemical Engineering
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 7 336 471, E-mail: alberto@cgf.co.cu

Mark Your Calendar

30 November–3 December 2004 • Agriculture • Jesenik, Czech Republic
Chemistry for Agriculture
Dr. Adam Pawelczyk, Wroclaw University of Technology, Smoluchowskiego 25, 50-370 Wroclaw, Poland, Tel.: +48 (0) 71-3202930, Fax: +48 (0) 71 3203469, E-mail: adam.pawelczyk@pwr.wroc.pl

6–8 December 2004 • Fats, Oils, and Oilseeds Analysis and Production • Tunis, Tunisia
IUPAC-AOCS Workshop
<www.aocs.org/meetings/>

2005

14–17 February 2005 • Crop Protection Chemistry in Latin America • San Jose, Costa Rica
International Workshop on Crop Protection Chemistry in Latin America: Harmonized Approaches for Environmental Assessment and Regulation
<www.iupac.org/symposia/2005/crop-protection-chemistry/index.html>

27 February–2 March 2005 • Heterocyclic Chemistry • Gainesville, Florida, USA
6th Florida Heterocyclic Conference
Prof. Alan R. Katritzky, University of Florida, Dept. of Chemistry, Gainesville, FL 32611-7200, USA, Tel.: +1 352 392 0554, Fax: +1 352 392 9199, E-mail: katritzky@chem.ufl.edu

17–21 July 2005 • Organometallic Chemistry • Geneva, Switzerland
13th International Symposium on Organometallic Chemistry Directed Towards Organic Synthesis (OMCOS-13),
Prof. E. Peter Kündig, Department of Organic Chemistry, University of Geneva, 30 Quai Ernest Ansermet, CH 1211 Geneva 4, Switzerland, Tel.: +41 22 379 6526, Fax: +41 22 328 7396, E-mail: Peter.Kundig@chiorg.unige.ch

17–22 July 2005 • Carotenoids • Edinburgh, Scotland
14th International Symposium on Carotenoids
Prof. Andrew J. Young, School of Biological and Earth Sciences, John Moores University, Byrom St. Liverpool L3 3AF, UK, Tel.: +44 151 231 2173 / 3575, Fax: + 44 151 207 3224, E-mail: a.j.young@livjm.ac.uk

13–21 August 2005 • IUPAC 43rd General Assembly • Beijing, China
IUPAC Secretariat, Tel.: +1 919 485 8700, Fax: +1 919 485 8706, E-mail: secretariat@iupac.org

14–19 August 2005 • IUPAC 40th Congress—Innovation in Chemistry • Beijing, China
Prof. Xibai Qiu, IUPAC-2005 Secretariat, c/o Chinese Chemical Society, PO Box 2709, Beijing 100080, China, Tel.: +86 (10) 62568157, Fax: +86 (10) 62568157, E-mail: qiuxb@iccas.ac.cn

11–15 September 2005 • Boron Chemistry • Sendai, Japan
12th International Meeting on Boron Chemistry
Prof. Yoshinori Yamamoto, Department of Chemistry, Graduate School of Science, Tohoku University, Sendai, Japan 980-8578, Tel.: +81 22 217 6581, Fax: +81 22 217 6784, E-mail: yoshi@yamamoto1.chem.tohoku.ac.jp

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