# Contents

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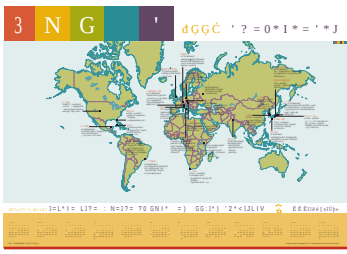

*A complementary map/2006 calendar is enclosed with this issue.*

# IUPAC—An Optimistic Future

*by Bryan R. Henry*

**As I begin my term as President of IUPAC, I would like to share with you a few personal reflections on some aspects of our 2005 General Assembly (GA), and on the corresponding ICSU (International Council for Science) General Assembly held two months later in October.**

I am very optimistic about the prospects for IUPAC. We have both the abilities and resources to serve the international chemistry community, and to use chemistry to contribute to solutions for the many problems facing our planet. We can and should help the world to meet the Millennium Development Goals.*

Our principal strengths lie in the talent, knowledge, and commitment of the more than 1000 scientists worldwide who are involved in the IUPAC project system. The reports and presentations at the GA of the division presidents and standing committee chairs were both impressive and inspirational, as they detailed their accomplishments over the last two years. My *Vice President's Critical Assessment* provides an overview of the project system as we near the conclusion of the second biennium of its full operation. In summary, the project system is a success. In financial terms alone there has been a 65 percent increase in project commitments from the transition years of 2000–2001 to the first years of the project mode. The financial state of the Union is strong with no significant problems on the horizon. This is particularly true when we compare ourselves with other Unions.

*We can and should help the world to meet the Millennium Development Goals.*

As was the case in 2001, the most controversial topic at our GA in August was the proposal to eliminate the Bureau in an attempt to streamline IUPAC governance. The vote to proceed with that process failed by a substantial margin, primarily because of the perception that it would lead to less direct influence by division presidents and standing committee chairs. However, many delegates expressed the view that we should be investigating further efficiencies in governance. I made the commitment that one of my first acts as IUPAC president would be to set up two small committees. The first, chaired by the secretary general, would examine revisions to our statutes and bylaws. The second, that I will chair, will attempt to find more efficient ways to govern IUPAC within its current structure. Hopefully by the time you read this article both committees will have begun their work.

*. . . the IUPAC Executive believes that we need to work more closely with ICSU.*

Past President Piet Steyn and I represented IUPAC at the ICSU General Assembly in October. ICSU was founded in 1931 and is a nongovernmental organization with a membership that includes over 100 countries, about 30 scientific unions, and about 25 scientific associates. (For an overview of the International Council for Science, see Nov.-Dec. 2004 *CI*, p. 4.) Its stated mission is to strengthen international science for the benefit of society, and it deals directly with national governments and international organizations, several of which are associated with the

*For details on the eight UN Millennium Development Goals, see <www.un.org/millenniumgoals/>.

## The United Nations Millennium Development Goals

Goal 1: Eradicate extreme poverty and hunger

Goal 2: Achieve universal primary education

Goal 3: Promote gender equality and empower women

Goal 4: Reduce child mortality

Goal 5: Improve maternal health

Goal 6: Combat HIV/AIDS, malaria, and other diseases

Goal 7: Ensure environmental sustainability

Goal 8: Develop a global partnership for development

United Nations. Highlights of its Assembly included final plans for the establishment of the International Polar Year (2007–2008), a report on the Millennium Ecosystem Assessment, a review of Science and its Interactions with Society, and a discussion of the newly accepted ICSU Strategic Plan (see also IUPAC Wire, p. 21).

One interesting recent development is the plan to establish four ICSU regional offices. The African office was opened last September in Pretoria, South Africa, an office for Asia and the Pacific is currently being set up in Kuala Lumpur, and offices are being planned for Latin America and the Caribbean, and the Arab world.

In my view almost all of the scientific programs of ICSU involve chemistry, yet IUPAC has not been fully involved over the last few years. Increasingly many of our own programs have a worldwide outreach. If we are to maximize our global opportunities, the IUPAC Executive believes that we need to work more closely with ICSU. As a first step, we became involved with the ICSU strategic planning process by providing input to many of their planning documents.

ICSU functions through a Secretariat in Paris that serves an Executive Board. The latter oversees the operations of ICSU, and is made up of seven officers and eight additional members, four each elected as representatives of the Scientific Unions and the National Members. At their General Assembly, I was elected as a Scientific Union member of the ICSU Executive for the next three years. I am hopeful that an IUPAC officer as a member of the ICSU Executive will provide an exciting opportunity to enhance the global aspects of IUPAC's programs.

I very much look forward to the privilege of serving as your president over the coming two years, and hope that together we can truly make the world a better place through chemistry.

**Bryan Henry <chmhenry@uoguelph.ca> starts his IUPAC presidency this January 2006. He is a professor of chemistry in the Department of Chemistry and Biochemistry at the University of Guelph, Canada. He has been a member of the Canadian National Committee for IUPAC since 1995, and served as chair from 1998–2003.**

## 2006–2007 Bureau

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Committee on Chemistry and Industry

# "Inner Chemical Life" of Solids

*by Joachim Maier*

**A quick glance at our environment is enough for us to realize the significance of the solid state in our daily life. Solids are advantageous over other forms of matter mainly because of their rigidity: durable structuring is inconceivable without solid matter which is characterized by low diffusion coefficients, at least for one component. Nonetheless, other components may exhibit perceptible or even fast diffusion without letting the solid lose its structural stability. Such a mobility is not only important to enable electrochemical performances, it is also a prerequisite for solid-state reactions to occur. In materials in which all atomic constituents are immobile, the electrons still can be fairly mobile, which means that electronic transport can be tuned reversibly. Solids exhibiting both ionic and electronic mobility are important for specific applications as well. Hence, apart from mere mechanical functionality, solids offer the possibility of subtly and reproducibly tailoring chemical and electrochemical functionalities.**

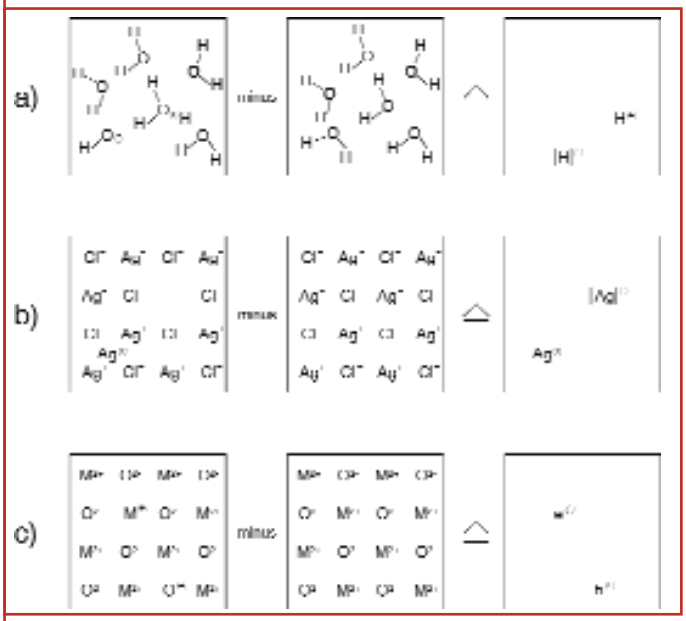



*Figure 1: a) As the compositionally unperturbed structure (chemical ground structure) is subtracted from the real structure, the point defects shown on the right remain. Naturally each is surrounded by a distorted region (effective radius of the point defect) which affects at least the immediate neighborhood. In the case of fluid phases (see above) this procedure can only be regarded as an instantaneous picture. (Owing to the absence of defined sites no distinction is made between various types of defect reactions as is done in the solid state.) b) Frenkel disorder is sketched in the second row. c) The third row shows the case of purely electronic disorder whereby localized charge carriers are assumed for the sake of clarity.* Reprinted with permission from reference 1.

Reactions involving solids are used extensively in laboratory research. Despite this fact, the chemists' relationship to solids resembles that of a stepmother with regard to an unloved child, and is often more characterized by tolerance than by understanding. The chemists learned to prepare solid compounds of great complexity and to understand in detail perfect structure and bonding. However, this conception of the solid state is static and superficial, and does not hold the key for the tailoring of properties. Nor does it enable the understanding of kinetic processes in solid-state materials. Solids are still considered to be more "dead than alive"; they are, within the range of their stability, considered as chemically invariant entities. Only the surface is recognized as a site of chemical reactivity. The conception that solids have an "inner chemical life," which makes it possible for us to tune their properties like we do with liquids, still sounds adventurous to most chemists. On the other hand, many materials scientists, ceramicists, and even physicists appreciate the chemical tunability of solids more than chemists.

A comparison between the liquid and solid phases of water (figure 1) makes it immediately clear what is lacking in the naive chemical description of the solid state. As regards water, chemists are not so much interested in the bulk structure (in fact studying the detailed structure of water was largely the subject of physics), rather they are focusing on the deviations from the ideal water structure, namely the chemical excitations $H_3O^+$ and $OH^-$. These species are, indeed, the acid-base active particles of relevance, and together with the dissolved species they determine the inherent acid-base and redox-chemistry. In addition, they are the relevant centers to be considered with respect to mass transport and electrical conductance. On the other hand, concerning the solid state (e.g., an ionic crystal such as AgCl), the historical situation is diametrically different. Consideration of the perfect solid-state structure was and still is the domain of chemistry while the genuine chemical issues such as mass transport, ion conduction, and the kinetics of compositional change are almost unaccounted for in the realm of chemistry. It is exactly this issue that prevents the solid state from being included in the familiar concept of chemical kinetics.

This article emphasizes that it is the field of *defect chemistry in solids, which represents the missing link in the conception.*[1] Defect chemistry not only provides the pertinent fundamental insight, it also enables optimization of solids with regard to technological applications. It should become implicitly clear that the physico-chemical consideration of the "mixed conductor," which exhibits ionic and electronic mobility, allows generalization of semiconductor physics, solid-state ionics and electrochemistry.

The key to the "opening" of the solid, which in fact was provided as early as the 1930s by Frenkel and in particular by the physicist Schottky and the chemist Wagner,[2] is the identification of the relevant centers in solids which are analogous to $H_3O^+$ and $OH^-$ in water. These are the so-called point defects. This is easy to demonstrate. Just remove from the dissociation equation

$$H_2O + H_2O \rightleftharpoons H_3O^+ + OH^-, \qquad (1)$$

or more concisely from

$$H_2O \rightleftharpoons H^+ + OH^-, \qquad (2)$$

an additional water molecule, as it is displayed in figure 1, then obviously we are left with two defects, viz. the excess proton $H^+$ and the proton vacancy $|H|^-$

$$Nil \rightleftharpoons H^+ + |H|^- \qquad (3)$$

The same procedure is possible with an ionic crystal such as AgCl. As above, it is entropy not energy that favors a disorder, as shown in figure 2. To a certain extent, excess $Ag^+$ ions (interstitial ions) are formed at the expense of ($Ag^+$) vacancies:

This $Ag^+$ transfer may also be written as

$$AgCl + AgCl \rightleftharpoons Ag_2Cl^+ + GCl^- \qquad (4)$$

(Owing to the rigidity of the lattice we have—in contrast to reaction (1)—to consider the vacancy (G) explicitly.)

Most concisely (subtraction of two AgCl) it reads

$$Nil \rightleftharpoons Ag^\bullet + |Ag|' \qquad (5)$$

This is not a mere formalism, in fact the perfect AgCl crystal, even though AgCl is dissociated into $Ag^+$ and $Cl^-$, is not dissociated in terms of being split into free particles. In the perfect state, the $Ag^+$ and $Cl^-$ ions are strongly bound and can only vibrate around the lattice positions. In this sense equation (5) describes the "superionic" dissociation. Only this thermal disorder (together with dopants and neighboring phase effects) leads to mobile particles. In addition, the particles $Ag^\bullet$ and $|Ag|'$ (the old-fashioned symbols $^\bullet$ and $'$ are used to highlight the significance of the relative charge they possess), formed for entropic reasons, not only exhibit an appreciable mobility, they also exhibit a higher local energy, and thus a higher reactivity that unfolds when they are in contact with reaction partners (e.g., at the surface).[1]

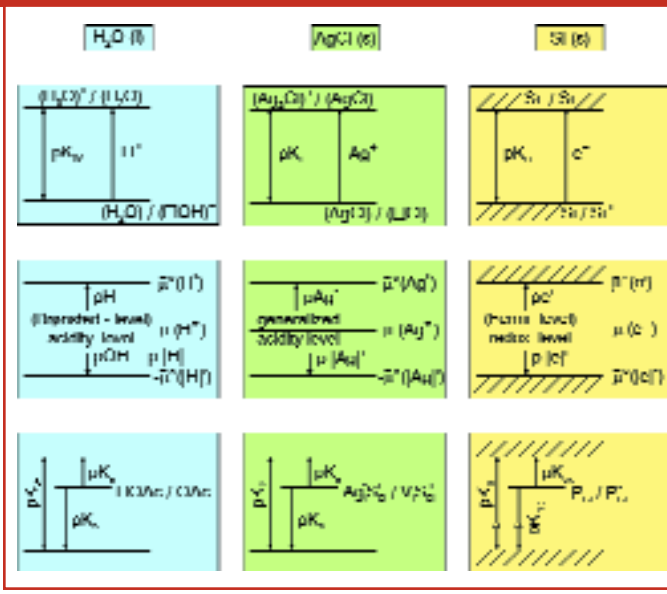


***Figure 2: In the same way as the concentration of protonic charge carriers characterizes the acidity (basicity) of water and in the same way as the electronic charge carriers characterize the redox activity, the concentration of elementary ionic charge carriers, that is, of point defects, measure the acidity (basicity) of ionic solids, while associates constitute internal acids and bases. The definition of acidity/basicity from the (electro-)chemical potential of the exchangeable ion, and, hence, of the defects leads to a generalized and thermodynamically firm acid-base concept that also allows to link acid-base scales of different solids (In order to match the decadic scale the levels are normalized by ln 10).[2]*** *Reprinted with permission from reference 3.*

In fact, the correspondence is so complete (figure 2) that one can show that a thermodynamically firm acid-base concept can (and in fact shall) be based on counting the equilibrium point defects in the same way that water pH and pOH reflect acidity and basicity in $H_2O$.[3]

Together with the electronic carriers, the ionic defects constitute the internal acid-base and redox

chemistry. Analogously to the ionic disorder described by equations (4) or (5), the electronic disorder is described by

$$Ag^{\cdot} + Cl^{-} \rightleftharpoons Ag^{\circ} + Cl^{\circ} \qquad (6)$$

or more concisely (subtracting $Ag^{+}Cl^{-}$ on both sides) by

$$Nil \rightleftharpoons e' + h^{\cdot} \qquad (7)$$

(Equation 7 is to be preferred since it avoids double counting and is independent of the band structure. In AgCl the valence and conduction bands are only approximately due to Cl-p-orbitals and Ag-d-orbitals only.)

The presence of defects also allows the interaction with the neighboring phase. Every solid phase possesses a finite phase width. Even if the variability of the stoichiometry in $MO_{1+\delta}$ may be so small that it does not perceptibly affect the total free energy, its influence on the defect budget and hence on all the parameters that directly rely on the presence of the charge carriers (conductivity, reactivity), is of first order. So the equilibration under different oxygen partial pressures can change normal conductors into superconductors, n-type conductors into p-type conductors, or ion conductors into electron conductors. Dopants in solids are comparable to, and are in fact as important as, impurities in water (e.g., consider traces of HCl in $H_2O$ with respect to pH or conductivity, see figure 2). Whilst in water both impurity cation and impurity anion are usually soluble, in solids most impurities are introduced substitutionally. Hence, the charge difference between dopant and substituted particle matters significantly. In fact, this effective charge is the only quantity that has to be known in most examples in order to predict the consequence of doping: a substitutional doping by a lower-valent cation, for example, introduces a negative relative-excess charge resulting in an enhanced concentration of positively charged carriers (holes, oxygen vacancies) and a depression of negatively charged carriers (e.g., conduction electrons, oxygen interstitials). It is therefore expected that Gd doping of $CeO_2$ turns $CeO_2$ from an electronic into an ionic conductor, and that Sr doping in $La_2CuO_4$ ($Sr^{2+}$ replaces $La^{3+}$) increases p-conduction (conduction via $h^{\cdot}$). Simple internal mass-action laws even show in a straightforward way that the concentration of hole pairs ($2h^{\cdot} \rightleftharpoons (h^{\cdot})_2$) has to increase in the latter case. To explain, however, their amount or the fact that the formation of these so-called Cooper pairs enable superconductivity at finite temperatures requires a subtle understanding of the underlying quantum mechanics.

In addition, point defects can internally react with each other: such association between ionic centers represents internal acids or bases (see figure 2, bottom center), while association of ionic with electronic particles represents internal redox centers (see figure 2, bottom right hand side); association between electronic carriers are of no less importance, examples are excitons ($e'h^{\cdot}$) or the already mentioned Cooper pairs ($(e')_2$, $(h^{\cdot})_2$).

A further point that is equally important and is of significance in solid-state science is the influence of interfaces on the charge-carrier density.[4] As in the case of solid/liquid interfaces, double layers at solid-solid surfaces result in an enormous change in concentration compared to the bulk values. It can be shown that based upon this concept new electrolytes or novel sensors can be created. This is particularly of importance when considering a high density of interfaces as is the case in nano-sized systems[5] (see figure 3).

In the extreme case of minuscule interfacial spacings, the interfaces begin to perceive each other and

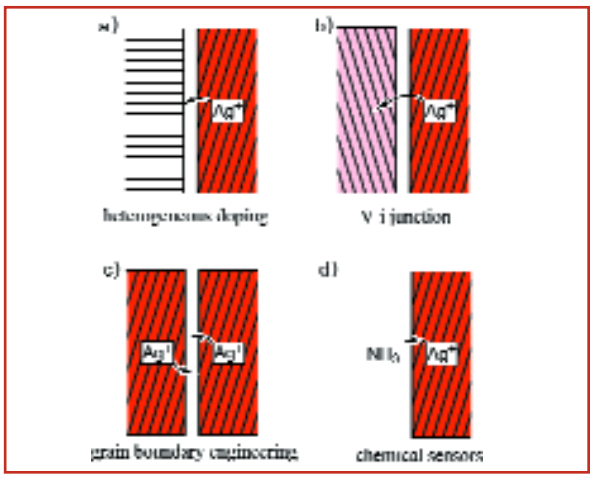



***Figure 3: Four basic space charge situations involving ionic conductors (here silver ion conductor): a) contact with an insulator that adsorbs Ag+ leads to an increased vacancy concentration adjacent, b) contact with a second ion conductor leads to a redistribution over two space charge layers, c) grain boundary that traps silver ions increases vacancy concentrations on both sides, d) contact with a fluid phase; the increase of the vacancy concentration if $NH_3$ is adsorbed can be used as a selective sensor signal.[4]*** *Reprinted from J. Maier, in* Modern Aspects of Electrochemistry, *(B. E. Conway, ed.), vol. 38 (2005) 1, with permission from Springer, New York.*

we are met with size effects. The field of nano-ionics, which is concerned with size effects on ionic transport properties, is expected to play a similar role for electrochemical applications as nano-electronics does for semiconductor devices.[5]

A further key point is chemical kinetics. The major difference to solution chemistry lies in the heterogeneity of the reactions. They start at the surface (e.g., at the gas/solid contact) and are followed by transport steps. Realizing that the hopping process in diffusion kinetics (hopping from one site to the next equivalent one) just refers to the simplest possible chemical kinetic problem, namely a "reaction" involving a symmetrical reaction profile (i.e., equal rate constants for forward and backward reactions), may remove a further hindrance for chemists to enter the field.[1,6]

Figure 4 shows how, using the example of oxygen incorporation into an oxide, the variation of the stoichiometry proceeds. On changing the outer oxygen partial pressure, three basic kinetic modes for the kinetics of stoichiometry change in a perovskite ($SrTiO_3$) can occur as displayed.

Defect chemistry is not only a prerequisite for adequately understanding the fundamental aspects of the internal chemistry of solids or the proper understanding of catalysis, it is also a prerequisite for enabling functionality and designability of solids, as far as many important applications are concerned: Oxygen ion or proton conductors are the key component of high-temperature fuel cells (SOFC); oxide electrodes that may incorporate oxygen or lithium are relevant electrodes in SOFCs and Li batteries, respectively. The latter are mixed conductors and are also relevant for permeation membranes or catalysts. Also, gas sensors rely on the interaction of solids with the neighboring gas phase mediated by point defects. (For an overview on such devices, see this article online.) As far as the engineering of relevant functional materials is concerned, tuning of ionic and electronic conductivities is a key issue.

Even if one is exclusively concerned with semiconductor devices, stoichiometric aspects are crucial. Defect chemistry offers the possibility to understand and predict the fine composition in the frozen-in state that is otherwise only accessible in terms of empirical preparation procedures or via an a posteriori analysis.[7]

These are only a few examples out of the whole spectrum of relevant applications, but they may suffice to show (i) that the internal chemistry of solids is conceptually a viable subset of chemistry, (ii) how efficiently electrochemical and kinetic properties can be purposefully tuned given a pertinent understanding of this topic, and (iii) how subtly the understanding of electroceramic applications is connected with defect chemistry.

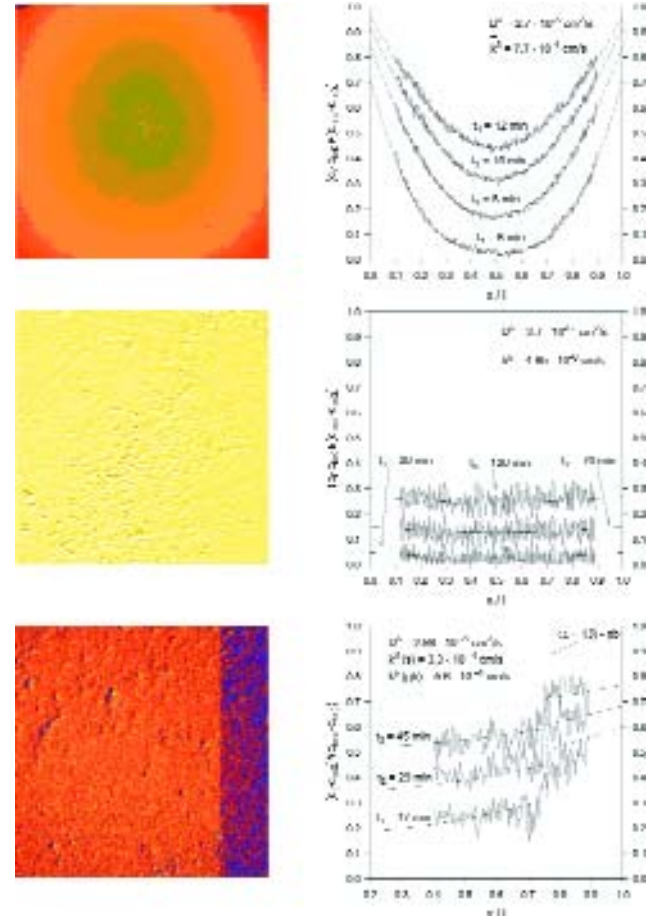


***Figure 4: Three limiting cases of oxygen indiffusion into $SrTiO_3$ as recorded by spatially resolved in-situ spectroscopy. L.h.s.: snapshots during the experiment. R.h.s.: The evolution of the corresponding stoichiometry profiles. Top: diffusion control. Centre: Surface reaction control. Bottom: Grain Boundary control.*** *Reprinted from J. Maier,* Solid State Ionics *135 (1-4) (2000) 575, with permission from Elsevier.*

**Joachim Maier is a professor and director at the Max Planck Institut fuer Festkoerperforschung in Stuttgart, Germany. He has also been a titular member of the IUPAC Physical and Biophysical Chemistry Division.**

References

1 J. Maier, *Physical Chemistry of Ionic Materials. Ions and Electrons in Solids*, John Wiley & Sons, Chichester, 2004.
2 C. Wagner, W. Schottky, *Z. Phys. Cem.* **B11** (1930) 163; C. Wagner, *Z. Phys. Chem.* **B32** (1936) 447.
3 J. Maier, *Chem. Eur. J.* **7** (22) (2001) 4762.
4 J. Maier , *Prog. Solid St. Chem.* **Vol. 23** (3) (1995) 171.
5 J. Maier, *Nature Materials* **4** (11) (2005) 805.
6 H. Schmalzried, *Chemical Kinetics of Solids*, VCH, Weinheim, 1995.
7 J. Maier, *Phys. Chem. Chem. Phys.* **5** (11) (2003) 2164.

# Does It Have a Sporting Chance?

*by Alan Smith*

**It's been hard to miss the hype that's surrounded nanotechnology the past few years. On one side, industrialists and academics hype nanotechnology's wideranging potential applications, hoping to garner government funding. On the other side, advocacy groups agitate about the potential dangers of exposure to nanoparticles, working to stir up public awareness—and gain membership fees, to boot. As usual, the truth about nanotechnology lies somewhere inbetween the two sides' positions, but it is important that the debate does not go the same way as the dispute over genetically modified foods.**

Nanotechnology is debated as though it were a new technology, but it's not. Our own bones are composed of self-assembling nanostructures; car tires have included carbon black nanoparticles for decades; the red and yellow colors in sunsets are caused by nanoparticulate pollution (both volcanic and from chimneys); and many food products are nanoemulsions or particulates.

*Nanotechnology is debated as though it were a new technology, but it's not.*

Scanning tunnelling microscopy enabled us to observe objects at the nanoscale, revealing that at that level, thermal, optical, mechanical, electronic, magnetic, and surface properties change. This realization has driven the search for new products, and the sporting goods industry has lead the way.

## From Bowling Balls to Tennis Balls

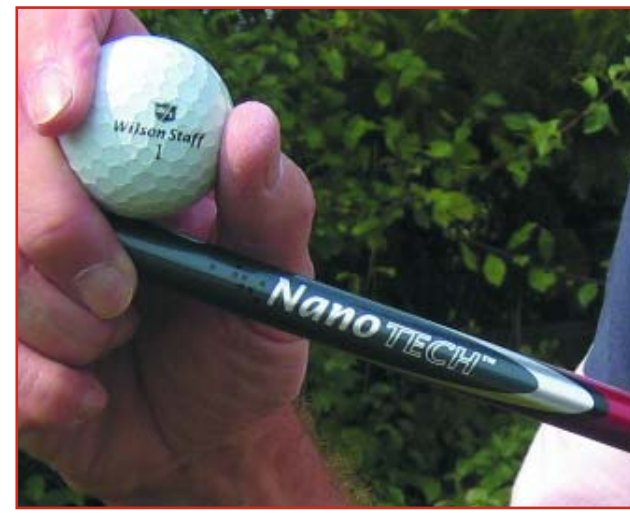
For example, bowling balls are usually covered in scratches; hardly surprising when they hit the pins at the end of the alley with such force. One enterprising company used nanoparticulate coatings to give the balls a scratch-resistant surface, enabling them to look pristine for months. A similar technology is being used for the final lacquer coating on a number of Mercedes vehicles, and the results have been impressive.

Wilson Sports recently introduced a nanocomposite tennis racquet, currently used by Switzerland's Roger Federer. Use of the racquet has enabled Federer to consistently hit the ball harder. Wilson also offers a new "Double Core" tennis ball that keeps its pressure longer, even when Federer and others hit it in excess of 150 mph. The new balls have a butyl rubber nanocomposite coating inside that acts as a barrier, preventing air from getting out. This same technology is also being used for footballs and for food packing, helping slow degradation by preventing flavor from getting out of the packaging and oxygen and ultraviolet light from getting in.

## Golf Clubs, Fly Rods, and Racing Bikes

Nanocomposite materials are also being used in fly-fishing rods from Redington's; the rods' "nano-titanium" resin layer gives them a lighter weight and stronger frame than has previously been possible. Nanocomposite golf balls are on the market, and Wilson is leading the way with "Nanotech" golf clubs. These new drivers and fairway woods have a nanocomposite material that reduces the weight of the crown of the club, lowering the center of gravity and giving longer and straighter drives. These clubs also have carbon nanotubes in the tip section of the shaft to improve stability and add to the length of the shot. Padraig Harrington, Ireland's leading golfer, attributes his recent success to the new clubs. His caddy is grateful for nanotechnology as well-Harrington's golf bag is made from a new nanofabric that has reduced the weight of the bag by 52 percent.

Nanotechnology has also made inroads in the textile industry. Stain-resistant clothing has been available for the past few years, and a new fabric has been designed specifically to repel grass stains and help "whites stay



whiter"-an advance sure to be welcomed by cricketers around the world. Socks are available that are based on the antimicrobial properties that silver nanoparticles impart. And many sunscreens now on the market contain nanoparticulate titanium dioxide, which blocks so-called "bad" ultraviolet rays while letting tan-giving rays through. Surfers and other athletes who cover their lips and noses with sunscreen will appreciate the distinction.

BMC, the leading Swiss bicycle brand, has developed a revolutionary bike for the number-one Pro Tour Team Phonak for the latest Tour de France. The company's enhanced resin system contains carbon nanotubes and exploits the fact that nanotubes have a strength-to-weight ratio a hundred times better than that of aluminium, and far better than that of normal carbon fibers. The combination of good riders and excellent bikes has put Team Phonak at the top of the worldwide UCI ProTour ranking.

## In the Cold and In the Shower

Winter sports are also benefiting from nanotechnology, with nanofibers being used to windproof and waterproof ski jackets. And skis and snowboards themselves are being coated with a high-performance nanowax that produces a hard, fast gliding surface.

Microelectromechanical systems (MEMS)—small, integrated devices that combine electrical and mechanical components—are commonplace nowadays, and top range cars often contain 50 to 100 sensors. As the trend from micro to nano continues, the sports industry will see increasing use of sensors in sports goods. Suunto markets a wide range of sensor-packed, wrist-top computers. One of their golf models has GPS incorporated into it and can indicate which club to use to reach the pin and avoid water and bunkers. Who needs a caddy—especially because the golf bags are so lightweight?

*. . . even a 1 percent share of the market will add more than $5 billion to a country's economy.*

The use of nanotechnology in Formula One motor racing has not been widely discussed, but lighter-weight materials and nanosensors offer an advantage that will likely be seized upon. To the extent that the race depends heavily on the type of tires used, there is a good chance that manufacturers such as Bridgestone and Michelin are investigating replacing their carbon black nanoparticle tires with better-wearing and lighter nanocomposite products.

Even the changing rooms at the gym will be using more and more nanotechnology, as easy-to-clean and antimicrobial products become more prevalent. Nanocoated glass surfaces are already available for showers that prevent water droplets from sticking to the glass, keeping the surfaces cleaner longer. Samsung is using this technology to keep refrigerators fresher, and black mold in showers will become a thing of the past as tile and sealant manufacturers adopt this development.

*The author in action.*

## A Trillion-Dollar Market

Markets of between one-half to one trillion dollars for nanotechnology are being forecast in 10 years time, so even a 1 percent share of the market will add more than $5 billion to a country's economy. MEMS sensors and nanomaterials are predicted to reach $100 million in 2009 for the sporting goods market.

High-tech sporting goods are leading the way for nanotechnology, but other industry sectors are quickly jumping on board. If concerns about exposure to nanoparticles continue to be addressed successfully at an international level, all industries utilizing nanotechnology will have a sporting chance of success.

**Dr. Alan Smith is an associate director of the UK government's Micro Nano Technology Network, which is coordinating activities in nanotechnology throughout the United Kingdom. He was reelected as a member of the IUPAC Bureau in Beijing.**

# The Quest for a Universal Format

*by Robert Lancashire and Tony Davies*

**To quote a recent report from the International Council for Science (ICSU)[1]:**

> *"Because of the critical importance of data and information in the global scientific enterprise, the international research community must address a series of new challenges if it is to take full advantage of the data and information resources available for research today. Equally, if not more important than its own data and information needs, today's research community must also assume responsibility for building a robust data and information infrastructure for the future."*

IUPAC has been intimately involved with this challenge for many years, particularly with respect to getting instrument vendor consensus while creating and maintaining internationally recognized vendor-neutral scientific data formats suitable for interchange between analytical instruments, laboratories, reference data collectors, and archives. With the additional importance now being placed on this work—especially by ICSU—it is worthwhile to review the situation with respect to scientific data and to examine some of the prospects for the development of a universal spectroscopic data format.

## IUPAC Scientific Data Standards

Many of the ideas that predominated when standard file formats were originally designed in the 1980s are perhaps no longer appropriate, given the rapid technological changes that have made file storage less expensive and more reliable and the interconnection of equipment so much faster. New industrial regulations may require exact copies of original data to be made available electronically for inspection for many years after the actual experiments are performed. This has been especially relevant in the pharmaceutical industry, where the U.S. Food and Drug Administration in 2000 brought out a set of guidelines (21 CFR Part 11) outlining the steps needed to make electronic records legally equivalent to paper records. These rules were initially accompanied by explanatory guidelines that interpreted the rules in an extremely strict manner—one that could actually not be met by any of the scientific computing equipment currently available. At that time, one of the only data migration solutions that could even come close to meeting the regulation's requirements was the IUPAC JCAMP-DX series of data standards. Although the standards provided the essential framework to satisfy the regulators, the implementations that were commercially available had to be enhanced outside the published IUPAC standard definitions to be fully compliant. More recently, the U.S. Environmental Protection Agency brought out similar requirements on long-term electronic data storage.

Lawmaking aside, one point remains clear—if you need to produce and work with electronic analytical data, it should be stored in a standard, well-documented, vendor-neutral format. Even ignoring hardware compatibility issues, experience has shown that many instrument vendors themselves cannot produce the correct documentation or converters for their older legacy data formats.[2]

## State of the Art

So what is the current state of affairs? A survey of spectroscopic data types in common use suggests that more than 100 different formats are being used to store essentially similar information types. This is a substantial increase from 1997, when a review of the common formats then in use and the applications available for their manipulation was published.[3] However, just listing applications and file extensions misses one of the more fundamental problems involved with tackling the long-term availability of analytical data stored in electronic form. Behind each file format often lies a series of different formats or versions in which each instrument software release has slightly changed the format, despite retaining the old file extension. Instrument manufacturers often attempt to maintain backward compatibility within their own software, but doing so makes the life of the archivists very difficult. In one notorious case, a pharmaceutical company was generating files with a particular file extension from an analytical spectrometer in a completely different binary format than that documented by the manufacturer. Upon closer investigation, it turned out that a development prototype software version had been installed at the customer's site without the knowledge of the main company, just because doing so solved a

few technical problems for the installation engineer. The development prototype had never made it through the software validation cycle, and the development direction stopped. But the pharmaceutical customer was not told that the instrument software they were relying on was an unvalidated, unreleased prototype with essentially no support. One more reason to move to independent, vendor-neutral standard formats for long-term archiving!

If other scientific data formats are included, it is particularly surprising that many of these formats—at least 50 alone—are for molecular graphics files. Given that the object of many of these formats is for recording x, y, and z coordinates, this is unusual, although the *de facto* industry standards such as CIF, PDB, and MOL file formats probably account for more than 85% in terms of overall acceptance. The JCAMP-CS protocol supported by IUPAC,[4] one of the initial attempts by an international standards body in this arena, has not been adopted by software developers to any great extent.

With respect to spectroscopic instruments and data, the situation does seem to be improving. Although the number of proprietary data formats is large, it appears to be relatively stable; furthermore, with instrument company mergers taking place, the number may well be decreasing. A measure of the success of an IUPAC project on data protocols is the uptake by both instrument vendors and software developers. The IUPAC/JCAMP-DX standards project should therefore be considered a success: Almost all spectroscopic instrument manufacturers include an export option to JCAMP-DX, and more than 30 different software packages use JCAMP-DX for both import and export of data files.[5] Most commercial spectroscopic database packages incorporate data entry through files in JCAMP-DX format, as do the chemometrics packages found in the analytical field. (For more information on this project or to receive copies of the published protocols and latest drafts of new versions, go to <www.jcamp.org>.)

The new International Spectroscopic Data Bank, which went live in 2003, has adopted the IUPAC JCAMP-DX standards for spectroscopic data deposition and presentation via the Internet (see <www.is-db.org> for more information).

## Educational Use

From an educational perspective, the availability of spectral data that can be displayed and manipulated in a Web browser via plug-in or Java applets has opened up numerous possibilities that have been grasped both as teaching aids and learning tools. The release in 1997 of the MDL CHIME plug-in, with JCAMP-DX spectral support, served as a catalyst in this development. It is estimated that there have been more than 2 million downloads of the free version of MDL CHIME. Examples of its use include linking IR spectra to vibrational mode animations (see figure on page 12) and linking from NMR spectra to highlight H or C atoms.

## XML and Joint Developments

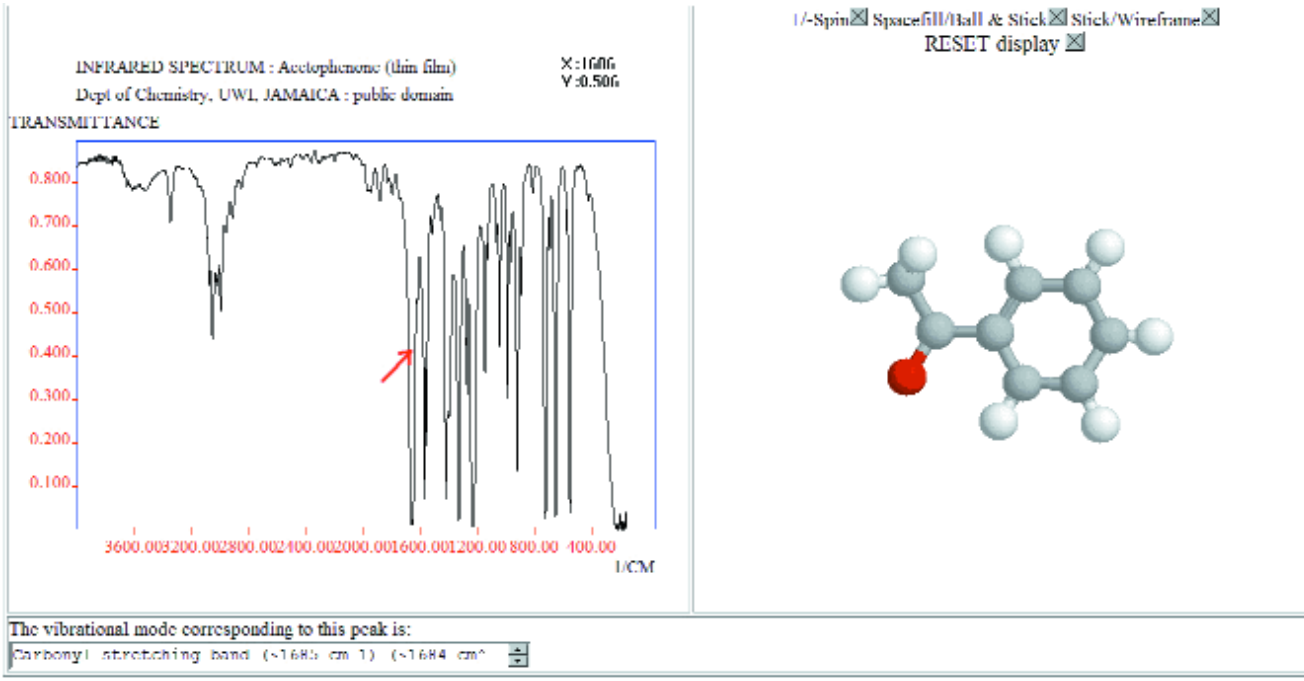
XML has become a buzzword in recent years, and many efforts have been made to generate scientific data storage formats based on this language.

IUPAC started to worry about the proliferation of standard formats and organized a meeting on the subject during the 2001 IUPAC General Assembly in Brisbane, Australia; IUPAC later reported on the meeting in *Chemistry International*.[6] In addition, the Committee on Printed and Electronic Publications (CPEP) Subcommittee on Electronic Data Standards is working with ASTM International Committee E13.15 on an XML standard for analytical data—the Analytical Information Markup Language, or AnIML for short.

The development team is working to make AnIML:

- validateable
- extensible
- able to accommodate any type of data
- able to offer an audit trail
- able to utilize digital signatures

Learning from the mistakes of previous standardization efforts, the team has adopted a flexible approach, allowing vendors and organizations to include their own specific fields while standardizing the data dictionaries at a core and technique level. This initiative is taking account of the new world in which we find ourselves—one in which science is facing increasing legal and regulatory scrutiny.




***Display of an IR spectrum on a web page using a browser plug-in.*** *Interpretation of the IR of acetophenone.*

## Ontologies

To avoid "reinventing the wheel," the IUPAC JCAMP-DX and ASTM ANDI ontologies form the basis of the current AnIML draft standard, which is currently being developed and reviewed by various experts.

Development has been split into three main phases:

- phase 1: UV/VIS, MS, NMR, IR, IMS, chromatography
- phase 2: EPR/ESR, NIR, crystallography
- phase 3: chemometrics

For more information, go to the AnIML project Web site hosted by SourceForge at <animl.sourceforge.net>.

Another XML-based IUPAC standardization project focused on analytical data is being led by Michael Frenkel. This standard, ThermoML, is being designed for experimental and critically evaluated thermodynamic property data and is in its final stages (see provisional recommendation on page 27).

## Conclusion

IUPAC can be proud of playing a leading role in the increasingly important field of the digital preservation of scientific records. In this area, only an independent international standardization body can hope to make headway and navigate the politics of differing instrument vendor positions.

References

1. International Council for Science. December 2004. *ICSU Report of the CSPR Assessment Panel on Scientific Data and Information.* ISBN 0-930357-60-4.
2. For more information on the digital preservation of scientific records, see "Cometh A Digital Dark Age?" by Tony Davies, *Chem. Int.* Nov-Dec 2002, p. 7 or <www.iupac.org/publications/ci/2002/2406/darkage.html>.
3. R.J. Lancashire, "An Introduction to Data Formats," *Spectroscopy Europe*, 1997, 9(2), 22–24.
4. J. Gasteiger, B.M.P. Hendriks, P. Hoever, C. Jochum, and H. Somberg, "JCAMP-CS: A Standard Exchange Format for Chemical Structure Information in Computer-Readable Form," *Applied Spectroscopy*, 1991, 45(1), 4–11.
5. For a list of some spectroscopic applications using JCAMP-DX and other data format types, see this article online.
6. A. N. Davies, "XML in Chemistry," *Chem. Int.* Jul-Aug 2002, p. 3 or <www.iupac.org/publications/ci/2002/2404/XML.html>.

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# IUPAC in Beijing—Division Roundups Part II

**Part I of the Division Roundups from the 2005 General Assembly (GA) in Beijing appeared in the Nov.-Dec. 2005 *CI* (page 7). That article covered Division I. Physical and Biophysical Chemistry, Division II. Inorganic Chemistry, Commission II.1. Isotopic Abundances and Atomic Weights, Division IV. Polymer, Division VIII. Chemical Nomenclature and Structure Representation, and CHEMRAWN.**

## Division V. Analytical Chemistry
### *Roger Smith, Secretary*

The Analytical Chemistry Division (ACD) includes a symposium or workshop in its annual meetings. These explore emerging and challenging areas in analytical chemistry, with a view to identifying potential new projects and suitable task groups. The several guests and young observers at the ACD meeting in Beijing contributed to worthwhile discussions and brought new perspectives.

This year's symposium on Future Opportunities and Challenges for Analytical Chemistry covered the following topics: Separations Science, Molecular Spectroscopy, Analytical Atomic Spectrometry, Nuclear Methods in Radioanalytical (and Radio-Pharmaceutical) Chemistry, Bioanalytical Chemistry, Emerging Needs in Developing Countries, Opportunities for New Critical Evaluations, and Metrology and Quality Assurance. The division also hosted a successful and well-attended interdivisional meeting on metrological traceability concepts in chemical analysis.

The ACD focuses its effort on a series of core activities and emerging areas. The four core activities are critical evaluation, quality assurance, terminology, and communication. The emerging areas are bioanalytical chemistry, nanotechnology, and emerging needs for developing countries. Each theme has an associated team of titular members, associate members, and national representative. An assessment of our commitment to these priority areas was an important aspect of discussions in Beijing. Communication within the division is aided by the circulation of the division newsletter *Teamwork* to all committee and task group members involved in project work.

An important activity of the meeting was to review all of the current ACD projects. This task was aided by the regular progress reports supplied by the task group chairmen of each project. These reports are subsequently posted on the project web pages. An important consideration for each project evaluation is the proposal for dissemination. As well as projects on important analytical topics, such as the comparability of pH measurements and the chemical speciation of environmentally significant heavy metals, each of the division's priority areas is well represented in the project portfolio.

A number of projects will assist the updating of the terminology in the Orange Book. The Subcommittee on Solubility and Equilibrium Data has continued to evaluate a wide range of chemical data important to industry, which has lead to numerous publications. Interdivisional projects include the *Critical Compendium of Pesticide Physical Chemistry Data*, and Analytical Capacity Building in Africa. The Interdivisional Working Party on the Harmonization of Quality Assurance has continued its work in areas such as Terminology for Soil Sampling, Proficiency Testing Methods, and Metrological Traceability Concepts in Chemical Analysis.

*The ACD is very conscious of the need to make its work both public and relevant.*

The ACD is very conscious of the need to make its work both public and relevant. A particularly visible activity has been the series of articles in *Chemistry International* on "Emerging Issues in Developing Countries," which is coordinated by Jan Åke Jönsson. The most recent article was also featured in *Gallium*, the special newsletter published for the GA.

The division officers for 2006–2007 will be Ryszard Lobinski (president, France), Ales Fajgelj (vice president, Slovenia), Kip Powell (past president, New Zealand), and Roger Smith (secretary, UK). Professors Paul De Bièvre (Belgium), Walter Lund (Norway), and Jan Labuda (Slovakia) were elected as new titular members.

## Division VI. Chemistry and the Environment
### *Ken D. Racke, President*

A total of 18 division committee members and 3 visiting contributors participated in the Division VI meeting, which proved to be an interesting event as some challenging issues were discussed. Among these were a fundamental dialogue on strategic issues, establishment of stronger linkages with other IUPAC divisions, and priorities for new initiatives.

Although it was concluded that the communication among division members and revitalization of the sub-

committees need further attention, the efforts and output of the project teams were found to be most encouraging. Since the beginning of the 2004–2005 biennium, eight projects have been completed, one project was abandoned, and seven new projects have been initiated. Most active projects appear to be making solid progress versus milestones, but it was agreed upon that one project lacking such progress should be terminated. This leaves the division with 21 active projects, several of which have interdivisional cooperation.

Several new areas of project activities were discussed, including an ambitious new book series on biophysico-chemical processes in environmental systems. Two specific project proposals are currently under review, and a call for new project proposals in priority areas of interest will be made in the near future, with funding expected to arise from the 2006–2007 biennium budget. Major conferences related to crop protection chemistry and food chemistry are planned for 2006 and 2007, respectively.

*. . . the ongoing arsenic remediation project has generated a lot of interest since it deals with a topic of major concern in many countries.*

The subcommittees reported a great deal of activity. The Subcommittee on Biophysico-Chemical Processes in Environmental Systems had Volume 9 of the Wiley series on *Analytical and Physical Chemistry in Environmental Systems* published during 2004, with Volumes 10 and 11 close to completion and another book project approved in 2004 on metals and metalloids. Within the Subcommittee on Chemistry of the Environmental Compartments, the ongoing arsenic remediation project has generated a lot of interest since it deals with a topic of major concern in many countries. The Subcommittee on Crop Protection produced an impressive list of projects, including the highly successful International Workshop on Crop Protection Chemistry held in Costa Rica. Finally, a prolonged debate was organized to thoroughly discuss the future of the Subcommittee on Food Chemistry.

The results of the 2005 election of titular members by e-mail ballot were confirmed and 7 associate members and 10 national representative positions were agreed upon. Ken Racke is continuing as division president (to 2007) and Willie Peijnenburg is the new division secretary after Patrick Holland steps down from this post after 20 years of meritorious service to IUPAC.

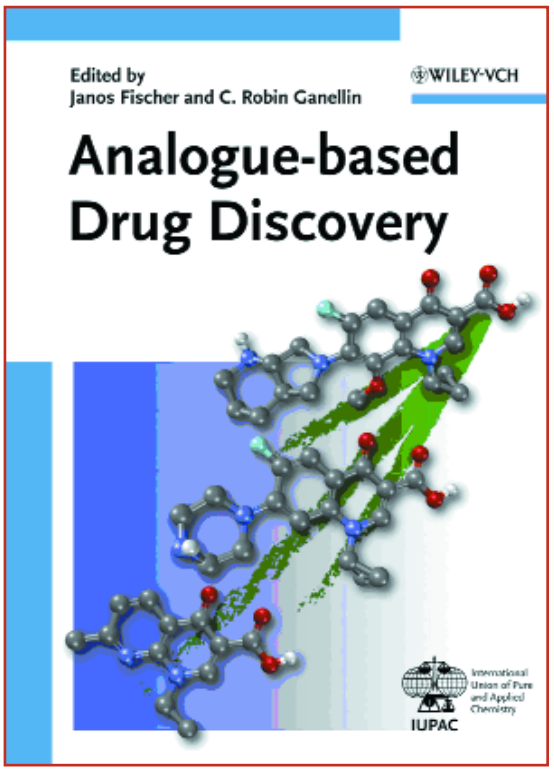
It was agreed that the next face-to-face meeting of the committee will be in Bilthoven, Netherlands, during July 2006, with at least one phone conference to be held in advance of this session.

## Division VII. Chemistry and Human Health

### *Paul W. Erhardt, President*

For its meeting, Division VII developed a very useful tool for evaluating the status of numerous ongoing projects. For the first time, a short update form was distributed by the three subcommittee chairpersons to each of the project leaders within their respective technical areas. There were approximately 10 projects completed in the current biennium, about 25 active projects, and nearly 15 projects undergoing serious consideration at various stages of subcommittee, divisional, and IUPAC review. Taking just one highlight from each subcommittee's activities, the following examples demonstrate the breadth of topics being addressed by the division.

Within the Subcommittee on Nomenclature, Properties, and Units (NPU) in Laboratory Medicine, the C-NPU database <http://dior.imt.liu.se/cnpu> has



been upgraded with codes for the most common properties associated with clinical chemistry using mass concentrations along with identifiers for clinical molecular biology, transfusion medicine, and immunoheamatology. Within the Subcommittee on Medicinal Chemistry and Drug Development, a thorough examination of the role that analog-based drug discovery has played toward bringing both improved and novel therapeutics to the clinic was completed. This important topic is the subject of a book recently published (John Wiley & Sons, GMbH, 2005) and replete with numerous case studies. Finally, within the Subcommittee on Toxicology and Risk Assessment, the second edition of the popular text *Fundamental Toxicology for Chemists* will soon be released (Royal Society of Chemistry).

Thanks to a proactive and rigorous effort by the nomination committee, the division's elections were a resounding success. Among the 10 titular members, 3 associate members, and 8 national representatives, all of which will be participating at the divisional level in 2006, a total of 19 different countries are represented. Dr. Pedro Soares de Araujo (Brazil) was elected vice president.

Finally, the entire division is extremely excited about the recent formation of the IUPAC-Richter Prize in Medicinal Chemistry. Funded by a generous donation from Richter Pharmaceuticals, Ltd. (Budapest, Hungary), this award will recognize one scientist every two years whose work has made a significant contribution to medicinal chemistry within the context of drug discovery and development. Awardees will receive a cash prize of USD 10 000 at an IUPAC-associated scientific meeting wherein they will be expected to deliver a lecture about their work. Funding has been allocated for 5 such awards across 10 years. (For more information, see www.iupac.org/news/Richter_prize.html)

## Interdivisional Subcommittee on Materials Chemistry

### *John Corish, Chairman*

The project to define "materials chemistry" has received IUPAC approval, with Peter Day as project leader. In his absence, Dr. Graham McCann of the Royal Society of Chemistry updated the subcommittee on the project's progress. The objective of the project, which will run for two years, is to produce a statement showing how materials chemistry can fit within the overall IUPAC structure. (See Sept.-Oct. 2005 *CI*, p. 22).

Following discussion, it was agreed that materials chemistry is clearly an interdisciplinary area that crosses the borders of several divisions within IUPAC, although Inorganic is its current principal home. To promote discussion, McCann presented the following first draft of a definition of materials chemistry based on his experience as editor of the *Journal of Materials Chemistry*:

> "The synthesis, processing, characterization, and exploitation of compounds that have useful, or potentially useful, properties and applications. The focus of the research is the creation, understanding, and development of substances or systems with improved properties that will impact positively on business and personal life. To use chemistry to create compounds that may lead to new technological opportunities or significant improvements in existing technology."

As expected and hoped, this generated a considerable amount of positive discussion.

Another hot topic during the meeting was a proposal by Sanjay Mathur to produce a glossary of nano-related terminology. This suggestion was received with much enthusiasm from the subcommittee; in particular, such a project it was thought could perhaps form the first step in a much wider glossary of terminology in materials chemistry. Considerable helpful discussion followed concerning how to establish an agreed terminology in an emerging area such as this.

As reported on page 35, the very successful IUPAC New Directions in Chemistry—Workshop in Advanced Materials (WAM III) attracted more than 150 participants to South Africa on 4–9 September 2005.

It was noted that several of the subcommittee members have continued membership in Division II and therefore the immediate future is assured. However, new recruits are certainly needed.

**Interested In Hosting WAM IV in 2008?**

Contact the subcommittee chairman:

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www.iupac.org/divisions/II/205

## Committee on Chemistry Education (CCE)

***Morton Z. Hoffman, U.S. National Representative***

The meeting of CCE, which was chaired by Peter Atkins, began with descriptions by committee members of the chemical education issues that confront their countries. In Europe, the focus is on the implementation of the "Bologna Process," in which all undergraduate university programs will follow a very similar pattern that leads to a uniformly recognized EuroBachelor; the quality of the curricula, the broadening of the diversity of students, and their future employability are current concerns. Russia and the other countries of the former Soviet Union are struggling to complete the reforms that were begun over the past 15 years; the result is that many old wheels have been reinvented. Asian countries are working to adjust their educational systems to reflect their newly developed economic opportunities. Questions have been raised within the provinces in Canada about the licensing of chemists as professionals in the same way that engineers are licensed. Sadly, chemical education in the developing countries around the world is just barely hanging on. In the United States, the American Chemical Society is playing an important role in producing materials across the educational spectrum, reaching out to high school teachers, encouraging research in educational practices and teaching and learning, and working to reflect the changes that are taking place within chemistry and the other molecular sciences in curricular content and pedagogical approaches.

*Peter Mahaffy and Peter Atkins hard at work during the CCE meeting.*

One of the very interesting issues that was discussed, which could have wide ramifications in the publishing world, was the recent directive from the Chinese Ministry of Education requiring that in as little as three years science and mathematics must be taught in English in China's many colleges and universities. The Chinese government is providing funds for faculty members to spend time in anglophone countries in order to perfect their English; institutions are eager to host visits by native English speakers or those for whom English is a well-developed second language. Whether or not this move will succeed in the absence of draconian measures remains to be seen, but clearly, China is looking toward taking a great leap forward in chemical education.

The Subcommittee on Chemistry Education for Development reported on its work in India to develop web-based interactive quizzes for high school chemistry students in several Indian languages in order to motivate students toward further studies in chemistry. The "Flying Chemist Program" seeks to provide the expertise needed to strengthen chemistry education on the primary, secondary, and tertiary levels through visits by chemists who will catalyze the establishment of partnerships among schools, industries, and governments (see Project Place, p. 24). Another project continues to be the development of microscale chemistry for Indian high schools in order to implement low-cost, hands-on experiences.

The Subcommittee on the Public Understanding of Chemistry issued a report that detailed the important role of IUPAC in enhancing the public appreciation of chemistry. The conclusion was reached that chemistry activities aimed at supporting teachers and students within the formal school system are often more effective than those aimed at the general public. The targeted public should be chemists and educators who would understand and work with a variety of other publics. IUPAC would focus on activities such as helping scientists to identify and understand their publics, influencing international organizations, supporting science education systems (particularly in countries in transition), communicating relevant findings from IUPAC projects and activities, and supporting national chemical societies (particularly in countries in transition). The subcommittee also reported on the Young Ambassadors for Chemistry initiative to enhance the public understanding of chemistry through teacher and school audiences in target locations within regions in transition.

Attention was brought to the latest issue of *Chemical Education International* <www.iupac.org/

publications/cei>, the online newsletter of CCE, that contains the texts of the plenary and keynote papers from the 18th International Conference on Chemical Education (ICCE), held 3-8 August 2004 in Istanbul, Turkey. The 19th ICCE will be held in Seoul, Korea, 12-17 August 2006 <www.19icce.org>. Consideration was given to an application from chemists in Mauritius to host the 20th ICCE in 2008.

The committee elected Peter Mahaffy (King's University College, Edmonton, Alberta, Canada) as the new chairman of the committee, and voiced acclamation for the leadership of Peter Atkins since 2002.

## Committee on Chemistry and Industry (COCI)

### *David A. Evans, Chairman*

In essence, COCI's role is to act as a key focus for the "A" (i.e., Applied) in IUPAC by promoting topics and activities of interest and relevance to the chemical industries. So what can be said about COCI after its meeting in Beijing? The clear answer is that COCI is alive and kicking, as evidenced by the attendance of more than 95 percent of committee members, from over 20 countries, who were active contributors to the meetings. Over the years, a great deal of social cohesion has developed amongst group members, again in evidence during the formal meetings, visits, and social gatherings organized in Beijing.

The undoubted highlight was a delightful banquet graciously hosted by Mr. Xianghong Cao and senior colleagues from SINOPEC which set the scene for a magical stay in Beijing. Another key event was a visit of the group to the Beijing Research Institute of Chemical Industry (BRICI), organized and hosted by Jinliang Qiao, one of our long-serving Chinese delegates. COCI is particularly indebted to colleagues at SINOPEC for making our visit to China such a success.

*Former COCI Chairman David Evans and Michael Droescher, German National Representative on COCI.*

*COCI Members and Safety Training Program participants at a tour of SINOPEC research facilities in Beijing (from left): Isiaka O. Bakare (Rubber Research Institute of Nigeria), Esma Toprak (National Representative on COCI from Turkey), and Aldo B. Alles (member from Uruguay).*

With regard to formal committee events, mention must be made of the Safety Training Program Workshop held as part of the Congress. A parallel event was held at the Ottawa Congress in 2003, which I have often described as the best session of that Congress, but regrettably poorly attended. I can report that the symposium in Beijing was also the best session of the Congress (at least in my opinion!) and was well attended! The Safety Training Program and associated Workshops are COCI's flagship activities and the event in Beijing acted as a fitting tribute to its continuing success.

Other notable successes include progress with new projects in Responsible Care, from Bernard West, and nanotechnology, with Alan Smith, and a developing interest in biometrics from Colin Humphris. In the area of the public appreciation of chemistry, the joint CCE/COCI/CHEMRAWN meeting featured a lively and informative discussion of an important paper by Peter Mahaffy (CCE) in which it was concluded that a key to gaining a better image for our craft is education of ourselves as to how best to communicate issues. This is an important pointer for future programs in this area.

COCI regards the Company Associates (CA) program as crucial to its ability to engage chemical companies in IUPAC affairs. There have been several notable achievements during the biennium including a stalwart effort in recent months by Ms. Khalida al-Dalama of Kuwait who has recruited three new CAs. However, one key objective that remains for the future is to streamline the recruitment process with active cooperative engagement of the NAOs, the Secretariat, and COCI.

Mark Cesa, of Innovene, USA, is the new chairman of COCI.

## Chemistry Enrollment in Germany: Bucking the Trend

*by Terry Mitchell*

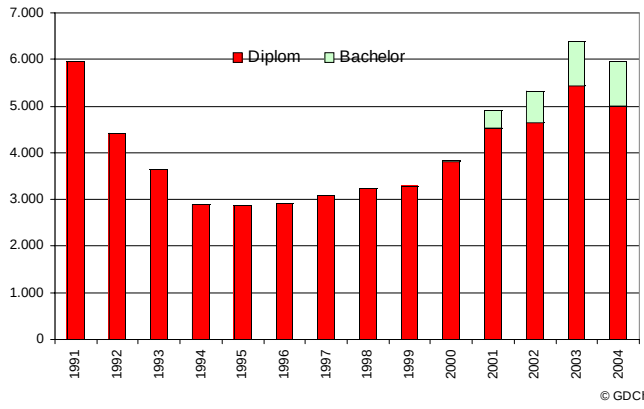
**The German Chemical Society (Gesellschaft Deutscher Chemiker, GDCh) has been collecting statistics on chemistry students in Germany for many years so that a huge amount of data on trends is now available. At the beginning of the 1990s German universities were happy with the way student enrolment was going in science and engineering. Then the slide started, and by the mid-1990s the press was full of stories about a lack of qualified graduates in the near future. When one asked around, this was not just a German situation, but also a European one; further inquiries indicated it seemed almost to be a world-wide problem!**

The fall in numbers was dramatic in many German universities, down to a third or even a quarter of the former figures in many cases, though some institutions did not seem to suffer quite as badly. In 1991 the total enrolment in chemistry was close to 6000, but by 1995 it had dropped to under 3000 (see figure). The number of students studying biochemistry and food chemistry is quite small in comparison, with a total of around 600 in 1995.

There is also (as in several European countries) a second set of institutions offering chemistry degrees, generally slanted towards chemical engineering, called "Fachhochschulen" (they are now called "universities of applied sciences," but the term "polytechnic" might also be appropriate in some countries). Their chemistry enrollment in 1993 was around 1400 and dropped to 850 in 1998.

The traditional first degree is the Diplom, which (on paper) takes five years, but Germany was unusual in that often around 90 percent of the chemistry graduates with this degree went on to obtain a Ph.D. (no other subject shows this kind of behavior). Presently, German institutions are in the throes of the "Bologna Process," which means giving up the Diplom and changing to Bachelor and Master, but most universities have not yet enrolled students for these, and very few have graduated any new Bachelors as yet.

*Entry into chemistry courses at German universities.*




Of course, the fall in enrollment meant that the number of Ph.Ds. coming out of the system would also fall, but with a big time lag. At the peak, about 2200 Ph.Ds. were graduated each year, but this number will continue to fall for a while yet: the number for 2004 was close to 1300.

Towards the end of the 1990s the picture began to change again: numbers started to rise, but not everywhere at first. There was a steady rise in the total numbers, however, and by now they are almost exactly back to where they were at the 1990s peak, with 6000 freshmen in Diplom and Bachelor courses in 2004 (the figure was very slightly higher in 2003).

In fact, the total enrollment is higher. As in 2004, around 1400 students began courses in biochemistry or food chemistry, while the Fachhochschulen attracted 1600. However, a recent round-the-table survey of other European countries showed that Germany is still really bucking the trend. In other countries numbers are either constant, dropping slowly each year, or rising slowly from a very low baseline.

So why is the situation in Germany different? The short answer has to be "nobody knows." It cannot be the change from the Diplom to a Bachelor/Master system, since in 2004 only around 1000 (17%) of the freshmen went into these courses, exactly the same number as in 2003.

The number of students entering biochemistry, which has increased by a factor of nearly three since 1995, may give us a clue (the change in food chemistry is only very small over that period). The prefix "bio" certainly has an influence on the way young people think. Two cases from my own university will serve as examples: Our chemical engineering departments were desperately short of students until they introduced a new course dealing with biochemical engineering. They were swamped with beginners in the first two years and had to limit the numbers! Chemical engineering itself remained uninteresting.

A year later, my own department changed to Bachelor/Master and offered two courses: chemistry and chemical biology. Chemistry attracted around 50 freshmen, chemical biology 120; the next year there

*continued on page 21*

# A First-Class Event for First-Class Young Chemists—37th International Chemistry Olympiad 2005

**The 37th International Chemistry Olympiad (IChO), held in Taipei from 16 to 25 July 2005, was a great success. This year, 59 countries competed and 6 countries attended as second-time observers, bringing 225 high school student competitors, 117 mentors, 37 scientific observers, and 34 guests to this great event.**

*Olympiad participants take the theoretical exam in the auditorium of the National Taiwan Normal University.*

Both the competitors and their escorts expressed enthusiastic appreciation of the excellent conditions under which the competition took place and of the program organized by the Department of Chemistry and Science Education Center of the National Taiwan Normal University (NTNU). The event helped draw the public's attention to the importance of the natural sciences, and of chemistry in particular. The chair of the International Steering Committee, Dr. Kurt B. Nielsen of Denmark, noted that it was "a very good IChO. Everything worked. It was a good example to follow."

*A member of the Russian federation accepts the absolute first prize from Yuan-T Lee.*

The five-hour practical laboratory competition was held on 19 July at National Taiwan University, and the five-hour theoretical examination on 21 July at the NTNU College of Science, where the students stayed during the IChO. The two unforgettable international jury sessions for tasks discussion and translation were held at the National Academy of Educational Research, which housed the mentors, scientific observers, and guests from 15 to 20 July. A gala reunion dinner for students and teachers was held 21 July at the Grand Hotel, which housed the teachers from 21 to 24 July. In addition, during the competition and while the mentors were grading and arbitrating the exams, many cultural, social, and science-related events were held for both students and teachers.

*The practical exam was held in the six big labs of the National Taiwan University.*

An Informal Steering Committee meeting was convened on 22 July, and the final jury session on 23 July to discuss IChO business and decide on the winners. The distribution of awards was as follows: ranks 1–26, 26 golds (11.5%); ranks 27–74, 48 silvers (21.3%); and ranks 75–154, 80 bronzes (35.2%). In addition, six honorable mentions and three special awards were given: the absolute first prize award, the best theoretical examination award, and the best practical examination award. Award winners received prizes from the 1986 Chemistry Nobel Laureate, President Yuan-Tze Lee; Premier of the Executive Yuan, Chang-Ting Hsieh; Ministers Tu (Education) and Wu (Science Council); and the president of the Chemical Society.


*Organizers of the 37th IChO 2005 meet the press on 15 July 2005.*

The next IChO will be held in Gyeongsan, South Korea, 2 to 11 July 2006.

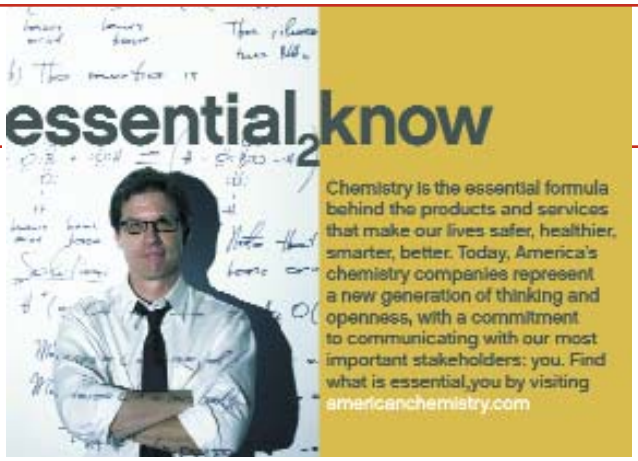
http://icho2006.kcsnet.or.kr

## Essential to You

**In September 2005, the American Chemistry Council (ACC), the trade association for the world's leading companies engaged in the business of chemistry, launched a major public education campaign to increase awareness of the chemistry industry's contributions to modern life, from innovations in everyday products to its contribution to the U.S. economy.**

The educational campaign demonstrates how the American chemistry industry is essential to ("essential$_2$℠") safety, health, innovation, the economy, and the environment. The campaign encompasses advertising, public relations, a new website, and employee communications.

"The initiative makes use of 'essential$_2$' as an homage to the traditional display of a chemical compound formula one would see on the periodic table of elements in any science classroom," said Michael Campbell, Chairman, President and CEO of Arch Chemicals and Chairman of the Board of Directors of ACC in a press release issued by ACC. "The campaign is a constructive way for us to engage and have a dialogue with the very people who use, enjoy and benefit from our products."




This is an inspiring undertaking for America's chemical makers and for industries that use the products of chemistry," said ACC President and CEO Jack N. Gerard in the ACC press release. "'essential2' makes a powerful statement about how connected we all are and how central chemistry is to the health and growth of our nation. For example, the chemistry industry is America's leading exporter, accounting for 10 percent of all U.S. exports, and we generate more than half a trillion dollars for the U.S. economy each year."

A central feature of the campaign is a new website <www.americanchemistry.com> highlighting the industry's contributions to technological advances and economic performance. The site also demonstrates the economic contributions of the industry to each state, including employment, exports, and tax data.

**www.americanchemistry.com**

## Two New CAs Join IUPAC

**Two industrial companies from the United Kingdom have joined IUPAC as Company Associates. AstraZeneca R&D Charnwood and Syngenta will now take part, with more than 100 companies from around the world, in the work of the Committee on Chemistry and Industry to influence the IUPAC agenda.**

The United Kingdom is one of the major hubs of AstraZeneca—one of the world's leading pharmaceutical companies. The company's Charnwood site is focused on finding new medicines for respiratory diseases such as asthma, chronic bronchitis, and emphysema (diseases often associated with smoking and for which new medicines are desperately needed) as well as inflammatory diseases such as rheumatoid and osteoarthritis.

Syngenta's Jealott's Hill, established in 1927, is a center of excellence for discovery and bio-performance research and is a key site for environmental sciences. It is the company's largest research site, employing over 800 scientists and support staff. Jealott's Hill houses the company's main collection of hundreds of thousands of chemical compounds. Over 200 000 chemicals are added to the collection from a variety of sources each year. It is also the Syngenta global center for environmental sciences and works closely with Syngenta CTL to ensure all products are tested for safety in the environment.

**AstraZeneca R&D Charnwood**
Dr. John Dixon <john.dixon@astrazeneca.com>
Vice President; Drug Discovery
<www.astrazeneca.com>

**Syngenta**
Jeollot's Hill International Research Station
Bracknell, Berkshire
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<www.syngenta.co.uk/about/syngenta-jealotts-hill.asp>

**www.iupac.org/links/ca.html**

## Strengthening International Science—A Recurring Catchphrase from ICSU

**In an unprecendented statement to the U.N. General Assembly, the leadership of international scientific, engineering, and medical organizations urged the heads of state and government meeting in New York in September 2005 to strengthen worldwide capacities in science, technology, and innovation. Stronger capacities in science and technology are required to allow humanity to achieve the U.N. Millennium Development Goals (MDGs), the statement concludes. In September 2000, 147 heads of state and government, and 189 nations in total, committed themselves by year 2015 to reduce significantly global poverty and the related problems of illiteracy, hunger, discrimination against women, unsafe drinking water, and degraded environments and ecosystems.**

Among the signers of the statement was ICSU President Jane Lubchenko, who, along with leaders of the other organizations, made a commitment to help strengthen global capacities for achieving the Millennium Development Goals. The group stated that "sustained progress in reducing poverty and related problems require strengthened institutions for science, technology, and innovation throughout the world, including in each developing nation."

In a press release, Thomas Rosswall, Executive Director of ICSU stated that "ICSU is committed to help implement the challenges to the international scientific community in line with its pledges to the World Summit on Sustainable Development. Science is essential for sound decision making as well as for technological development and national innovation systems. The MDGs can be met if international science is strengthened for the benefit of society. Science and technology are necessary, but not sufficient, prerequisites for achieving the MDGs."

More recently, at its General Assembly this past October in Suzhou, China, ICSU released a new strategy to strengthen international science for the benefit of society. Acknowledging that the world of scientific research has not lived up to its full potential in addressing some of society's most pressing concerns, including the terrible impact of natural disasters, ICSU announced an ambitious plan of action to strengthen international science for the benefit of society. It will focus on interdisciplinary science in key areas of policy uncertainty, including sustainable development, and efforts to mitigate the impact of disasters such as the recent earthquake in Kashmir, Hurricane Katrina, and the tsunami in the Indian Ocean.

"The tsunami and Hurricanes Katrina and Rita have demonstrated the devastating consequences to people and property of the removal of natural storm surge barriers such as wetlands, mangroves, and coral reefs," said ICSU President Jane Lubchenco in a press release. "When coastal development ignores scientific information about the critical protecting functions of these ecosystems, people are at greater risk. The world needs natural, social and economic scientists to work together, tailor their research and share their findings more effectively," she continued.

www.icsu.org

## Up for Discussion *continued from page 18*

was no change in the number for chemistry, but in chemical biology it was now 150! So for 2005 we shall have to limit the number of students.

So are chemistry departments in other countries not offering the right courses? This cannot be the answer, as traditional chemistry is still a popular option in Germany, but not elsewhere in Europe. How about the image of chemistry? Germany had a "year of chemistry" in 2003, which certainly did make an impression, but will have virtually no effect on the numbers for 2004 (which in fact dropped slightly in any case!).

Can it be the career prospects? Well, we do not know exactly how young people perceive things, but in real terms the situation of the chemical industry in Germany has not been improving lately: Of the original "big three," Hoechst and Bayer no longer exist in their original form (Hoechst not at all!), and only BASF is still flying the flag and referring to itself as "The Chemical Company."

So we have an unanswered question. What can chemists in other countries learn from the present German situation? Well, if you are looking for doctoral students or postdocs, Germany will still be a good source of them for the next few years!

**Terry Mitchell <terence.mitchell@uni-dortmund.de> is a professor at Dortmund University (Germany); he is national representative on the IUPAC Committee on Chemistry Education.**

# The Project Place

Information about new, current, and complete IUPAC projects and related initiatives.
See also www.iupac.org/projects

## Developments and Applications in Solubility

Solubility is a basic phenomenon underlying most industrial processes. The objective of this project is to produce a book that will bring together recent developments in solubility studies that have a bearing on industrial applications, especially the rigorous work that is underpinned by thermodynamic considerations.

The book will highlight important areas of new research involving theory, techniques, results, modeling, simulation, and industrial applications related to solubility. It will include chapters on super-critical fluids, data banks, "green chemicals," molten salts, liquid-liquid phase equilibria, nanotechnology, industrial solutions including cryogenic solutions, predictions, simulations and molecular modeling, gases in polymers, metallurgical and hydrometallurgical processes, separation processes, and the food, pharmaceutical, and cosmetics industries.

**For more information or to comment on this project, contact Task Group Chairman Trevor M. Letcher <trevor@letcher.eclipse.co.uk>.**

**www.iupac.org/projects/2005/2005-016-1-100.html**

Trevor M. Letcher's most recent book, *Chemical Thermodynamics for Industry*, was published in October 2004 by the Royal Society of Chemistry (ISBN 0 85404 591 0). It presents the latest developments in applied thermodynamics and highlights the role of thermodynamics in the chemical industry. To learn more about the book, go to <www.iupac.org/publications/books/author/letcher04.html.>

## Glossary of Terms Related to Solubility

This project will define terms related to the phenomenon of solubility, including both experimental and theoretical aspects of gas-liquid, liquid-liquid, and solid-liquid solubility. The terms and definitions will be presented in glossary format and published as IUPAC Recommendations in *Pure and Applied Chemistry*. The glossary will be made available for inclusion in the *IUPAC Compendium of Chemical Terminology* (the Gold Book) and the *Compendium of Analytical Nomenclature* (the Orange Book) as well as in other non-IUPAC publications.

**For more information, contact Task Group Chairman David Shaw <ffdgs@uaf.edu>.**

**www.iupac.org/projects/2005/2005-017-1-500.html**

## e-Quiz for Promoting Chemical Education

A chemistry quiz titled "Rasayanika" ("chemistry" is "rasayan" in Sanskrit) was conducted in Delhi in 2003 under the auspices of the JK Foundation for Human Development (JKFGD). JKFGD is a part of the JK Organization, one of the most prestigious industrial houses in India. The quiz was an adaptation of the pioneering Australian National Chemistry Quiz developed by Dr. Charles Fogliani under the auspices of the Royal Australian Chemical Institute. Dr. Fogliani has been conducting his quiz in the Australasian region since the 1980s.

Rasayanika was designed to improve awareness of the role that chemistry plays in everyday life in a developing country like India. The highly enthusiastic response from students and teachers in 2003 led to the idea of conducting the quiz outside Delhi in 2004.

Moving Rasayanika to an online format is now desirable; doing so will allow the quiz to reach a wider audience and will professionalize the assessment tools and techniques, allowing Rasayanika to become a catalyst for improving student interest in chemistry. To enable the participation of schools where chemistry is not taught in English, the online version will also be accessible in local languages.

The objective of this project is to design the online version of the exploratory trials conducted in 2003 and 2004. An online quiz will allow students from across India to participate in the 2005–2006 quiz and

will pave the way for its regional extension. Participants in the program will need to take the following consideration into account:

- A question bank will need to be designed and developed, and the questions categorized. Each question should test conceptual ability, application ability, numerical ability, or another specified skill.
- Participants' performance will be analyzed for each question on a five-point scale. The analysis will be made available to all the schools with comments and suggestions for follow-up. It is hoped that this step will motivate many schools to begin a capacity-building program in chemical education.
- The analysis will also be used to validate the items in the question bank. This will permit labeling of questions in the bank by the so-called discrimination index, which indicates the efficacy of an item for assessing student performance.
- To attract large student turnout, Rasayanika 2005 will be held under the IUPAC CCE banner, and all quiz certificates will be signed by the IUPAC president, the CCE chairman, and the chairman of the IUPAC Subcommittee on Chemistry Education for Development.
- To facilitate the participation of students from non-English medium schools, the quiz will also be conducted in local languages. Because India shares some languages with some of its neighbors, the geographical scope of the quiz could be extended, helping to foster regional cooperation in chemical education.
- The program should establish a platform for bringing together specialists (for creating the Question Bank and for validating the items in the bank), school teachers (for providing feedback), industry and government agencies (for instituting awards), and university teachers (for initiating capacity-building programs for schools and teachers).

In summary, the task group envisages the online quiz as a catalyst for enhancing student appreciation of chemical science as a creative and a dynamic field. Although India is the focus of the current project, once an online tool is created, the quiz can be expanded into other geographic regions.

**For more information, contact Task Group Chairman K.V. Sane <sitah@bol.net.in>.**

**www.iupac.org/projects/2005/2005-003-2-050.html**

## Solubility Data Series: Transition and 12 to 14 Main Group Metals, Lanthanide, Actinide, and Ammonium Halates

A volume of the *Solubility Data Series* will include compilations and critical evaluations for the solubility of transition metal, lanthanide, and actinide halates. The solubility data for the halates of metallic elements in groups 12 to 14 will also be included. Whereas the solubility of ammonium iodate has been compiled and evaluated previously, data on ammonium chlorate (and bromate) have been lacking. Data related to ammonium chlorate are now available and are included in this volume.

Compilations for the solubilities of the title halates in water and organic solvents (such as methanol, ethanol, and dimethyl sulfoxide) and those in aqueous-organic solvent mixtures, aqueous electrolytes, and buffer solutions are included in this volume. The critical evaluations and compilations of the halate solubilities deal only with the simple salts of a type of $MX_y$ (M = metal; X = halate) and do not treat complex compounds such as hexaamminecobalt(III) halates, $[Co(NH_3)_6]X_3$.

The halates of these metals are related to industrial processes. For example, some halates are essential as catalysts, heat stabilizers, and blanching reagents for manufacturing polymer products such as textiles and resins. Some halates are used in pyrotechnic compounds for weather modification and colored smoke generation. The nonlinear halate crystals are important for the construction of optical devices.

**For more information, contact Task Group Chairman Hiroshi Miyamoto <rmiya@cc.hirosaki-u.ac.jp>.**

**www.iupac.org/projects/2005/2005-033-1-500.html**

## Flying Chemists Program—A Visit to India

In July 2005, Professors Peter Atkins and Ram Lamba (IUPAC Committee on Chemistry Education [CCE] and Subcommittee on Chemistry Education for Development) participated in a one-week program in India coordinated by Professor K.V. Sane. The program included seminars and discussions with academics, industrial houses, and government agencies. The aim of this visit—the first under the new CCE Flying Chemists Program—was to identify viable strategies for professional development of in-service and preservice teachers. These strategies include the design of an Internet-linked system that will equip chemistry teachers with some of the skills needed to become an effective teacher—specifically, skills related to promoting student interest by using a discovery-based approach to teaching and learning.

During the week-long program, lectures, workshops, and interactive sessions were presented for an audience that included teachers, principals, and school management. The program was organized by the DAV College Management Society and the Gujarat Education Society. The two societies have a combined network of more than 600 schools and colleges across India.

A follow-up project on capacity building, drafted by Professor Sane in consultation with Professors Atkins and Lamba, will integrate relevant portions of the proposals on microscale chemistry and e-quizzes and will focus on:

- curriculum development
- development of new assessment tools
- design and implementation of hands-on experiences at all levels of chemistry education, using the microscale approach wherever feasible
- promotion of partnerships among universities, between universities and industries, and among universities, industries, and governments
- development of self-learning and self-assessment approaches based on state-of-the-art technological tools; this exercise will yield items to be included in a Question Bank set up by teachers for fellow teachers
- creation of international and intranational networks for real and virtual partnerships for sharing and monitoring innovative practices

The project will attempt to revitalize the teaching-learning process through an e-cooperative formed by teachers for teachers.

**For more information contact Task Group Chairman K.V. Sane <sitah@bol.net.in>.**

**www.iupac.org/projects/2005/2005-004-1-050.html**

## What is the Flying Chemists Program?

In January 2005, the Committee on Chemistry Education (CCE) embarked on a new initiative: the Flying Chemists Program (FCP). The aim of the program is to help emerging countries improve the teaching and learning of chemistry at the primary, secondary, and tertiary levels. FCP will provide a country with the expertise needed to strengthen its chemistry education program and will assist in the program's development.

FCP will generally be implemented in economically disadvantaged countries. The host country will provide boarding and lodging for the FCP experts, and CCE will provide the airfare. Visits will be considered only if invitations are received from a national society, a ministry of education or technology, or other comparable organization.

FCP is intended to:

- assist in the development of curricula
- help develop or recommend new assessment tools
- help develop different approaches to the teaching of chemistry, including hand-on experiences
- help develop and implement teacher training and preparation programs
- assist in the establishment of partnerships among universities, industries, and governments
- develop successful international conferences to gain expert advice on a particular aspect of chemistry education
- help identify and approach sources of funding

The host country is expected to make thorough preparations for the visit and to coordinate all activities related to achieving the specific goals and objectives of the visit. In addition, the host country should plan meetings with academics, industry representatives, and government agencies in order to identify future viable strategies for strengthening chemistry education.

**For more information, contact Program Coordinator and CCE Subcommittee on Chemistry Education for Development Chairman Ram S. Lamba <rlamba@cayey.upr.edu>.**

**www.iupac.org/standing/cce/FCP.html**

## Global Climate Change—Translation and Dissemination of a Monograph for Secondary Schools

A booklet on global climate change has been produced by the Italian Consorzio Interuniversitario Nazionale (INCA) "La Chimica per L'Ambiente." The booklet constitutes one of the early chapters of the senior secondary textbook *Introduction to Green Chemistry*, which will be produced by INCA as part of its Green Chemistry Series. The monograph is gaining considerable popularity in Italy and has been adopted by numerous science teachers for inclusion in their curriculum.


To serve as a resource for secondary schools in other parts of the world, the booklet must be translated into other languages—ideally, into English, Portuguese, and Spanish, to start. Translation into these languages will permit the booklet's wide distribution, including to parts of Europe, the United Kingdom, Australia and New Zealand, South Africa, and most of the countries in the North and South American continents.

Accordingly, the objectives of this program are to:

- translate the booklet into the designated languages
- provide 2 000 copies of the translated booklet for initial dissemination and evaluation by relevant secondary school authorities, professional science teaching bodies, and secondary teachers in Australia, Portugal, Spain, and other selected countries
- demonstrate the central role of chemistry in global issues and highlight the contribution of green chemistry
- determine the potential demand for this booklet in secondary schools

In the original version of the booklet, the "Perspectives" section was dedicated to the Kyoto protocol and issues closely tied to Europe and Italy. In the translations, this section will be updated and customized to address the issues facing each user country.

**For more information, contact Task Group Chairman Pietro Tundo <tundop@unive.it>.**

**www.iupac.org/projects/2005/2005-015-1-300.html**

## Distance Learning in Toxicology: Effective Teaching through Technology

In the past few years, distance learning has come of age: Registration is expanding, types of offerings are proliferating, and the skepticism surrounding this form of education is being dispelled by its common-sense, practical advantages. The rapid rate of development has been boosted by the increased awareness of programs by both teachers and students and their appreciation of its blend of electronic tools with pedagogy and asynchrony with synchrony.

The objective of this project is to present and clarify issues surrounding the development and delivery of online courses in toxicology—the effect of chemicals on humans, animals, and the environment. Instruction in the development of these courses and several examples of robust programs around the world will be presented. Discussions relating to the cost, delivery, effectiveness, and overall quality of these programs will be incorporated into a symposium organized in the framework of this project; both the thinking and the technological tools behind development of the courses will be presented. The task group overseeing the symposium is Jane Huggins and John Morris (Drexel University), Kristine Willett (University of Mississippi), John Duffus (Edinburgh Centre for Toxicology), and Paul Wright (Royal Melbourne Institute of Technology).

The symposium will be presented at the Society of Toxicology annual meeting in San Diego, California, 5–9 March 2006.

**For more information, contact Task Group Chairman Jane Huggins <dona.jane.huggins@drexel.edu>.**

**www.iupac.org/projects/2005/2005-013-1-700.html**

## IUPAC Stability Constants Database—Completion of Data Collection up to 2006

The IUPAC Stability Constants Database (SC Database) is the most comprehensive compilation of stability constants available, now covering the years 1877 to 2002. It is a major research tool for those involved in equilibrium modeling of environmental, biological, and industrial systems, and it is the primary source of data for the *Critical Evaluations of Stability Constants* that are published regularly by the IUPAC Analytical Chemistry Division (Division V).

The SC Database records solution equilibrium data (lg $K$, $\Delta H$, $\Delta S$) abstracted from 55 mainstream journals. It includes all of the data from the previous volumes published before 1972 by IUPAC and RSC. Publications from 1972 to 2002 were evaluated and abstracted through a series of projects by Commission V.6, then Division V. The database now contains some 105 500 records (pages of data) from 22 000 references for 9 000 ligands, forming a unique compilation of significant published solution equilibrium constants.

The SC Database can be searched by ligand (formula, name, fraction of name, structure fragment, ligand class), metal ion, author, reference, method, medium, or any combination thereof. Data resulting from an SC Database search can be exported to a powerful speciation program or to programs for temperature and ionic strength corrections. Coupled with its ancillary programs, it has no equivalent competitor.

There is no indication that the publication of articles on solution equilibria has declined in the past 10 years, although there have been changes in the popularity of specific journals for this work (e.g., an increasing use of biological journals and study of biologically relevant ligands). Furthermore, the average number of records derived from each article has remained essentially constant. This trend indicates a continuing interest in the field and also an ongoing need for literature evaluation and abstracting of data.

The continuing flow of publications and the shifting focus of experimental work (and published data) onto new classes of ligands (e.g., biological buffers, ligands used in medicinal and pharmaceutical applications, and macrocyclic ligands) ensures an ongoing demand for IUPAC's SC Database. It also ensures an ongoing need for IUPAC projects that will contribute to the *Critical Evaluation of Stability Constants*.

The current database can be ordered at <www.iupac.org/divisions/V> or <www.acadsoft.co.uk>. Each of these sites offers a downloadable demo version of the database.

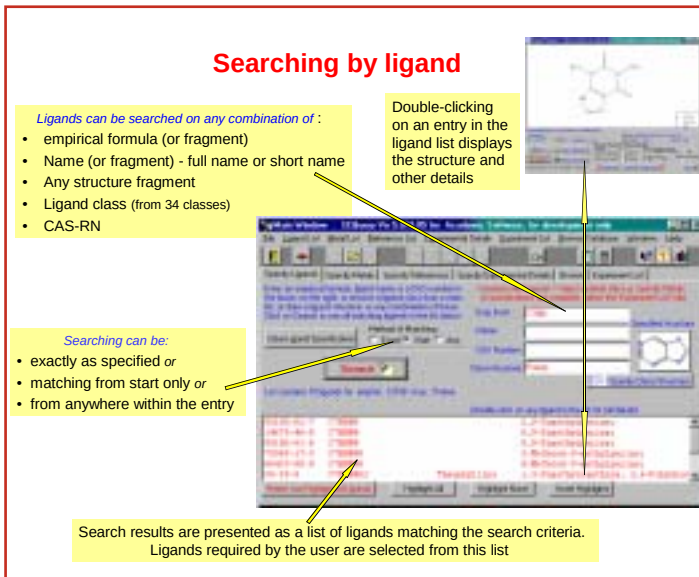
The aim of the present project is to:

- bring the literature coverage in the SC Database up to date to 2006, to be accomplished by 2008 (Coverage is currently complete to the end of 2002 for 26 mainstream journals, to 2001 for 11 journals, and to 2000 for nine journals of the 55 that are currently abstracted.)
- expand the team of experts who supervise data entry and oversee quality control
- establish a succession of experts to continue this work beyond the current project

Members of the project team who are responsible for literature abstracting, data evaluation, and data entry are Kip Powell (New Zealand), Tamás Gajda (Hungary), Igor Sukhno (Russia), and Erich and LanChi Königsberger (Australia). Expressions of interest from additional experts are welcome.

**For more information , contact Task Group Chairman Kip Powell <kip.powell@canterbury.ac.nz>.**

**www.iupac.org/projects/2005/2005-014-1-500.html.**



# Provisional Recommendations

## IUPAC Seeks Your Comments

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

www.iupac.org/reports/provisional

## JCAMP-DX for Electron Magnetic Resonance

In this document, we define a data exchange format initially formulated from discussions at the 35th Royal Society of Chemistry-ESR conference in Aberdeen 2002. The definition of this format is based on the IUPAC Joint Committee on Atomic and Molecular Physical Data Exchange (JCAMP-DX) protocols, which were developed for the exchange of infrared spectra and extended to chemical structures, nuclear magnetic resonance data, mass spectra and ion mobility spectra. This standard was further extended to cover year 2000 compatible date strings and good laboratory practice and the next release will cover the information needed for storing n-D data sets. The proposed recommendations aim at adapting JCAMP-DX to the special requirements for EMR, electron magnetic resonance.

**Comments by 31 January 2006**

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www.iupac.org/reports/provisional/abstract05/lancashire_310106.html

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

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

**Comments by 31 January 2006**

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## Quantities, Units and Symbols in Physical Chemistry, Third Edition

The purpose of this manual is to improve the exchange of scientific information among the readers in different disciplines and across different nations. As the volume of scientific literature expands, each discipline has a tendency to retreat into its own jargon. This book attempts to provide a readable compilation of widely used terms and symbols from many sources together with brief understandable definitions. This third edition reflects the experience of the contributors with the previous editions and we are grateful for the many thoughtful comments we have received. Most of the material in this book is "standard," but a few definitions and symbols are not universally accepted. In such cases, we have attempted to list acceptable alternatives.

The book has been systematically brought up to date and new sections have been added. As in previous editions, the first chapter describes the use of quantity calculus for handling physical quantities and the general rules for the symbolism of quantities and units and includes an expanded description on the use of roman and italic fonts in scientific printing. The second chapter lists the symbols for quantities in a wide range of topics used in physical chemistry. New parts of this chapter include a section on surface structure. The third chapter describes the use of the International System of units (SI) and of a few other systems such as atomic units. Chapter 4 outlines mathematical symbols and their use in print. Chapter 5 presents the 1998 revision of the fundamental physical constants, and Chapter 6 the properties of elementary particles, elements and nuclides. Conversion of units follows in Chapter 7, together with the equations of electricity and magnetism in their various forms. Chapter 8 is entirely new and outlines the treatment of uncertainty in physical measurements. Chapter 9 lists abbreviations and acronyms. Chapter 10 provides the references, and Chapter 11, the Greek alphabet. Chapter 12 ends with the indexes.

**Comments by 31 March 2006**

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www.iupac.org/reports/provisional/abstract05/stohner_310306.html

## Glossary of Terms Used in Photochemistry

The first edition of the *Glossary of Terms Used in Photochemistry* ("Glossary") prepared for publication in the Commission of Photochemistry of the IUPAC Division of Organic Chemistry by S. E. Braslavsky and K. N. Houk was published in 1988 [*Pure Appl. Chem.* **60**, 1055–1106 (1988)] and has been incorporated in the *Handbook of Organic Photochemistry* and in *Photochromism: Molecules and Systems*.

The second edition of the "Glossary" prepared by Jan Verhoeven and published in 1996 [*Pure Appl. Chem.* **68**, 2223–2286 (1996)] corrected some minor mistakes in the first one and was expanded especially to incorporate terms related to (photoinduced) electron transfer processes. Major photochemistry and photobiology journals have since adopted the "Glossary" as a guideline.

This third edition incorporates revisions and enhances the "Glossary" introducing terms related to molecular anisotropy, the use of polarized ultraviolet, visible, or infrared radiation, and nonlinear optical techniques, as well as the emerging field of computation of excited species. Some changes have been introduced in this "Glossary" regarding the terms related to radiation energy to make this collection fully compatible with internationally agreed upon terms.

**Comments by 31 March 2006**

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www.iupac.org/reports/provisional/abstract05/braslavsky_310306.html

## Postgenomic Chemistry (IUPAC Technical Report)

***Sergey Varfolomeyev, et al.***

*Pure and Applied Chemistry*
*Vol. 77, No. 9, pp. 1641–1654 (2005)*

Systematic investigation of DNA structures and the decoding of genomes of various microorganisms, plants, and humans established the basis for a quantitative leap in modern natural science. Numerous areas of chemistry can benefit from the ongoing genomic revolution. Recent outstanding achievements in genomics and proteomics illustrate considerable potential for chemists to investigate the structure and functions of biomacromolecules and biosystems.

The bulk of information currently available on protein-coding nucleotide sequences in genomes of different species is growing exponentially. Bioinformatics and chemoinformatics methods raise the challenge of identification of all molecular structures in biological systems. In turn, these developments may lead to new fields of chemistry. Development of new large-scale and high-throughput projects oriented toward the generation and application of genomic information suggests a model for the development of chemical projects on a similar scale. The use of chemistry in the development of new biomimetic structures that incorporate artificial amino acids or other compounds is of particular importance. The following avenues represent potential advances in postgenomic chemistry:

- combinatorial chemistry and automated chemical synthesis
- synthesis of new classes of unnatural amino acids and development of new biosynthetic methods to prepare proteins containing these amino acids; studies on altering aminoacyl-tRNA-synthetase specificity by methods of molecular evolution
- chemical management of biosystems at the molecular level
- new approaches for classification of enzymes on the basis of structures of enzymatic active sites
- creation of new polymer catalysts using the principles of enzyme catalysis
- self-multiplying polymers: chemical models of DNA-polymerases
- new methods of analytical chemistry that are based on microchip and nanochip technologies

Genomic and proteomic studies can significantly influence chemical education. At present, instruction in molecular biology, genetic engineering, genomics, and proteomics in chemistry departments at most universities is unsatisfactory and should rise to the postgenomic challenge. The development of new courses such as "chemical basis of genomic studies," "genes and genomes for chemists," and "bio- and chemoinformatics" is essential to increasing the attractiveness of chemistry as a field of study and accelerating the development of postgenomic chemistry. This report, based on the opinions of experts working in various fields of biomolecular chemistry, should be helpful in developing strategic directions for future development of chemical sciences.

**www.iupac.org/publications/pac/2005/7709/7709x1641.html**

## Measurement and Interpretation of Electrokinetic Phenomena (IUPAC Technical Report)

***A.V. Delgado, F. González-Caballero, R.J. Hunter, L.K. Koopal, and J. Lyklema***

*Pure and Applied Chemistry*
*Vol. 77, No. 10, pp. 1753–1805 (2005)*

Electrokinetic phenomena (EKP) can be loosely defined as all those phenomena involving tangential fluid motion adjacent to a charged surface. They are manifestations of the electrical properties of interfaces under steady-state and isothermal conditions. In practice, they are often the only source of information available on those properties. For this reason, their study constitutes one of the classical branches of colloid science, electrokinetics, which has been developed in close connection with the theories of the electrical double layer (EDL) and of electrostatic surface forces.

In this report, the status quo and recent progress in electrokinetics are reviewed. Practical rules are recommended for performing electrokinetic measurements and interpreting their results in terms of well-defined quantities, the most familiar being the $\zeta$-potential or electrokinetic potential. This potential is a property of charged interfaces, and it should be inde-

pendent of the technique used for its determination. However, often the $\zeta$-potential is not the only property electrokinetically characterizing the electrical state of the interfacial region; the excess conductivity of the stagnant layer is an additional parameter. The requirement to obtain the $\zeta$-potential is that electrokinetic theories be correctly used and applied within their range of validity.

Also in this report, basic theories and their application ranges are discussed and a thorough description of the main electrokinetic methods is given, with special attention paid to their ranges of applicability as well as to the validity of the underlying theoretical models. Electrokinetic consistency tests are proposed in order to assess the validity of the $\zeta$-potentials obtained. The recommendations given in the report apply mainly to smooth and homogeneous solid particles and plugs in aqueous systems; some attention is paid to nonaqueous media and less ideal surfaces.

www.iupac.org/publications/pac/2005/7710/7710x1753.html

## Evaluated Kinetic Data for Combustion Modeling: Supplement II

***D.L. Baulch, et al.***
*Journal of Physical and Chemical Reference Data*
*Vol. 34, No. 3, pp. 757–1397 (2005)*
doi:10.1063/1.1748524

This compilation updates and expands two previous evaluations of kinetic data on elementary, homogeneous, and gas phase reactions of neutral species involved in combustion systems [*J. Phys. Chem. Ref Data* **21**, 411 (1992); **23**, 847 (1994)]. The work has been carried out under the auspices of the IUPAC Commission on Chemical Kinetics and the UK Engineering and Physical Sciences Research Council. Individual data sheets are presented for most reactions, but the kinetic data for reactions of $C_2$, C, ethyl, *i*-propyl, *t*-butyl, and allyl radicals are summarized in tables. Each data sheet sets out relevant thermodynamic data, experimental kinetic data, references, recommended rate parameters with their error limits, and a brief discussion of the reasons for their selection. Where appropriate, the data are displayed on an Arrhenius diagram or by fall-off curves. Tables summarizing the recommended rate data and the thermodynamic data for the reactant and product species are given and their sources referenced. As in the previous evaluations, the reactions considered relate largely to the combustion in air of organic compounds containing up to three carbon atoms and simple aromatic compounds. Thus, the database has been expanded, largely by dealing with a substantial number of extra reactions within these general areas.

## Solubility Data Series—Recent Reports

**Gaseous Fluorides of Boron, Nitrogen, Sulfur, Carbon, and Silicon and Solid Xenon Fluorides in All Solvents (IUPAC-NIST Solubility Data Series 80)**
H. Lawrence Clever, et al.
*J. Phys. Chem. Ref. Data*, Vol. 34, No. 1, pp. 201–438 (2005)
<www.iupac.org/publications/sds/2005/80_abstract.html>

**Hydrocarbons with Water and Seawater—Revised and Updated (IUPAC-NIST Solubility Data Series, Vol. 81; part I to VIII)**
Andrzej Maczynski (volume editor)
*J. Phys. Chem. Ref. Data*, Vol. 34, No. 2 (2005)
Part I. C5 Hydrocarbons with Water, pp. 441–476
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Part III. C6H8-C6H12 Hydrocarbons with Water and Heavy Water, pp. 657–708
Part IV. C6H14 Hydrocarbons with Water, pp. 709-753
*J. Phys. Chem. Ref. Data*, Vol. 34, No. 3 (2005)
Part V. C7 Hydrocarbons with Water and Heavy Water, pp. 1399–1487
Part VI. C8H8-C8H10 Hydrocarbons with Water, pp. 1489–1553
*J. Phys. Chem. Ref. Data*, Vol. 34, No. 4 (2005)
Part VII. C8H12-C8H18 Hydrocarbons with Water, pp. 2261–2298
Part VIII. C9 Hydrocarbons with Water, pp. 2299-2345
<www.iupac.org/publications/sds/2005/81_abstract.html>

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www.iupac.org/publications/sds/volumes.html

## Biological and Synthetic Polymer Networks and Gels

F. Horkay and E.J. Amis (editors)
*Macromolecular Symposia*, Vol. 227
Wiley-VCH, 2005, pp. 1-382
ISBN 3-527-31330-3

Polymer science is by nature an interdisciplinary field, traditionally spanning chemistry, physics, and engineering. One of the most promising new developments in polymer science is its interaction with other disciplines such as biology and medicine.

This volume contains the text of selected presentations from the Polymer Networks 2004 Conference—a conference designed to provide an interdisciplinary forum for physical scientists, engineers, biologists, and clinicians to meet and discuss their work, exchange ideas, and assess the latest developments in the rapidly expanding field of polymer gels and networks. The most recent advances in eight categories were presented and discussed at the conference: phase transition in synthetic and biopolymer gels, associating/self-assembly systems, polyelectrolytes and intelligent gels, controlled synthesis of networks, tissue engineering and hydrogel scaffolds, nanoparticles in diagnostics and therapeutics, gene and drug delivery, and simulation and modeling of polymer networks.

The conference, organized and sponsored by the National Institutes of Health and the National Institute of Standards and Technology under the auspices of IUPAC, focused on all areas relevant to the formation, structure, properties, and applications of synthetic and natural polymer networks and gels, including materials science, nanotechnology, surface science, rheology, tissue engineering, and modeling. In particular, the conference explored experimental tools and theoretical models to describe biological phenomena with physical concepts that allow predictive, model-driven research. This knowledge is essential for understanding, designing, and controlling material properties and performance. The collection of papers in this volume illustrates that increased understanding of the behavior of complex gel systems is critical to developments in biomedical research, biotechnology, diagnostics, dentistry, and medicine.

www.iupac.org/publications/macro/2005/227_preface.html

## Magnituds, Unitats I Símbols en Química Física

Versio catalana de la segona edcio anglesa a cura de Josep M. Costa. Editat per l'Institut d'Estudis Catalans, Barcelona, Spain (2004), ISBN 84-7283-733-5

[Catalane translation of IUPAC "Green Book", *Quantities, Units, and Symbols in Physical Chemistry*, 2nd edition. Prepared for publication by Ian Mills, Tomislav Cvitas, Klaus Homann, Nikola Kallay, and Kozo Kuchitsu. Blackwell Science (1993)]

This Catalane translation of the 2nd edition of the IUPAC "Green Book" was prepared by Josep M. Costa I Torres from the University of Barcelona, a member of the Societat Catalana de Química.

# Innovation in Chemistry

*by Xibai Qiu*

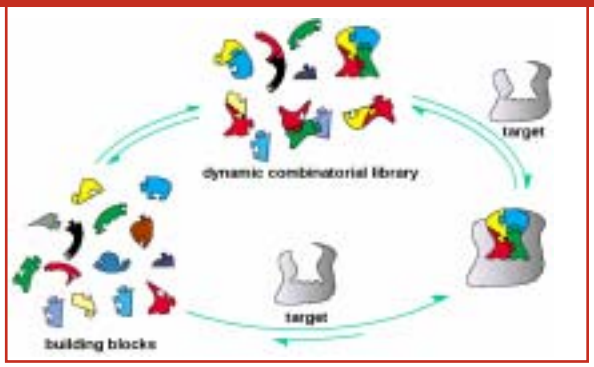
With nearly 1000 participants from 64 countries, the **40th IUPAC Congress**, held 14–19 August 2005 in Beijing, helped to build a bridge between Chinese chemists and the world. With 412 of the participants from China and 556 from other countries, the Congress was an excellent forum for encouraging cooperation and excellence in the chemical sciences and in the practice of chemistry.

The high-scientific value of the Congress was evident in the plenary lectures, which were delivered by eight distinguished chemists, including three Nobel Laureates and one Einstein Award Winner. A total of 1145 papers and 622 posters were presented in eight sessions of the Congress.

The Congress was held in parallel with the 43rd IUPAC General Assembly at the same venue, the Beijing International Convention Center. The Congress was sponsored by IUPAC, China Association for Science and Technology, Chinese Academy of Sciences (CAS), National Natural Science Foundation of China, Ministry of Science and Technology of China, Ministry of Education of China, and the SINOPEC Corporation. It was co-organized by the Chinese Chemical Society (CCS) and the Institute of Chemistry of CAS. The president of the Congress was Chunli Bai, president of CCS.

During the Opening Ceremony, IUPAC President Leiv K. Sydnes presented the 2004 and 2005 IUPAC Prize for Young Chemist Awards. On 19 August 2005, Professor Sydnes presented the IUPAC Poster Prize Awards to Zhou Jiehua from Wuhan University, China, Rattikan Chantiwas from Chiang Mai University, Thailand, and Kelly Anderson from Canterbury University, New Zealand.

*From left: Chunli Bai, president of the Chinese Chemical Society, IUPAC Poster Prize winners Zhou Jiehua (China), Rattikan Chantiwas (Thailand), and Kelly Anderson (New Zealand), and IUPAC President Leiv Sydnes.*




*Dynamic Combinatorial Library: recognize, select, stabilize and amplify—A Dynamic Combinatorial Chemistry Approach to Synthesizing and Screening Specific Ligands for RNA Ribozyme was investigated by Jiehua Zhou of Wuhan University.*

A session of the Congress on environmental and green chemistry, featured presentations on the distribution and transportation of organic and heavy metals, development of new catalysts, deep oxidation of pollutants for pollution control, investigation and characterization of high-efficiency adsorbents, and toxicities analysis.

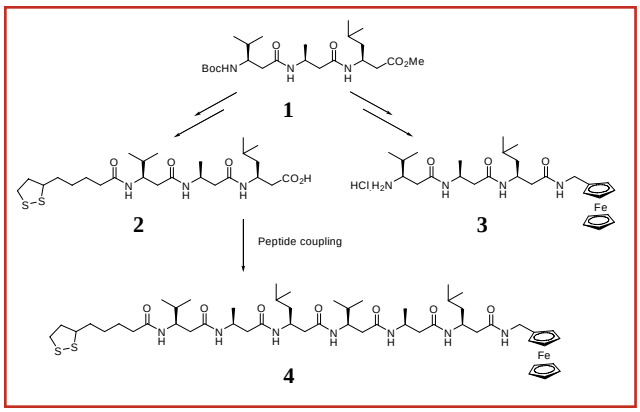
A number of presentations from the session on chemistry in the life sciences stimulated heated discussions and demonstrated the widespread enthusiasm for biological chemistry research. Many of these presentations involved recent research on nucleic acid, including "DNA Repair at Atomic Resolution" by T. Carell (Germany), "It's a Small RNA World that Makes a Big Revolution" by K. Taira (Japan), "Low Molecular Weight Protamines for Long-Acting Insulin Formulation" by Y.F. Li (Canada), and "DNA-RNA World" by P. Guga (Poland). Other presentations focused on natural compounds, including "Accessing Plant-Associated Microbial Diversity for Discovery of Small Molecule Bioactive Agents" by A.A.L. Gunatilake (USA) and "Marine Natural Products Sponge Mimics and the Role of Allelochemicals in the Field" by M. Garson (Australia).

Presentations in the session on Materials Chemistry, Supermolecular Chemistry, and Nanochemistry made it clear that the intersection of these fields will be the key to future developments in science and technology. The session on Information Technology in Chemistry and Computational Chemistry featured leading-edge research on the calculation and pharma-

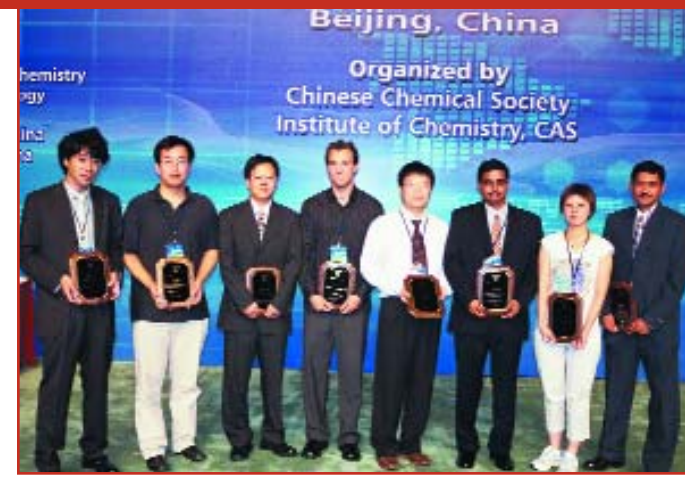
ceuticals design of bio-macromolecular systems, multi-scale analog for complex systems, progress in the quantum chemistry calculation method, chemical reactions with molecular ab initio calculation, and chemical informatics.

The session on Innovation in Physical Chemistry and Biophysical Chemistry—Research Methods and Techniques showcased the most up-to-date research in the areas of spectroscopy, catalyses, chemical dynamics, electrochemistry, thermodynamics, colloid and interfacial chemistry, and biophysical chemistry. Among the highlights were presentations on the physico-chemical properties of nano-materials and the development of new experimental methods, including imaging technology, probe technology, single-molecule reaction technology, and bio-single molecule detected technology. All of these presentations indicated the interdisciplinary nature of current research in physical chemistry.

Papers in the session on innovations in analytical chemistry related to the separation techniques of protein in human proteomics, protein zymohydrolysis, modification of nano-materials at the surface of sensor electrodes, biological nano-label techniques, new chromatographic stationary phases, monolithic columns, molecular imprinting techniques, enantiomeric separation, and analysis of chiral bio-active material and chiral pharmaceuticals. The interdisciplinary nature of analytical chemistry and life sciences was a frequent theme of this Congress. A number of lectures left a deep impression on attendees, including "Multidimensional Liquid Phase Based Separation Technique and Its Application in Proteome Study" by CCS academician Prof. Yukui Zhang, "Developments in Multi-dimensional Chromatography" by Chinese academician Prof. Erkang Wang, and "Novel Instrumentation for Electrochemical Impedance Spectroscopy" by Korean Prof. Su-Moon Park.




*Synthesis of the redox-active β-hexapeptide reported by Kelly Anderson (University of Canterbury) in her study on the electrochemical and structural properties of simple β-oligomers on gold surface.*




*Presentation of the 2004 and 2005 winners of the IUPAC Prize for Young Chemists at the Congress opening ceremony on 14 August 2005; L to R: Hiromitsu Maeda, Tokyo University of Japan; Xun Wang, Tsinghua University of China; Jiaxing Huang, University of California Berkeley; Zev Gartner, Harvard University; Zhipan Liu, Queen's University of Belfast, UK; Parag Acharya, Uppsala University of Sweden; Yu Huang, Harvard University; and S.G. Srivatsan, India Science and Technology University of Kanpur, India.*

The session on Innovation in Chemical Education and Teaching Methods attracted a large audience in addition to those who had registered in advance. The vivid and unique presentations brought participants up to date on the latest innovations in chemistry education. The first invited speaker, Viktor Obendrauf, gave a presentation on "Microscale Experiments Dealing with the History of Making Fire from Fire Drills to Jet Flame Lighters," which explained how to use microscale experiments to explain the chemical principles behind fire. Peter Atkins' lecture on "Communicating Chemistry: The Challenge" garnered big applause for its magical presentations and demonstrations.

The session on Innovation in the Chemical and Petrochemical Industries and "Responsible Care" for Society featured experts from world famous institutions such as ABB Lummus Global Inc. of the USA, UOP LLC., and the SINOPEC Corporation. Their practical and highly applicable lectures dealt with the technology of alkene, technical progress of aromatic hydrocarbons, synthesis technology of caprolactam,

branching technique development of toluene, and progress involving metallocene polyolefins.

Through the Young Chemists Program, CCS and IUPAC cosponsored 88 young chemists from 34 countries to attend the Congress. The program aims to promote young chemists' academic development and facilitate information exchange. In addition to helping the careers of these young chemists, the program provides a spark to the Congress through the valuable contributions of these chemists.

**Professor Xibai Qiu <qiuxb@infoc3.icas.ac.cn> was secretary of the 40th IUPAC Congress Program Committee; he is vice-chairman of the Committee on International Activities of the Chinese Chemical Society.**

## Solution Chemistry

*by Vojko Vlachy*

The **29th International Conference on Solution Chemistry** (ICSC) was held in Portoroz, Slovenia, 20–25 August 2005. The conference was organized by the faculty of chemistry and chemical technology at the University of Ljubljana, Slovenia.

The ICSC has been held biannually since 1967 and under the present name since 1988. The meetings, which have been held in locations ranging from Debrecen to Vaals and from Fukuoka to Vichy, are organized by a 10-member international steering committee. The present chairman of the committee is Professor Ingmar Persson from the University of Uppsala in Sweden.

The 29th ICSC was sponsored by IUPAC, and IUPAC representative Hitoshi Ohtaki gave a speech at the opening ceremony. Other guests at the opening ceremony were Bijoy Chatterjee from the Organization for the Prohibition of Chemical Weapons and Franci Demšar, director of the Slovenian Research Agency.

The theme of the conference was "the chemistry of solutions," but sessions were also held on supramolecular assemblies and nanostructures, interfaces, biophysical and pharmaceutical problems, aquatic chemistry, and others. In addition, a roundtable discussion on ionic liquids was held, sponsored by Merck. Andreas Heintz chaired the discussion, and the main contributors were Josef Barthel, Urs Welz-Biermann (Merck), Hartmut Krienke, and Chris Hardacre.

*Professor Jean-Marie Lehn during his plenary lecture "From Supramolecular Chemistry to Constitutional Dynamic Chemistry."*

A broad array of eminent scientists from around the world gave presentations and keynote lectures; a complete list can be found at <www.icsc2005.si>. The conference program also included 69 20-minute oral contributions and two poster sessions, with 160 posters in total. Moderated discussions followed each poster presentations, and each participant or group had an opportunity to show the conclusions of their study in a few slides and discuss them with the audience. An ad hoc committee chaired by Josef Barthel selected the most interesting posters, which received diplomas and practical awards. The recipients were:

- Yasuo Kameda and coworkers from Yamagata University, Japan
- Sylvia E. McLain, Rutherford Appleton Lab, United Kingdom
- Mónika Valiskó and coworkers from the University of Veszprem, Hungary
- Andrew W. Hakin, University of Lethbridge, Canada, and Harald Høiland, University of Bergen, Norway

An exhibition of scientific instruments included the participation of MicroCal LLC (United States), Mettler-Toledo (Slovenia), Merck (Germany), Sanolabor (Slovenia), and Anton Paar (Austria).

Altogether, the ICSC hosted almost 300 participants from 36 countries, including approximately 50 Ph.D. students who took advantage of the conference's reduced fees for students, and more than 40 accompanying family members.

The conference organizers made strong efforts to secure funds for participants from economically less developed countries; in fact, the organizing committee fully supported more than 30 participants and provided reduced fees for 25 others. This support would not have been possible without generous donations from the Organization for the Prohibition of Chemical Weapons, IUPAC, and the

Slovenian Research Agency. The conference organizers are also grateful for many other donors and sponsors, particularly general sponsor Lek, a new Sandoz company from Ljubljana, Slovenia.

The 30th ICSC will take place in Perth, Australia, 16–20 July 2007; for more information, go to <www.icsc30.murdoch.edu.au>.

**Dr. Vojko Vlachy served as chairman of the organizing committee of the 29th ICSC. He is currently a professor of chemistry and chemical technology at the University of Ljubljana, Slovenia, as well as an adjunct professor at the University of California, San Francisco campus, United States.**

**www.icsc2005.si**

# Advanced Materials—WAM III

## *by Piet Steyn and John Corish*

The very successful **IUPAC New Directions in Chemistry—Workshop in Advanced Materials (WAM III)** attracted more than 150 participants to South Africa on 4–9 September 2005.

The workshop was funded under IUPAC's program for conferences in emerging regions and was organized by the University of Stellenbosch's United Nations Educational, Scientific and Cultural Organization (UNESCO) Associated Center for Macromolecules and Materials, with professor Ron Sanderson chairing the local organizing committee. The first two workshops were held in Singapore (in July 1999) and Bangalore (in February 2002), respectively. Overall responsibility for the workshops rests with the IUPAC Interdivisional Subcommittee on Materials Chemistry.

*Left to right: Professor Ayusman Sen, Pennsylvania State University, plenary lecturer; Professor John Corish, Trinity College Dublin, chair of the international organizing committee; Professor John Boland, Trinity College Dublin, plenary lecturer; and Professor Ron Sanderson, University of Stellenbosch, chair of the local organizing committee.*


*Sanjay Mathur (1st on the left) and Ron Sanderson (5th) with some of the participants of the bilateral German-South African minisymposium. Funding from the national research foundations of South Africa and Germany enabled the participation of 10 young South African and German scientists.*

WAM III focused on nanostructured advanced materials and featured eight sessions addressing new synthetic routes for the production of nanostructured materials, nanoelectronics, nanotubes and fibers, design and self-assembly, biorelated materials, and device characterization and applications. The workshop was opened on behalf of IUPAC by past president Piet Steyn. C.N.R. Rao, another former president and the organizer of WAM II, also participated and presented a plenary lecture. The plenary and invited lectures will be published in a special issue of *Pure and Applied Chemistry*. The journal's scientific editor, James Bull, also attended the conference.

WAM III concentrated on the vital role played by chemists in the design and fabrication of nanostructured materials, with a particular emphasis on soft chemistry. The presentations covered an exhaustive range of established and novel synthetic techniques for the preparation of nanoparticles as well as nanotubes and a variety of nanostructured films, nanocomposites, and nanoporous materials. All of the principal characterization techniques were also covered, with particularly impressive presentations given on the latest developments in the use of scanning tunneling microscopy and atomic force microscopy on silicon surfaces. The current and future technological utilization of nanomaterials as coating materials, electrocatalysts, and electronic components, as well as their application in chemical separations, fuel cells, and other novel energy technologies and in medicine were also discussed, as was the potential offered by autonomous nanoscale motion through catalysis.

The WAM III program also incorporated a bilateral

German-South African minisymposium organized by Sanjay Mathur and Ron Sanderson and jointly funded by the National Research Foundation (South Africa) and the Deutsche Forschungsgemeinschaft (Germany). All of the presentations at the symposium were given by research students.

In addition, the South African Department of Science and Technology generously sponsored poster awards for young chemists. First prize was given to Ziboneni Godongwana of the South African Institute for Advanced Materials at the University of the Western Cape for the poster entitled "Inexpensive production of graphitic mesoporous carbon material." Second prize was given to Rushanah Mohamed and Ziboneni Godongwana, from the same institute, for a poster entitled "Preparation and characterization of proton conducting membranes for direct methanol fuel cell applications."

The success of WAM III in terms of its educational objective may best be judged by the fact that many more students than established scientists attended. Moreover, the rapidly growing interest in materials chemistry in general, and nanoscience in particular, is reflected in the fact that the workshop was significantly larger than its predecessors. Notably, it was attended by delegates and students from the African countries of Algeria, Ethiopia, Lesotho, Libya, Mozambique, Nigeria, Senegal, and South Africa.

**Piet Steyn <psst@sun.ac.za>, a professor at the University of Stellenbosch, was a member of the local organizing committee and the IUPAC representative. John Corish <jcorish@tcd.ie> is the chairman of the IUPAC Interdivisional Subcommittee on Materials Chemistry and the WAM III International Organizing Committee.**

## Young European Chemists

### *by Leiv K. Sydnes*

In August 2005, more than 120 European chemists between 20 and 35 years of age met in Brno in the Czech Republic to discuss chemistry research and compete for the European Medal and Prize. This was the fifth in a series of conferences run under the auspices of Science, Engineering, and Technology (SET) for Europe and its leader, Dr. Eric Wharton.

This meeting series—known as the "**Younger European Chemists' Conference"** series—is a concrete result of a discussion on measures that could be taken to increase European students' and Ph.D. candidates' interest in science and technology in the face of the declining number of chemistry graduates in many European countries. This special annual meeting, which emphasizes interaction and cooperation between young scientists working in the field of chemistry, is designed to inspire more students to opt for a career in chemistry and chemistry research.

***Poster presentations and discussions constitute the backbone of the Younger European Chemists' conferences. IUPAC President Leiv K. Sydnes discusses photochemical problems with Elena Tulyakova from M V Lomonosov Moscow State University in Russia.*** *(Photo: Frank Dumbleton)*

The conference series was created by a small group of enthusiasts headed by Eric Wharton from the United Kingdom. The first meeting was held in London in 2001, and subsequent meetings in Heidelberg, Grenoble, and Torino. Sponsors have been European chemical companies as well as the Royal Society of Chemistry.

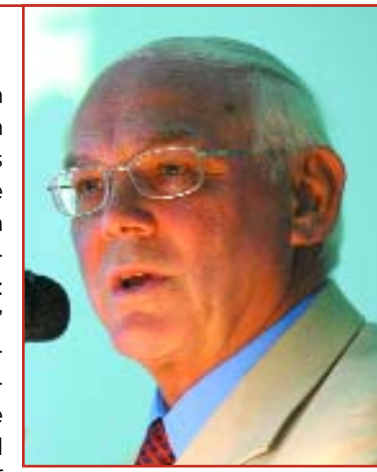
The conference serves as an international forum for the presentation of posters, short talks, and discussion of recent advances in chemistry research and development and is geared to the needs of younger European chemical researchers. A key goal is to foster networking and cooperation across Europe; with that in mind, extensive discussions are held at the meetings based on the posters presented by the young participants. These discussions are led by an international group of scientists that scrutinize every poster and quiz each presenter extensively. During this process, the participants are assessed and the winner of the medal and prize for "Excellence in Science, Engineering and Technology in Europe" is selected. The format is unique and means that the meetings

receive a level of attention rarely seen at other conferences.

This year, as in earlier years, participants came from all parts of Europe. More than 25 countries were represented, from the Artic to the Mediterranean and from the Atlantic Ocean to east of the Ural Mountains. And when the meeting was coming to an end after four hectic days, the international poster judges revealed that Dr. Javier Garcia-Martinez, a postdoctoral fellow from the Universidad de Alicante in Spain, was the winner of this year's European Medal and Prize.

In addition to the extensive, productive poster sessions, lectures were given by selected keynote speakers. This year IUPAC sponsored one of the lectures—the 2005 IUPAC Lecture—which was delivered by Professor Gerald Pattenden from Nottingham University in the United Kingdom. Pattenden talked about "The Excitement of Natural Products and Their Biomemetic Synthesis" with such vigor and enthusiasm that he appeared to be living proof of the title. Many participants indeed felt inspired to carry on with chemistry after his talk.

Another enthusiastic keynote lecturer was Pietro Tundo from Universita Ca Foscari di Venezia in Italy. Professor Tundo is a driving force in the field of green chemistry, not only in Europe, but also within IUPAC, where he has chaired the Subcommittee on Green Chemistry for a number of years. His lecture on "Green Chemistry: Research and Education" presented much interesting chemistry and also outlined how a sustainable (green) perspective could become an integral part of a modern chemistry curriculum. And he did not forget IUPAC: both the Union and the First International IUPAC Conference on Green Chemistry, to be held 10–15 September 2006 in Dresden, Germany, were well promoted.



***The IUPAC Lecture was delivered by Gerald Pattenden from Nottingham University in the United Kingdom.*** *(Photo: Frank Dumbleton)*

In addition, as president of IUPAC, I delivered a presentation entitled "IUPAC: Advancing Worldwide Chemistry and Chemistry Worldwide." For an audience that mainly associates IUPAC with rules for naming organic compounds, the talk contained a great deal of new material that generated both questions and discussion. Notably, several participants subsequently volunteered to become involved in IUPAC activities.

The 2006 Younger European Chemists' Conference will be held in Budapest on 22–27 August 2006.

**Leiv K. Sydnes <leiv.sydnes@kj.uib.no> was IUPAC president in the 2004–2005 biennium; he is a member of the Norwegian Chemical Society and professor at the University of Bergen.**

**www.setforeurope.org**

***Javier Garcia-Martinez, a postdoctoral fellow from Universidad de Alicante in Spain, was the winner of this year's European Medal and Prize. He received the medal and the certificate from Stephen Abbott, research director for Autotype International and visiting professor at the University of Leeds in the United Kingdom.*** *(Photo: Frank Dumbleton)*

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- Structure & Function of Biomolecules
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**Congress organization:** EuCheMS* executive committee: Gábor Náray-Szabó (chair), György Horvai (local chair)
**Congress host:** Hungarian Chemical Society
**Scientific programme committee:**
Jean-Marie Lehn (chair), E. Peter Kündig (co-chair)

*EuCheMS, the European Association for Chemical and Molecular Sciences incorporates 50 member societies which in total represent some 150,000 individual chemists in academia, industry and government in over 35 countries across Europe

## Advanced Materials

17–22 April 2006, Nara, Japan

The **14th POLYCHAR World Forum on Advanced Materials** will be held 17–22 April 2006 in Nara, Japan. Previous conferences in this series have attracted attendees from approximately 40 countries.

POLYCHAR 14 will encompass the many research fields of polymer science. The main topic areas include 1) predictive method; 2) synthesis; 3) nanomaterials and smart materials; 4) mechanical properties and performance; 5) dielectric and electrical properties; 6) surface, interface, and tribology; 7) rheology, solutions and processing; 8) biomaterials and tissue engineering; 9) natural and biodegradable materials and recycling; and 10) characterization and structure-property relationships.

POLYCHAR-14 will feature both oral and poster presentations. The presentation papers will be published in *POLYMER* after standard reviews. Prizes for young scientists and students will be awarded for outstanding poster presentations.

On 18 April, a special symposium will be held to discuss the future development of women researchers in the polymer science field as well as those in the various science fields. Some well-known female professors and young female scientists will be invited as panelists. In addition, a short course will be held on 16 April for students and young researchers who want to investigate polymer science.

**See Mark Your Calendar on page 42 for contact information.**

**www.unt.edu/POLYCHAR/polychar14/**

## Theoretical and Computational Chemistry

6–10 August 2006, Kunming, China

The **4th Worldwide Chinese Theoretical and Computational Chemistry Conference** (WCTCC), in conjunction with the 2nd International Conference on Theoretical Chemistry, Molecular Modeling, and Life Sciences (ICTCLS), will be held in Kunming, China, 6–10 August 2006. This conference series has become an important gathering of Chinese theoretical and computational chemists from around the world. The previous WCTCC conference's were held in Dalian (2000), Taipei (2002), and Hong Kong (2004).

The purpose of the conference is to provide a forum for Chinese scientists to disseminate and share the latest developments in theoretical/computational chemistry and related interdisciplinary fields, and to foster scientific research in China. The main themes include, but are certainly not limited to:

- methodological development in electronic structure theory
- first-principles simulations of molecular devices
- molecular dynamics based on molecular mechanics/quantum mechanics
- reaction dynamics
- modeling of biomolecules and functions
- computational materials sciences
- excited states and their dynamics
- novel computational methods and algorithm

The conference will be co-organized by the Institute of Chemistry, Chinese Academy of Sciences, and the Yunnan University. The International Advisory Committee will be chaired by the prominent theoretical chemists Prof. Guangxian Xu of Peking University and Prof. Weitao Yang of Duke University. The organizing committee consists of Prof. Zhigang Shuai (Chair), Prof. Jiushu Shao, Prof. Shushan Dai, and Prof. Xueyan Tu. The conference will consist of plenary lectures (40 minutes), invited lectures (30 minutes), selected lectures (20 minutes), and poster presentations.

Kunming is the capital city of Yunnan province. The city and the province are well known for their beautiful, breathtaking, and unique natural landscapes, for the folk cultures of the various ethnic groups, and its mild climate.

The official language of the conference will be English.

**http://wctcc2006.iccas.ac.cn**

## Combustion

6–11 August 2006, Heidelberg, Germany

The **31st International Symposium on Combustion** will be held 6–11 August at the University of Heidelberg, Germany. Hosted by the German Section of The Combustion Institute and the Interdisciplinary Center for Scientific Computing at the University of Heidelberg, the symposium is the largest international meeting in the field of combustion, bringing together the most renowned scientists from all over the world.

The purpose of this biennial event is to promote research and disseminate results in the field of combustion science. The symposium is open to anyone who is interested in the research of combustion phenomena. Participants have backgrounds in such diverse fields as physical chemistry, fuel technology, fluid dynamics, internal combustion engine design, fire research, environmental research, mechanical and aerospace engineering, and research on detonation.

The technical program of the 2006 symposium consists of oral sessions of contributed papers and poster sessions of works in progress. Invited lectures and topical reviews will be given by eminent specialists.

Selected topics include, among others:

- kinetics of hydrocarbon fuels, NOx and SOx mechanism generation, simplification, and reduction; and informatics of reaction systems
- development and application of diagnostic techniques and sensors for the understanding and control of combustion phenomena
- flames, including premixed, nonpremixed, and partially premixed flames, their ignition, extinction, stabilization, instabilities, and interactions with flows
- heterogeneous combustion, including fundamental aspects of combustion of solid fuels (e.g., coal, char, and biomass, including pyrolysis, gasification, and ash formation) as well as combustion of propellants and metals, catalytic combustion, and material synthesis, including nanoparticle synthesis

The well-rounded social program includes a reception at Heidelberg castle, a banquet at Schwetzingen castle, and a boat cruise on the Neckar River. For accompanying persons, there are various tours available, including visits to Strasbourg (France) and the Lorely.

www.combustion2006.org

## Advanced Polymers for Emerging Technologies

10–13 October 2006, Busan, Korea

The **IUPAC International Symposium on Advanced Polymers for Emerging Technologies** will be held 10–13 October 2006 at BEXCO in Busan, Korea. The symposium is being organized to commemorate the 30th Anniversary of the Polymer Society of Korea (PSK). The symposium is sponsored by IUPAC and many polymer, chemical, and pharmaceutical companies.

The scientific program comprises plenary lectures, invited guest lectures, contributed oral presentations, and poster sessions. More than 90 plenary and invited lectures will be given by renowned polymer scientists and engineers from many foreign countries. The official language will be English.

The aim of PSK30 is to present and discuss recent achievements in the fields of advanced polymers, multidisciplinary applications of polymers, and future developments. The main topics of the symposium will include the following:

- Advanced Polymers for Emerging Technologies
- Polymers for Electronics and Photonics
- Smart Polymers for Sensors and Intelligent Systems
- Biomedical Polymers
- Polymers for Energy Conversion and Storage
- Polymer Nanomaterials and Nanotechnology
  Contemporary Polymer Science and Technology
- Polymers Syntheses and Reactions
- Polymer Physics, Properties, and Characterization
- Environmental and Green Polymers
- Polymer Engineering and Processing
- Industrial Polymers

The deadline for abstract submission is 30 June 2006. Applications for pre-registration and hotel reservations will be accepted until 31 August 2006.

See Mark Your Calendar on page 44 for contact information.

www.psk30.org

## Phosphorus Chemistry

15–21 April 2007, Xiamen, China

The 17th International Conference on Phosphorus Chemistry will be held 15–21 April 2007 in Xiamen, China. The ICPC2007 program will concentrate on phosphorus chemistry in life science and material science. The conference will present new phosphorus-related chemistry in a wide range of disciplines, including organic, inorganic, polymer, human health, materials, environmental, analytical, biomolecular, biotechnology, and others. Dr. Yunfen Zhao is the general chairperson of the meeting.

The conference is typically attended by scientists from over 30 countries. The expected ICPC2007 attendance is 400 to 500. The Chinese Chemical Society will be the sponsor of this conference and is working together with the committee to help make it a success.

Main topics include:

- Phosphorus in Organic Synthesis and Stereochemistry
- Structure and Reactivity of Organic Phosphorus Compounds
- Structure and Reactivity of Inorganic Phosphorus Compounds
- Phosphorus Coordination Compounds and Their Use in Catalysis
- Bioorganic Aspects of Phosphorus Chemistry
- Dental and Medicinal Chemistry of Calcium Phosphates
- $^{31}$P NMR in Biological Systems
- Nucleotides-Chemistry and Delivery-From Basics to Therapy
- Phosphorus Chemistry in Agriculture, Industry and Materials Sciences
- Theoretical Aspects of Phosphorus Chemistry

The abstract deadline is 15 December 2006.

**See Mark Your Calendar on page 44 for contact information.**

**Web site to be announced.**

# Mark Your Calendar

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

## 2006

*IUPAC poster prizes to be awarded*

**10–13 January 2006 • Green Chemistry • Delhi, India**
*Second International Symposium on Green/Sustainable Chemistry*
Prof. M. Kidwai, Department of Chemistry, University of Delhi, Delhi-110007, India, Fax: +91 11 27666235, E-mail: kidwai_chemistry@yahoo.co.uk

**6–10 February 2006 • Photodynamics • Havana, Cuba**
*4th International Meeting on Photodynamics*
Prof. Jesus Rubayo Soneira, Instituto Superior de Tecnologias y Ciencias Aplicadas, Ave. Salvador Allende y Luaces, A.P. 6163, Havana 10600 Cuba, Tel.: + 53 7-2041188, Fax: +53 7-2041188, E-mail: jrs@fctn.isctn.edu.cu

**6–8 March 2006 • Combining and Reporting Analytical Results • Roma, Italy**
*International APAT-IUPAC Workshop on the Role of (metrological) Traceability and (Measurement) Uncertainty for Comparing Analytical Results*
Dr. Ales Fajgelj, International Atomic Energy Agency, Agency's Laboratories Seibersdorf, Wagramer Strasse 5, A-1400 Vienna, Austria, Tel.: +[43] 1 2600 28233, FAX: +[43] 1 2600 282221, E-mail: a.fajgelj@iaea.org

**12–15 March 2006 • Heterocyclic Chemistry • Gainesville, Florida, USA**
*7th 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

**2–7 April 2006 • Photochemistry • Kyoto, Japan**
*XXIst IUPAC Symposium of Photochemistry*
Prof. Masahiro Irie, Department of Chemistry and Biochemistry, Kyushu University, Graduate School of Engineering, Hakozaki 6-10-1, Fukuoka, Japan, Tel.: +81 92 642 3556, Fax: +81 92 642 3568, E-mail: irie@cstf.kyushu-u.ac.jp

**17–21 April 2006 • Advanced Materials • Nara City, Japan**
*POLYCHAR-14 World Forum on Advanced Materials (Polymer Application & Theory)*
Prof. Masaru Matsuo, Department of Textile and Apparel, Nara Women's University, Faculty of Human Life and Environment, Nara, 630 8263 Japan, Tel.: +81 742 20 3462, Fax: +81 742 20 3462, E-mail: m-matsuo@cc.nara.wu.ac.jp

**28 May–1 June 2006 • Macro- and Supramolecular Architectures and Materials • Tokyo, Japan**
*3rd International Symposium on Macro- and Supramolecular Architectures and Materials (MAM-06): Practical Nanochemistry and Novel Approaches*
Prof. Kurt E. Geckeler, Lab. of Applied Macromolecular Chemistry, Gwangju Institute of Science & Technology, 1 Oryong-dong, Puk-gu, Gwangju 500-712, South Korea, Tel.: +82 62 970 2316, Fax: +82 62 970 2338, E-mail: keg@kjist.ac.kr

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

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

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

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

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

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

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

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

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

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

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

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

**3–9 September 2006 • Radical Polymerization • Il Ciocco/Castelvecchio Pascoli, Italy**
*International Symposium on Radical Polymerization: Kinetics and Mechanism*
Prof. Michael Buback, Institut für Physikalische Chemie, Universität of Göttingen, Tammannstraße 6
D-37077 Göttingen, Germany, Tel.: +49 5-513-931401, Fax: +49 5-513-93144, E-mail: mbuback@gwdg.de

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

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

# Mark Your Calendar

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

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

## 2 0 0 7

*IUPAC poster prizes to be awarded*

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

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

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

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

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

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

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

## IUPAC Poster Prizes

IUPAC Poster Prizes can be awarded at Division—or Standing Committee—sponsored events. The events are flagged in the previous calendar pages. For more information, contact the IUPAC Secretariat.

## How to Apply for IUPAC Sponsorship

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

IUPAC

GEDEON RICHTER LTD.

# IUPAC and Gedeon Richter, Ltd. Announce the 2006 IUPAC-Richter Prize in Medicinal Chemistry

## *Call for Nominations*

The IUPAC-Richter Prize Prize is to be awarded to an internationally recognized scientist, preferably a medicinal chemist, whose activities or published accounts have made an outstanding contribution to the practice of medicinal chemistry or to an outstanding example of new drug discovery.

The prize has been established by a generous gift from the **Chemical Works of Gedeon Richter, Ltd.** (Budapest, Hungary) to acknowledge the key role that medicinal chemistry plays in improving human health.

Application is by NOMINATION only with one person needing to serve in that capacity, although a total of five (5) individuals should be listed as referees overall. The package should contain a complete resume, a professional autobiography of not more than two pages, and a one-page summary of what the individual considers to be his/her activities, accomplishments and/or publications that have had the most significant impact upon the field of Medicinal Chemistry. The material will be confidentially forwarded to an independent selection committee appointed by the IUPAC Subcommittee on Medicinal Chemistry and Drug Development.

The first IUPAC-Richter Prize will be presented in 2006 during the XIXth International Symposium on Medicinal Chemistry, 29 Aug–2 Sep 2006, in Istanbul, Turkey, where the recipient will also give a 45-minute plenary lecture on the subject of his/her research.

**Prize USD 10 000**

**Deadline: 31 March 2006**

For further information please visit <www.iupac.org/news/Richter_prize.html> or contact Professor C. Robin Ganellin, Chairman of the IUPAC Subcommittee on Medicinal Chemistry and Drug Development, by e-mail at <c.r.ganellin@ucl.ac.uk>.

**ISMC–2006**
29 Aug–2 Sept 2006
Istanbul, Turkey
The XIXth International Symposium on Medicinal Chemistry is being organized by the Turkish Association of Pharmaceutical and Medicinal Chemistry under the auspices of the European Federation for Medicinal Chemistry.
<www.ismc-2006.org>

Nomination materials should be submitted by **31 March 2006** to:

**IUPAC Secretariat**
by e-mail to <secretariat@iupac.org>

telephone: +1 (919) 485 8700
fax: +1 (919) 485 8706