

The News Magazine of the  
International Union of Pure and  
Applied Chemistry (IUPAC)

# CHEMISTRY

## International

September-October 2008  
Volume 30 No. 5

A close-up photograph of a hand holding a magnifying glass over a document. The magnifying glass is held by the thumb and index finger, and the lens is focused on the text of the document, which is slightly blurred. The background is a soft, out-of-focus grey.

**Creativity  
in Applied  
Polymer  
Science**

**Functional Foods**

**Computers in Clinical  
Laboratories**



# From the Editor

## CHEMISTRY International

The News Magazine of the  
International Union of Pure and  
Applied Chemistry (IUPAC)

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The feature “Computers in Clinical Laboratories” published in this issue (p. 5) caught my attention because of the underlying generalities of the challenges presented. The issues related to IT are numerous, but the key problems are basically how to design, develop, and implement a computer system that best serves its users.

“Best serves its users” is, in my view, the most challenging aspect. I am pretty sure we all have experienced that moment when using some software when we wondered why would someone want to do that? You know what I am talking about, “that” function tucked under the third



drop-down menu under “advance.” Maybe I don’t get it and as a consequence ignore these functions, acknowledging that there are other users with other needs. It seems that most of us have to make compromises between what is readily available and what we want to accomplish. Ideally, as systems are

further upgraded—hopefully in the spirit of best serving the users—the number of compromises shall decrease and our ability to use and exploit those systems become optimal.

The feature ends with a quote that sticks with me: “The real danger is not that computers will begin to think like men, but that men will begin to think like computers,” by Sydney J. Harris. What would Harris (1917–1986), a British-born U.S. journalist, think of IT today and of the progress and changes we have experienced over the last two decades?

I believe that it is essential that we keep thinking as “humans” and that we do not lose our logic and intuition. As computer users, we all have had experiences with new systems and software, and in the course of learning them have come to understand the logic by which the systems were developed. That does not make us think like computers, but only able us to understand how the concepts presented are related to each other, and how overall the system works for us.

Do I wish some days that my computer understood me better? Yes I do, but that is not to say that I wish my computer will ever think like me!

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*Cover photo: A plastic organic transistor that can operate under water and detect trace amounts of organic polluting chemicals. Image courtesy of Zhenan Bao, Stanford University. See related feature “Creativity in Applied Polymer Science” on page 3.*

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## Was Midas a Chemist?



by John Corish

**A** modern Midas among our members would be a unique and welcome asset in the current uncertain and predominantly gloomy global financial environment. However, even without the magic of the alchemist the Union remains on a sound

financial footing. For this I wish to sincerely thank my predecessor as treasurer, Christoph Buxtorf, and also the Finance Committee and John Jost and his colleagues at the Secretariat for their excellent management and husbandry of our resources. Buxtorf has generously agreed to extend his IUPAC service by now chairing the Finance Committee in which forum his experience will continue to be most beneficial.

Our financial statement for the year 2007, complete with an independent auditor's assessment, was issued in June of this year. It was a healthy report with IUPAC showing an admittedly modest increase in its overall assets. But this gain was after a very full and active year. On the income side, national and other subscriptions held up as might have been expected, but the values of the income streams from publications and investments were also thankfully maintained.

Taken together, these three sources provide the funds to drive our publication output and the work programs of our divisions and standing committees, to finance all the projects undertaken on our behalf, to let us maintain our position as one of the most active scientific unions in the world, and to maintain our infrastructure and administration. The two latter parts of our income are very necessary because they are instrumental in keeping the first, the annual subscriptions, at a reasonable and manageable rate. The budget for the current biennium has been set at just less than USD 2.94 million, which shows a small increase.

The Strategic Opportunities Fund, boosted by the

addition of unused monies recovered from completed or abandoned projects, was set at USD 120 000. This fund is intended to support projects that are particularly relevant to achieving IUPAC strategic plans, with allocations made by the Executive Committee on recommendation of the Project Committee.

A second source of additional funding for projects, over and above division and standing committee budgets, is available in the Project Committee reserve. This is intended for interdisciplinary projects, including joint projects with standing committees, and projects that are too expensive for a division to fund. This reserve fund provides real opportunities for new initiatives to increase the impact of the Union. The fund will greatly enhance our work programs if it can be fully utilized.

Perhaps it is again necessary to state that it is not the purpose of IUPAC to accumulate reserves per se nor is it the intention of the Finance Committee to attempt to do this. However, as all of us face a less certain financial future it is vital that the Union continues to have the funding necessary to support and even expand its work, as well as the flexibility to be able to seize strategic opportunities as they arise. The upcoming International Year for Chemistry is a prime example.

So, what are the most useful things a Midas could do for us? He could endorse the decision of the Finance

Committee to continue the prudent and defensive policy that it had adopted in 2007 and which has proved to be effective in managing the IUPAC portfolio in the current financial climate. He could advise us on how we can diversify to find novel income streams as this will almost certainly become necessary to compensate for the anticipated eventual decline in income from our current publications. It is most important that we all now

consider how best we can use our knowledge bases and our other service activities to generate new routes to boost our income. 🧪



John Corish <jcorish@tcd.ie> has been treasurer of IUPAC since January 2008. He has served IUPAC at many levels since 1979, including chair of the Subcommittee on Materials Chemistry, president of the Inorganic Chemistry Division, and member of the Finance Committee. He is a professor of physical chemistry at Trinity College in Dublin, Ireland.

# Creativity in Applied Polymer Science

by Dick Jones

**R**arely do applied scientists pursuing research within industry and confined by the requirements of patenting and commercial interest before publication receive wide recognition from the scientific community. For that reason, *Polymer International* has instituted the *Polymer International-IUPAC Prize*, an award for excellence in creativity and industrial application in polymer science, open only to scientists under the age of 40 <[www.iupac.org/news/archives/2007/PolymerInt-award.html](http://www.iupac.org/news/archives/2007/PolymerInt-award.html)>.

The award is to be presented every two years at the IUPAC World Polymer Congress, where the winner will present a lecture about his or her work. In addition to a cash prize, all travel and accommodation expenses incurred in attending the Congress will be covered. This year, following receipt of 24 nominations from all over the world and the deliberation of an international panel of judges representing major nations participating in polymer science, the first award went to Zhenan Bao, a professor of chemical engineering at Stanford University. The award was presented at the Macro 2008 Congress held in Taipei at the end of June (see July 2008 *CI*, p. 19).

Bao is a world leader in the field of organic and polymer electronics. Educated at Nanjing University in China and the University of Chicago in the United States, her first post was as a member of the technical staff of the Polymer and Organic Materials Research Department at Lucent Technologies in New Jersey, where she became a distinguished member of the technical staff. She is now a professor in the Chemical Engineering Department at Stanford University, with more than 100 refereed publications and 30 patents to her name.

Bao pioneered the materials design concepts for high-charge transport polymeric semiconductors and air-stable organic semiconductors capable of being processed using solution techniques. The high-performance materials she designed and realized subsequently led to the first demonstrations of all-printed organic transistors and organic transistor-driven electronic circuitry. Her research group at Stanford has also pioneered several new dielectric material systems that played significant roles in demonstra-

tions of printed circuitry as well as enabling a new type of water-stable sensor: A glass resin dielectric polymer that can be easily processed became the workhorse dielectric material that allowed the demonstration of the first-ever printed electronic paper powered by organic transistors. Another important polymer dielectric system contains a stable cross-linker that allows low-temperature curing. Ultrathin films cast from this new polymer are pinhole-free and behave as high-performance low-power consumption transistors. The low-voltage operation characteristic of transistors made using this new dielectric enabled chemical detection in an aqueous system, presenting possible applications of interest to the military, the health industries, and in environmental monitoring.

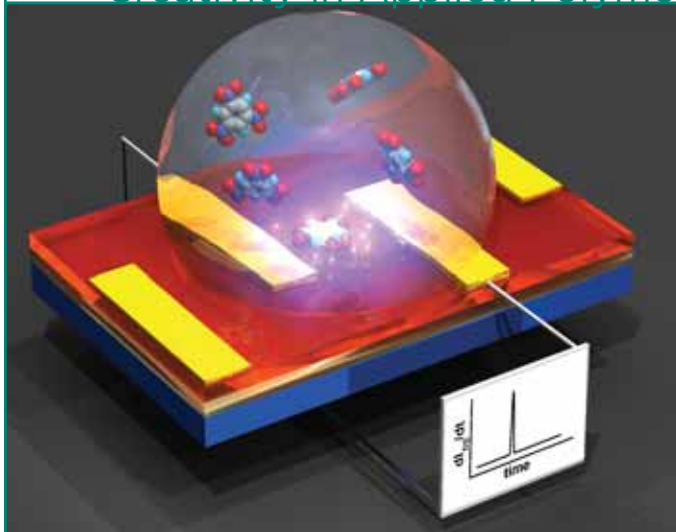
Recently, Bao's group at Stanford has developed chemistry for the synthesis of a new type of conjugated polymer containing pentacene. With high mobilities of over  $1.0 \text{ cm}^2\text{V}^{-1}\text{s}^{-1}$  and acceptable on-off ratios, the best-performing molecule as the active material in *p*-type organic transistors is pentacene. Pentacene is subject to rapid degradation in ambient conditions, but by incorporating it into a conjugated polymer, the processability and stability of the material is significantly improved without compromising its charge transport property. Bao has also led the synthesis of the first regioregular pentacene-containing conjugated polymers with 2,9 substitutions on the pentacene. These will have great potential as transistor materials as well as being low bandgap polymers.

A frequent recipient of scholarships, fellowships, and other awards, Bao's reputation has spread, leading to distinguished lecture invitations and external awards. Her work has been featured in various news media, including *CNET*, *New Scientist*, *Chemical & Engineering News*, *NanoWorld News*, *NanoTech Wire*, and *Nanowerk News*, and in top journals such as *Science* and *Nature*. *Science* noted Bao's work on large-scale integrated circuits based on organic materials as being among the top 10 research breakthroughs in 2000. That same year she was selected by the U.S. National Academy of Engineering as being among the top 100 young engineers in the world. In 2001 she was a lecturer at the Nobel Laureates in Polymer Chemistry Symposium at the American Chemical Society Polymer Chemistry Division. That same year



*Zhenan Bao delivers the Award Winning Lecture at MACRO 2008 on 4 July 2008 at the Taipei Convention Center, Taiwan.*

## Creativity in Applied Polymer Science



*A water droplet with a trace amount of trinitrobenzene resides on the surface of an organic transistor. The presence of the analytes in the semiconductor channel results in a disturbance to the charge transport, causing a change in output current. Plastic materials form the basis of new electronic sensors for chemical detection in air or water. See the article by Roberts et al. in PNAS early view online. Image courtesy of Stefan C.B. Mannsfeld, Mark Roberts, and Zhenan Bao, Stanford University.*

she was given the American Chemical Society Team Innovation Award, an R&D 100 Award for her work on printed plastic circuits for electronic paper displays, and was *R&D Magazine's* Editor's Choice of the "Best of the Best" new technology for 2001. In 2002 she was selected by the Women Chemists Committee of the American Chemical Society as one of 12 "Outstanding Young Woman Scientists expected to make a substantial impact in chemistry during this century," and in 2003 she was selected by MIT Technology Review as one of the top 100 young innovators for this century.

Since she hasn't even hit midcareer, we expect that Zhenan Bao will continue to make a mark on science and technology for years to come. We congratulate her on her achievements to date and wish her the very best in the future. 🌍

Richard G. Jones <r.g.jones@kent.ac.uk> is chair of the *Polymer International-IUPAC Prize Adjudication Panel*. He is emeritus professor of Polymer Science at the University of Kent in the UK and a long-time member of the IUPAC Polymer Division.

See also [www.iupac.org/publications/ci/indexes/stamps.html](http://www.iupac.org/publications/ci/indexes/stamps.html)

## Stamps International

### Erasers, Rubber Duckies, and So Much More

Natural rubber is a fascinating polymeric material derived from the milky white latex extracted from trees of the *Hevea* genus. It is essentially a polymer of isoprene (2-methyl-1,3-butadiene) and its distinctive physical and chemical properties, such as elasticity, durability, and impermeability, have resulted in its widespread use in modern society. Close to 10 million metric tons of natural rubber are produced in the world every year, with applications ranging from elastic bands and tires to containers and insulators. Although natural rubber is primarily an agricultural product, a variety of synthetic rubbers are also made in a large industrial scale from petroleum feedstocks, including isoprene, butadiene, ethylene, and styrene.



The stamp illustrated here was issued on the occasion of a Natural Rubber Conference held in Kuala Lumpur, Malaysia, in 1968. It displays an appealing space-filling model of isoprene and a representation of the traditional way of collecting natural rubber latex from a tapped tree. It is remarkable that most of the natural rubber latex produced in the world today is still harvested by this centuries-old process and that approximately 70 percent of the world production comes from only three countries, namely

Indonesia, Thailand, and Malaysia.

For a readable history of rubber, see: Loadman, J. *Tears of the Tree*; Oxford University Press, New York, 2005.

Written by Daniel Rabinovich <drabinov@uncc.edu>.

# Computers in Clinical Laboratories

by Josep M. Queraltó Compañó, Maria Àngels Bosch Ferrer, Josep Lluís Bedini Chesa, Jaume Raventós Monjo, and Xavier Fuentes-Arderiu

Information technology was introduced in clinical laboratories around 30 years ago, although some analytical instruments had already been empowered with microprocessors, or “intelligent systems,” for simple calculations. At that time, not even the most forward-thinking scientists could envisage the speed at which IT would race ahead, evolving from microprocessors embedded in instruments to specifically designed laboratory information systems (LIS).

Laboratory instrumentation manufacturers played a critical role in the implementation of IT, creating an unusual market. At the onset, computers were simply attached to analytical instruments to facilitate the flow of data. The main reason for implementing a “laboratory computer” was a high workload. New uses and applications soon appeared, such as transactions from the laboratory to the mainframes of hospital information systems (HIS). What we now know as data warehouses were in fact the result of the natural evolution of information science and technology. Laboratory and institutional computers today contain an incredible amount of data and, surely, knowledge. This flood of information raises a number of questions: Is the computer just a powerful typewriter with a memory, as it seemed 30 years ago? Will natural or artificial intelligence be able to transform data into useful knowledge? Will information technology be able to meet the challenges of the future?

In order to discuss basic questions along these lines, the 2007 symposia\* was structured in three sessions:

- current laboratory information systems and their management
- relationships and communication between laboratories and users

\* This report is an account of the discussions held during the 2007 symposium of the ACCLC (the Catalan Association of Clinical Laboratory Sciences) on information technology in laboratory medicine. A forum was set up featuring professionals from clinical laboratories, the *in vitro* diagnostics industry that provides laboratory information systems, and from various health administrations. The symposium, organized in Barcelona from 1-2 March 2007, started straight off with the chairperson raising a series of questions previously developed by the advisory board and the ACCLC board.

- implementing intelligent expression of laboratory results

## Laboratory Information and Management Systems

Many aspects should be taken into consideration when a laboratory information and management system is under analysis. These include, for example, connections with other laboratory instruments, point-of-care devices, computer platform architectures, languages and standard protocols, robotics, and wireless technology. However, the 2007 symposium debate was centered on the purchasing, dimensioning, and staff training that is necessary before an LIS becomes operative.

### Purchasing a Laboratory Information System

To fulfill its information management needs, a laboratory must decide whether to develop its own software or to buy “off the shelf.” In Spain, LIS are mainly provided by *in vitro* diagnostic manufacturers and only by a few independent software companies, though these are increasing. The situation differs in the rest of Europe where the diagnostic industry is rarely involved in the information systems business. Experts agree that the involvement of the diagnostic industry may have some advantages:

- The large companies have powerful computer facilities and personnel who can participate in efficient software development. Moreover, some of these companies in Spain now have substantial experience in this field.
- The diagnostic industry’s profound knowledge of the needs and organization of clinical laboratories can positively influence the design of the software products.
- LIS can be continuously updated and improved



## Computers in Clinical Laboratories

as a consequence of commercial pressure to sell reagents or instruments.

- For many public laboratories with strict budget limitations, purchasing reagents can be the only way to obtain or improve their IT.

However, there are also a number of disadvantages:

- Clients can feel too tied to a single manufacturer, who appears to be in a dominant position. This may condition negotiations for the purchase of the reagent or instrument.
- Technical and commercial relations may not be optimal when IT is not the core of the company business.
- Investment in software development may reduce investment in reagent or instrument improvements.

In summary, the most important criteria to take into account when selecting an LIS are that:

- The performance of the systems should fit the individual laboratory requirements.
- The development, configuration, and/or adaptation of the LIS should be user friendly.
- Software should be sufficiently flexible to fit the global laboratory organization, allowing communication with other information systems, adapting to future environment changes, and incorporating the possibility to implement new features.
- Purchasing decisions should be made freely and independently.
- Ideally, each laboratory should have a specific budget available for IT.

Each laboratory's specific budget was considered the most crucial issue, for if laboratories themselves can manage the acquisition of information systems, a greater number of software development companies would be interested in the clinical laboratory market, and the available options would increase.

### Dimensioning the Laboratory Information System

LIS size depends on multiple technological factors such as the corporate IT system in use. Economic issues such as budget and personnel resources also obviously play a major role, as does the workload of the laboratory. It is

a general observation that in recent years, the dimension of HIS has increased in relation to LIS.

### Training In the Use of the Laboratory Information System

Before an LIS can be implemented, it is essential to establish an appropriate training plan for users. The aim is not only to guarantee correct operation, but also to attain optimal performance. According to some experts, the use of LIS is frequently less than 40 percent of its potential. However, training should be adapted to the different levels of users' needs and skills: basic, intermediate, or advanced. The training period is not completed when LIS is implemented, but must be permanently updated through a "continuous education" strategy, such as through meetings with software users from other institutions.

It may be helpful to appoint an information system coordinator in the laboratory. This coordinator, preferably a member of the faculty staff, an IT expert, or a laboratory technician, should have a sufficiently global vision of the laboratory in order to define:

- laboratory quantities and processes (e.g., codes, lists, etc.)
- interactions, cooperation, or synergies with other centers and institutions

### Communications and Users' Relationships

Originally, LIS acted as a connection between analytical instruments. As they gained power, LIS progressively became a consistent, permanent communications network among all information systems, including HIS, associated institutions, and practitioners, as well as health authorities. The relationships between

health authorities and LIS staff have become considerably stronger through their participation in external quality surveys and exchange of useful epidemiological information. Consequently, for the near future, the essential point is not simply to implement an efficient communication system, but to achieve integration of all information systems. In other words, both LIS and HIS must not be only able to talk each to other, but efficiently work together.

In this context, five topics were discussed in depth: electronic clinical records, technol-





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ogy boundaries, changes in cultural paradigms affecting LIS integration, ethical and confidentiality issues, and the introduction of intelligent systems into this scenario.

Nowadays, there are no technological limits and all kinds of information can be integrated and shared. Consequently, the data structural model appears to be crucial and is now clearly more important than technological issues. This implies, however, that a previous step of data standardization is required before the transmission of information can be implemented:

- Proper patient identification is essential and patient confidentiality must be ensured at all times.
- Formal aspects of laboratory data such as nomenclature or units must be standardized.
- Standard catalogs should substitute corporate repertoires. Ideally, the same repertoire, such as the IUPAC/IFCC, should be used.
- The information content to be transferred to the clinical workstation should also be standardized, including the presentation of laboratory results in a validated report format.

Information transference from LIS constitutes a unique opportunity to provide laboratory users with optimal advice, information, or knowledge before they perform an analytical request. Clearly, LIS should be ready to help with questions such as: "What do clinicians want from the laboratory?", "How can the services be best delivered?", and "How can laboratory services be improved?"

Science and technology have influenced culture and society since time began. In recent years, a new paradigm, the Internet, has produced real, dramatic changes not only in our social life but also in science and technology<sup>1</sup> and has almost defeated the client-server paradigm. Today, there is no doubt about the global role the Internet and its many tools play in providing previously unimagined options.

A second cultural change we are experiencing is the progressive substitution of competitive systems for cooperative systems. As previously mentioned, the new role devised for the relationship between HIS and LIS, that of sharing instead of competing, may be a general trend.

We can, therefore, consider that the conventional clinical workstation is evolving towards a knowledge portal for all participants in the clinical process. The new clinical workstation should act as an intelligent manager integrating all information systems, including LIS and HIS.

During this process, however, it is unavoidable that as some problems are solved, other new challenges will appear. In other words, as the amount of communication increases, so do the network knots. Of major concern is the need to clarify privacy issues, access to information, and patient consent, for example. The confidentiality of clinical data is of maximum priority. Moreover, as patients are the owners of their clinical records, including laboratory information, their agreement to manage this information is mandatory. This must be kept foremost in the minds of developers so as to anticipate the eventual use of Internet, SMS (text messaging), or other communication technology, by patients wishing to access their own clinical (and laboratory) data.

The LIS must guarantee that access to sensitive data is limited to persons involved in the clinical process. Safety of sensitive data can be achieved by limiting or registering access to computer files. However, too many passwords or other security procedures for a single consultation, for example, is not only tedious and time consuming but can create negative feelings among healthcare workers. We need

*The conventional clinical workstation is evolving towards a knowledge portal for all participants in the clinical process.*

to reach a compromise between the patient's right to privacy and/or confidentiality and the best possible patient care; i.e., a compromise between professional activity, technology, and ethics. A final point here is that the LIS can also be useful to remind us of the need to obtain patient consent to perform some procedures.

There is general agreement that laboratory data is under-utilized from the point of view of scientific performance. To reverse this tendency, two objectives have been clearly identified for the LIS: (1) to improve the request of analytical services by providing knowledge about the biological properties of the laboratory quantities, and (2) to enhance the utilization of results.

### Intelligent Laboratory Results

Two relevant factors played a key role in transforming information from data to knowledge: the huge increase in the amount of laboratory data requested, and the continuous appearance of new biological quantities. Concerning this latter point, the new analytes greatly improve and refine the clinical laborato-

## Computers in Clinical Laboratories

ry's role in healthcare, but, paradoxically, complicate the interpretation of what is sometimes very complex information.

The LIS appears to be the most promising tool to deal with both these challenges, helping to modulate the demand in the preanalytical phase, and helping to interpret the data in the postanalytical phase. LIS should therefore display a series of "intelligent" features. Some are related with strictly formal aspects, such as the ability to:

- help in analytical validation, for example, by showing previous results and using "autovalidation" devices that use clinical and biological consistency criteria<sup>2</sup>
- estimate uncertainty in the patient's analytical results
- present and interpret relevant changes from previous results
- add plots, pictures, and color to the laboratory report in order to enhance interpretation

Others express the semiological value of the analytical report, and can:

- expand the semiological information (e.g., including predictive values and likelihood ratios)
- calculate the laboratory's own reference intervals
- provide diagnostic advice, using the historical records and the appropriate decision algorithms

From the point of view of laboratory organization and management, LIS seems well fitted to accomplish the following:

- control the activity of laboratory services, providing clues about the opportunity (or not) to request for a particular exploration
- decrease the number of redundant requests or errors in patient preparation by providing the appropriate suggestions to the laboratory consumers
- maintain, select, and distribute extremely valuable laboratory information, both internal (e.g., related to the quality system) and external (e.g., relevant information for consumers)


Finally, an appropriate use of LIS should allow the laboratory to implement applied research:

- taking advantage of modern data mining techniques
- safely exporting data to other software

The resulting LIS architecture would, therefore, be a combination of three components:

- an analytical information subsystem, oriented to share information
- a knowledge-based subsystem, oriented to analyze data and trends
- a transactional data warehouse subsystem, able to communicate with other information systems

Although we previously mentioned that technology today knows no boundaries, at the present time no single information system is efficient enough to simultaneously provide all these items. This is possibly because each aspect requires a different database structure. However, it is probably just a matter of time before a comprehensive solution for all three aspects is found. Meanwhile, a number of developments are growing in the clinical laboratory in the professional domain (proteomics, metabolomics), in closely-related disciplines (bioinformatics), and in the general framework of the knowledge society (knowledge globalisation). Applications that have been running for several years—such as expert systems, neural networks, and genetic algorithms—can benefit from the performance and capacity of today's computer science and technology.

It is difficult to forecast the evolution of IT and how it will continue to influence the clinical laboratory. The rather candid scepticism of 60 years ago: "I think there is a world market for maybe five computers" (Thomas Watson, chairman of IBM), has now evolved to a lawless optimism: "I do not fear computers. I fear the lack of them" (Isaac Asimov). It cannot be overlooked that the aim of information is to achieve knowledge and the aim of knowledge is to achieve wisdom. A word of caution may be advisable: "The real danger is not that computers will begin to think like men, but that men will begin to think like computers" (Sydney J. Harris). 

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# Functional Foods

## Reflections on an Expanding Market

by A. Monge et al.

In 2006, IUPAC supported the study of Nutraceuticals in Latin America as a scientific opportunity of commercial interest for the entire community. This initiative, promoted by the IUPAC Subcommittee on Medicinal Chemistry and Drug Development, chaired by C.R. Ganellin, resulted in Latin American researchers uniting efforts to successfully carry out this study. This project consists of a general presentation of the topic followed by discussions of specific situations in different Latin American countries.

The term nutraceutical is the result of a contraction between nutrition and pharmaceutical. In 1989, Stephen Defelice defined nutraceutical<sup>1</sup> as “any substance that is a food or a part of a food and provides medical or health benefits, including the prevention and treatment of disease.”

Not long after, the definition was modified by Health Canada, which defined nutraceutical as “a product isolated or purified from foods, and generally sold in medicinal forms not usually associated with food, and demonstrated to have a physiological benefit or provide protection against chronic disease.”<sup>2</sup> In the *Merriam-Webster Dictionary* this term is defined as “foodstuff (as a fortified food or dietary supplement) that provides health benefits in addition to its basic nutritional value.”

Functional food (FF) is that which has a beneficial effect for health, be it for its constitution or for having added a nutraceutical to the original foodstuff, more specifically in certain Latin American countries. Thus, according to Health Canada,<sup>2</sup> a FF is “consumed as part of a usual diet that is similar in appearance to, or may be, a conventional food, and is demonstrated

to have physiological benefits and/or reduce the risk of chronic disease beyond basic nutritional functions” (beyond energy and essential nutrients). For example, yogurt promotes beneficial microflora in the gut; cereals provide a significant source of fiber believed to decrease the risk of certain types of cancer; papaya, which contains papain, helps the digestion of protein and provides other benefits (see below).

### Background

The concept of FF is very old: “Let food be your medicine and medicine be your food. Whosoever gives these things no consideration and is ignorant of them, how can he understand the diseases of man.” Hippocrates ca 400 B.C.<sup>3</sup> Interest in functional foods emerged in Japan in the mid-1980s, with the following objectives:

1. control healthcare costs
2. improve quality of life
3. increase life expectancy

Indeed, the term functional food was first introduced in Japan and refers to processed foods containing ingredients that aid specific bodily functions in addition to being nutritious (Foods for Specified Health Use, FOSHU).<sup>4</sup>

In the past few years, consumption of functional foods has increased considerably and is a growing market. In many developed societies, there is a subset of the population that is preoccupied with these types of food, which have beneficial properties or incorporate extracts or compounds such as vitamins. In addition, these people are often focused on avoiding the ingestion of saturated fats, controlling alcohol intake, doing daily exercise, and following other healthy habits.

The situation is quite different in developing countries, where people consume functional foods to resolve nutritional problems and hunger and as a substitute for more expensive medicines. There are millions of people for whom these compounds not only prevent a loss of health but are, in fact, the only form of treating a disease.

We are living in an important time in which the developed countries are very interested in functional food that can be made available from the developing countries. With regard to variety as well as quantity, the majority of the plants under consideration as good sources of phytochemicals—extracts that are added to food such as fruit juice—are found in developing countries. It might be opportune to appeal to corporations'



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social responsibility so that developing and developed both benefit.

### Questions To Be Resolved

Frequently, knowledge of specific phytochemicals and their uses is limited to different native communities, which have a long history of using these compounds. However, these communities lack the modern scientific training to translate the benefits of these phytochemicals in such a way that the developed world will understand.

There are three principal issues to resolve. First, there is the question of scientific validation and verification of the claims of healthful effects from these products. The second issue involves the need to determine if the benefit can be obtained at the doses ingested with routine intake of the food. The third issue is related to safety issues; nothing justifies the affirmation that a natural product is equivalent to a non-toxic product.

### Functional Foods in Latin America

The Latin American region extends from Mexico to Chile and Argentina. It includes countries of diverse geography and culture, but nearly all possess a long history of using plants for health-related treatments, with innumerable oral and written testimonies to the curative effects of plants. Quinine, for the treatment of malaria, is probably the most well know of these.

Traditionally, plants have been associated with medicinal agents; hence, the interest shown by medicinal chemistry. Typically, scientists isolate and optimize

*Latin America's wealth in plants with potential applications as functional foods is remarkable, for its variety as well as for the associated traditional knowledge regarding the plants.*

Research can be carried out on the plant itself in such a way that the final product can be created completely within the developing countries, which results in local growth and maintains biodiversity.

compounds synthesized by plants for clinical use. The product that is finally introduced into clinical trials is usually a chemical modification of that which was originally found in the plant. Consequently, there is a loss of interest in the original material of vegetable origin.

The scenario is very different when considering functional foods.

Latin America's wealth in plants with potential applications as functional foods is remarkable, for its variety as well as for the associated traditional knowledge regarding the plants. This article presents examples of functional foods from many different countries. It is hoped that disseminating this knowledge will encourage companies and researchers to consider the importance of the issue and to take an interest in it. However, it should be pointed out that exploiting these plants can be sensitive because in many cases native groups are apprehensive about revealing discoveries that are part of their cultural heritage.

This situation is especially important and representative of the Amazon, where there are isolated groups that have their own languages, social structures, and nutritional habits. It is interesting to see how different isolated tribes use the same plants for the same use. For example, in the treatment for obesity,<sup>5</sup> the Yanumansi from the Venezuelan part of the Amazon (250 persons) use *Smilax dominguisis* in the same way as the Aba Conoeiros of Brazil (Fuentes del Totacntis) (50 persons) or as the Mamainde, also Brazilians (Rondônia-Alto Rio Curimbiara) (200 persons). Another example could be the use of *Turnera ulmifolia* for the treatment of something as generic as debility by the Apiaca of Brazil (Mato Grosso Norte (100 persons) or by the Kayapu (200 persons), also from Brazil (Moto Grasso) or by the Maku (300 persons) from the valleys of Uneixi del Urubaxi in Brazil, or by the Piriutiti (110 persons) of Rio Curian or by the Sinabo (320 persons) of Bolivia (Bajo Yata). Far from the Amazon, in Mexico, (Chihuahua) the Taramaras (500 persons) also use this plant for the same purpose.

With regard to these countries that are so rich in biodiversity, it is important that the aforementioned comments regarding experiences based on human groups composed of small numbers of people be verified scientifically. Continuing on with the area of the Amazon and focusing on Brazil, one example to be considered is *Taraxacum officinale*, an *Asteracea* containing a family of compounds which are claimed to be an antioxidant, have antiinflammatory and diurectic effects, and even be useful in the treatment of diabetes, without having scientific evidence to back up these claims,<sup>6</sup> and yet with well-known side effects and interactions.

This plant, known as Dandelion (Diente de León), is abundant throughout the Northern Hemisphere and is cultivated in East European countries such as Bulgaria, Hungary, Poland, and Romania. It is used in the form of infusions, decoctions of the roots, and also extracts from the leaves. This is an example of a plant that

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presents activity of interest that is still not confirmed and whose side effects should be taken into consideration, and yet it is being used with clear benefits of exploitation. It is an example of a relationship between different societies and continents that clearly reflects the difficulty regarding the establishment of the therapeutic use and innocuity of a plant regardless of the society being considered.

In Brazil, the root vegetable “racacha” or *Arracacia xanthorrhiza* is a major commercial crop. Purees and soups made from the root are considered excellent for children and babies. Racacha is rich in minerals and vitamins A and B and in calcium and phosphorus. It is easily digested and is indicated for convalescents and the elderly. Racacha roots are used as the basis of a food regimen in the district of Coroico, Bolivia, accompanied by yacón (*Smallanthus sonchifolius*) juice; yacón is a sweet root vegetable whose pulp contains inulin, an agent that can be related to the control of diabetes.<sup>6,7</sup> Many claim that Racacha provides energy, boosts the immune system, and prevents infections. It is necessary to demonstrate whether or not these claimed benefits correspond to the traditional use of the plant.

The institutional support given to the cultivation of Racacha has helped to improve the species, and its industrialization<sup>8</sup> benefits Andean countries. This is a clear example of how technical aid can benefit entire regions.

Sarsaparilla, *Kajahuatena* (*Smilax regeli* Killipel Morton Griseb), is another example of a root frequently used in America for its diuretic and purifying effects and for its effective treatment of psoriasis. Both the root and the rhizomes are used.

It is not surprising that governments, such as Bolivia's, have invested in research related to the production and determination of the properties of these plants, which have been known about in certain areas for a long time.

The American continent is very rich in fruits that can be used in food regimens, in their original form as well as in the form of juices. One example is Papaya (*Carica papaya*), of Mexican or Andean origin, according to diverse authors. Its use has extended throughout the entire world. Papaya pertains to *Caricaceas* and consists of 70 species. It is known for its content of papain which helps the digestion of protein, and it is also a source of potassium, vitamin C, pro-vitamin A and fiber.

While papaya is well extended throughout the world, knowledge regarding Noni juice (*Morinda citrifolia* L.) is different; the latter has been recognized for

over 2000 years in many villages, cultivated throughout Central America, and commercialized by different companies.<sup>9</sup> According to traditional knowledge, it has beneficial effects, such as for treating hypoglycemia, cholesterol levels, menstrual cramps, and blood pressure.<sup>10</sup> It is also a typical situation that demonstrates the resistance of developing societies to further study on traditional activities. Nevertheless, Noni juice is commercialized throughout the entire world, but at an elevated price. It is an example of a plant that not only has possible beneficial effects for health but is also commercial. The climatic conditions of the Caribbean are very favorable for this crop. This plant is an example of a value-added crop whose complete process from cultivation to market can be carried out in developing countries, thereby contributing to their industrialization.



“Racacha” or *Arracacia xanthorrhiza*.

Guayaba (*Psidium spp.*), guava in English, is one among more than 100 very popular species in Central America and the Caribbean. The trees of the Myrtaceae family produce an edible fruit that contains vitamins A, B and C; *Psidium guajara* is the most popular.<sup>11</sup> It is often used as an anti-influenza agent. This fruit is used in an ample variety of foods, frequently found in yogurt dairy products. In Mexina Calvillo, Aguascalientes, Mexico, within the Huajacar valley, the most important plantations of Guayaba are found. This could be considered a model of high yield sustained agriculture where, in addition to the beneficial effects of the fruit as a FF, the possibility of attaining great benefits for the development of the country can be taken into account.

Mango (*Mangifera indica* L.) is also an important fruit but, at present, the application of mango bark is considered for a pharmaceutical preparation (Vimang),

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made in Cuba.<sup>12</sup> This preparation is a raw extract with antioxidant, analgesic, antiinflammatory and immunomodulating activity. The activity has been demonstrated in more than 7 000 patients during a period of ten years (1994–2004). It is a clear example of the use of natural resources because, in addition to the fruit itself which has its interest in nutrition, the Cuban scientists have extended their studies and carried out scientific experimentation based on tradi-

tional observations; this offers the opportunity to introduce new products, as nutraceuticals or FF, in health treatment.

Naturally, when considering medicinal application of a plant, it is necessary to gather information that comes forth from its traditional use. One such case occurs in Costa Rica de Hombre Grande (*Quassia amara* L.ex. *Blom*). This plant, which extends from Mexico to the Amazon, is used in Europe as an appetizer, diuretic, and agent against dyspepsia and anorexia among others, which allows it to be considered as a nutraceutical. It also has an important use as an insecticide,<sup>13</sup> as can be deduced from the important importation of this plant for said use by the USA since 1940. The latter example offers a good reason to develop and conserve the biodiversity of these countries in addition to promoting research for additional uses other than the traditionally observed medical use.

### Industrialization of Functional Foods

Industrialization of FF is an important question that should be considered with great care, for the benefit of the developing countries. For example, in Mexico, the plants which are traditionally used for medicinal purposes are estimated to number 3000 (approximately 10 percent of the country's plants), of which the number estimated to be commercialized is approximately 250;<sup>14</sup> principally, their origin is in the central and southern areas of the country.

The project, "Mercados Verdes Herbolarios," supported by the USA is an example where farm workers

have acquired the ability for the sustained use and management and in the processing of medicinal plants.



However, as Bentacourt cites,<sup>15</sup> studies on this material that also consider the commercialization of these plants are scarce.

It is important to appreciate that if the use of plants for health purposes does not include industrial exploitation it will be impossible for them to reach societies which need them, and there will be no profitability

for the societies that possess the plants. Likewise, a series of actions common among all countries is required for the management of plants as nutraceuticals or FF. In general, there is a need for national programs such as PRONAPLAMED (National Program of Medicinal Plants), in Mexico. The objective of these types of programs is to guarantee sustained cultivation, which permits conservation of the plants and an improvement of the species, whenever possible. It should be kept in mind that a great number of these plants that are used for nutraceuticals or FF are wild plants. In addition, the cultivators should be educated in this matter because, if not, certain aspects will be negatively affected. One such example is the quality, which is sometimes affected during the process "plant to finished product." This is largely due to lack of knowledge or poor habits that are sometimes observed in the handling of the plants.

One possible solution for these cases lies in the formation of microcompanies, an activity much used today in developing countries; they are becoming accepted by the cultivators as they are beginning to realize the need for them.

There is a need for technology for the different phases that are involved in the preparation of these compounds. Storage and treatment can be real problems where there is a lack of properly ventilated warehouses and refrigerators.


The reasons behind the interest shown in plants by the national companies appear to be commonly shared by the native population whereas the transnational companies only seem to show interest in relation to the sectors that possess adequate economic

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availability.

In the Latin American countries a series of common characteristics appears, one being that their great tradition in the use of plants as FF or nutraceuticals corresponds to only 10 percent of their rich variety of plants. The most immediate consequence in this world of climatic changes and general aggressions on nature is the danger of losing the species.

The countries being considered here have formed organizations that support the producers through training of the cultivators, sustained management of the plants, and proper production of the final product. It should always be kept in mind that this action for the development of communities will result in good products, and efforts should be made so that the products may have the greatest possible added value. Producing fruit is not the same as producing juice, and the trade of plant extracts reduces the transportation costs and increases economic profit when compared with the commercialization of plain dried vegetable materials. Such development, in many cases, is out of the reach of plant producers and requires a technological input in order to establish, optimize and scale—up such processes. Organizations are being established through the creation of microcompanies in all of these countries and they reflect a great sense of solidarity.

The training of these cultivators is becoming an important aspect of this action because in many cases, the plants are wild and there is a possibility of unscrupulous exploitation which, in some cases, could result in mixing up some plants with others in a fraudulent attempt to satisfy possible market demands. An additional risk associated to this issue is the permanent lost of valuable species in their natural environments, which is a patent problem when roots are the organs of traditional use. The increasing concern in environmental affairs of the population from developed societies—consumers of natural resources produced in developing countries—could effectively contribute to the preservation of such resources, demanding the sustainable production of the raw material for the production of nutraceuticals and phytomedicines. 

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# Nikolai Izmailov

## An Essential Contribution to Physical Chemistry

by *Nikolay O. Mchedlov-Petrosyan*

**T**he V.N. Karazin National University, formerly Kharkov State University, has a long-standing tradition in physical chemistry dating back almost 150 years,<sup>1</sup> in which the renowned Russian chemist, Nikolai Beketov (1827–1911), played a pioneering role. As early as 1860, he took the first initiative in a series of lectures entitled “Special Course of Organic Chemistry and Interrelation Between Physical and Chemical Phenomena.” Within a few years a decisive milestone was reached when he founded the Physico-Chemical Division of the University in 1864 and delivered the first course of lectures on physical chemistry in 1865.

During the last years of the 19th century and the early years of the 20th century, a succession of scientists—among them P.D. Khrushchov, V.F. Timofeyev, N.D. Pilchikov, D.P. Turbaba, and G.E. Timofeyev—played a major role in building the university’s reputation and contributing significantly to the field of physical chemistry, mainly in the specialized area of solution chemistry. This tradition was continued in the years before the outbreak of World War II, with a succession of outstanding physical chemists in Kharkov. Along with the notable achievements of G.E. Mukhin, A.N. Shchukarev, I.S. Teletov, P.P. Kosakevitch, E.N.

Gapon, S.S. Urazovskiy, and I.N. Frantsevich, the career foundation of Nikolai Arkadievich Izmailov was laid at this time, before he went on to head the Department of Physical Chemistry of the Kharkov State University from 1944 to 1961.

Nikolai Izmailov (1907–1961) was born in Sukhumi in the southern region of the Russian Empire on 22 June 1907. During his early years he endured hardships, which most certainly contributed to his personal growth and maturation into what can aptly be characterized as a self-made man. When Nikolai was two years old, his father died. At the outbreak of the October Revolution in 1917, the family happened to be in Kharkov, and at the tender age of 10 Nikolai was obliged to assume the mantle of responsibility as the senior male member of the family and to support his mother, grandmother, and sister. Thus, he started a battle for survival in the face of daunting obstacles.

Despite these demands, he was able to persevere with his education and enrolled at the Financial-Economical Technical School in 1922. Here he was first introduced to chemistry and developed a deep and enduring interest in the discipline that was destined to shape his future. After graduating in 1926 he took a teaching position in a primary school, which gave him the opportunity to provide elementary instruction in chemistry. In the first formal step of his subsequent scientific career, in 1928 Izmailov enrolled as a Ph.D. student at Kharkov State University (at that time called the Kharkov Institute of Public Education). He initially conducted research, under the guidance of Professor Kosakevitch,<sup>2a</sup> into sorption of gases. Thereafter, he investigated the influence of salts on adsorption of organic molecules on the interface between water and air.<sup>2b</sup>

Shortly after these introductory ventures, Izmailov began to pursue independent research activities. In 1934 he started on a joint appointment at Kharkov Pharmaceutical Research Institute, and his scientific interests developed along two main directions: static and dynamic properties of sorption from solutions, and the influence of the solvent on dissociation of electrolytes. Both of these branches of pure chemistry were driven by the needs of applied science. Furthermore, his lively inventiveness and scientific insight enabled him to recognize and pursue inquiries to a practical outcome. This is vividly exemplified by his search for new methods for pharmaceutical analysis in which he collaborated with Maria Shraiber to introduce in 1938 the “drop-chromatographic method,”<sup>3</sup> which later became known as thin-layer chromatography. This



*Young Nikolai Izmailov in the chemical laboratory of the Financial-Economical Technical School.*



finding is widely recognized and acclaimed and continues to play an essential role in everyday laboratory practice.

Izmailov was awarded a Ph.D. in chemistry at Kharkov State University in 1937. Shortly thereafter he made a start in his Sc.D. dissertation; however, the outbreak of World War II forced him to postpone any plans to complete and submit it. In October 1941, Izmailov, along with his wife and two children, were evacuated to his birthplace, Sukhumi, where they remained for the next three years. This was a period in which he was engaged in hard work for the needs of defense. After the liberation of Kharkov from the Germans in 1943, Izmailov received a government decree to return to the city and head the Department of Physical Chemistry at the university. In May 1944, the Izmailov family returned.

A long and difficult period of restoration followed because Kharkov had suffered extensive destruction during the conflict and occupation of 1941 through 1943. However, Izmailov managed to reconcile his duties as department head with his research in the Pharmaceutical Institute. He resumed work on the preparation of his Sc.D. dissertation, entitled "The Influence of Solvents on the Strength of Acids," which he eventually presented in January 1948 to the Ukrainian Academy of Sciences in Kiev. Later in the same year he was appointed a professor.

This was the start of an extraordinarily creative phase in Izmailov's career. A review on the subject of his dissertation<sup>4</sup> and his systematic studies throughout the 1950s, dealing with behavior of electrolytes in solution, provided the basis for the definitive understanding of dissociation at that time.<sup>5</sup> His most monumental contribution was the treatise *Electrochemistry of Solutions*, which was published in Russian in 1959.<sup>6</sup> Major sections of this voluminous 958-page work—devoted to the detailed scheme of electrolytic dissociation, differentiation action of solvents, and solvation, among other topics—were completely reviewed in the excellent monograph by A.I. Shatenshtein, which was translated into English<sup>7</sup> and thus became available to international readership.<sup>5a</sup> This major contribution is well known to those working in the field of solution chemistry and is still frequently cited.

Izmailov also continued his early studies on the behavior of glass electrodes in different solvents and made notable contributions to the theory of physicochemical analysis. He authored more than 280 scientific publications during his career and supervised 31 people in their Ph.D. degree studies.



*Izmailov in his laboratory in the 1930s.*


Eleven of his coworkers later received Sc.D. degrees (V.N. Eremenko, A.M. Shkodin, V.D. Bezugliy, V.V. Aleksandrov, E.F. Ivanova, E.V. Titov, Yu.A. Krugliyak, O.M. Konovalov, V.P. Georgievskiy, V.I. Lebed, and V.D. Chmil). In 1955 the title "Honored Scientist of Ukraine" was conferred upon him, and in 1957 he was elected to the Academy of Sciences of the Ukrainian Soviet Republic. He was also honored by the Mendeleev award for *Electrochemistry of Solutions*.<sup>6</sup> In 1973, in recognition of his achievements in the field of glass electrode studies, he was posthumously included into the group of U.S.S.R. state prize winners.

Izmailov died suddenly on 2 October 1961 as he was discussing scientific problems with one of his coworkers. His untimely death while thus absorbed in his work is perhaps an expression of the man and his scientific style. He always believed that there was no time to be lost and usually began his working day at 5:00 a.m. He spent much time in consultation with his Ph.D. students and coworkers and also maintained regular sittings of scientific seminars in the physical chemistry department. Although he worked tremendously hard and was clearly driven by a consuming interest in science, he also led an active social life. He also was an enthusiastic sportsman and particularly enjoyed swimming, alpinism, and tennis. Among his extramural interests, he authored a set of publications devoted to the history of physical chemistry in Kharkov University. He also served the university as vice-rector from 1948 to 1953. In addition, Izmailov and his wife Alexandra Izmailova (Glukhovtseva) had a daughter, Victoria, and a son, Alexander. Victoria Nikolaevna Izmailova (1930–2002) spent a significant part of her career at Moscow State University, where she became a professor and was a well-known expert in the field of colloid chemistry. Alexander Nikolaevich (1938–1990) was a physicist.

## Nikolai Izmailov

An International Conference on Modern Physical Chemistry for Advanced Materials was held in V.N. Karazin National University 26–30 June 2007 to commemorate the centenary of the birth of Professor Nikolai Izmailov. This event was held under the sponsorship of IUPAC and the European Society of Chemical and Molecular Sciences. Just before the opening of the conference, the book *Scientific Heritage of N.A. Izmailov and Topical Problems of Physical Chemistry*

(eds. V.I. Lebed, N.O. Mchedlov-Petrosyan, Yu.V. Kholin, Kharkov University Press, Kharkov, 2007) was ceremonially presented to the academic community and the media at the Kharkov National University Museum.

The conference provided an opportunity to pay tribute to Nikolai Izmailov and to salute his achievements. A majority of the eminent international scientists who delivered plenary lectures at this event have contributed works to a collection of papers in *Pure and Applied Chemistry* [2008, Vol. 80, Issue 7; <[www.iupac.org/publications/pac/80/7/](http://www.iupac.org/publications/pac/80/7/)>]. This volume serves as a permanent archival record of the event and of the man who inspired it. 

**Supplementary material.** A short bibliography listing the sources of some seminal contributions by N.A. Izmailov, analysis of his scientific activities written in English and in Russian, as well as some recollections are available at <[www-chemistry.univer.kharkov.ua/izmailov](http://www-chemistry.univer.kharkov.ua/izmailov)>.



**Nikolai Izmailov**  
(1907–1961)

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ChemSpider—a free-access service providing a structure centric community for chemists—continues to expand its list of supported publishers. In July 2008, ChemSpider added Royal Society of Chemistry articles and IUPAC's journal *Pure and Applied Chemistry* to the sources feeding its literature search. Users can now conduct Chemrefer text-based searches of 12 sources of chemistry literature.



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 [www.chemspider.com/blog/iupacs-pure-and-applied-chemistry-text-now-indexed-on-chemspider.html](http://www.chemspider.com/blog/iupacs-pure-and-applied-chemistry-text-now-indexed-on-chemspider.html)

## Craig Hawker Wins DSM Performance Materials Award

Craig J. Hawker, professor of chemistry, biochemistry, and materials, and director of the Materials Research Laboratory at the University of California, Santa Barbara, USA, has been awarded the DSM Performance Materials Award 2008 in recognition of his exceptional contributions to the advancement of the materials sciences. Hawker is one of the world's leading scientists in the field of polymeric performance materials. His fundamental and applied research and his dedication to innovative science have earned him a high reputation and a large following in the academic world.



Craig Hawker (right) receives the award from Professor Joseph Put, Chief Technology Officer of DSM.

An international judging committee, chaired by Joseph Put, chief technology officer of DSM, selected Hawker from among several candidates shortlisted by an international nomination committee. Hawker received the award—which carries a cash prize of EUR 50 000—from Put at the IUPAC Macro 2008 Congress in Taipei (Taiwan) on 30 June 2008. Speaking on the occasion, Put said “A real paradigm shift took place in synthetic chemistry in the past 15 years, which resulted in the building up of well-defined large functional systems mimicking biological systems. This was made possible by a combination of very well-controlled chemistry, noncovalent interactions and biotechnological approaches. Professor Hawker played a vital role in this development, both by opening up new synthetic pathways and by looking into possible applications in microelectronics and biomedical.”

Craig Hawker was born in Australia, where he received his early education and graduated in chemistry with a First Class Honors degree from the

University of Queensland in 1984. He went on to study at Cambridge University in the UK, where in 1988 he obtained his Ph.D. From 1988 to 1990 he worked as a post-doctoral research associate at Cornell University.

Hawker started his professional career as a Queen Elizabeth II Research Fellow at the University of Queensland in Australia, a position he held from 1990 to 1993. In 1993 he went to the USA again to take up the position of research staff member at the IBM Almaden Research Center in San Jose, California. Since 2004 he has held his current positions at the University of California, Santa Barbara. His research group there is doing pioneering work on novel polymers and nanostructured materials for application in areas as diverse as electronics and biomedical and has focused on the interface between organic and polymer chemistry with emphasis on the design, synthesis, and application of well-defined macromolecular structures in biotechnology.

Hawker has been honored with a large number of international awards, including the 2000 Young Scientists Award from IUPAC and the 2005 ACS Award in Applied Polymer Science from the American Chemical Society. He is editor of the *Journal of Polymer Science Polymer Chemistry* and serves as a consultant to many U.S. and international companies.

At the presentation ceremony in Taipei, Hawker gave an award lecture on "Design of Performance Polymers for Microelectronic and Biomedical Applications."

The DSM Performance Materials Award forms part of DSM's Innovation Awards Program and was presented for the first time this year in cooperation with IUPAC. DSM grants the award every two years in recognition of scientific work that has significantly contributed to the advancement of the materials sciences, with special emphasis on polymeric materials.

 [www.dsm.com](http://www.dsm.com)

### Le VIM Nouveau Est Arrivé!

**A**fter 10 years in the making, the third edition of *International Vocabulary of Basic and General Terms in Metrology* (VIM) is now available. The VIM provides a set of definitions and associated terms, in English and French, for a system of basic and general concepts used in metrology, together with concept diagrams to demonstrate their relations. Additional information is given in the form of examples and notes under many definitions. This vocabulary is meant to be a common reference for scientists and engineers, as well as teachers and practitioners, involved in planning or performing measurements, irrespective of the level of measurement uncertainty and irrespective of the field of application. It is also meant to be a reference for governmental and inter-governmental bodies, trade associations, accreditation bodies, regulators, and professional societies.

This third edition has been approved and adopted by each of the eight Joint Committee for Guides in Metrology (JCGM) member organizations: International Bureau of Weights and Measures, International Electrotechnical Commission, International Federation of Clinical Chemistry and Laboratory Medicine, International Organization for Standardization, IUPAC, International Union of Pure and Applied Physics, International Organization of Legal Metrology, and International Laboratory Accreditation Cooperation.

This edition cancels and replaces the second edition published in 1993. The full text of the VIM is available online at no charge.

 [www.bipm.org/en/publications/guides/vim.html](http://www.bipm.org/en/publications/guides/vim.html)

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## Biophysico-Chemical Processes of Anthropogenic Organic Compounds in Environmental Systems

Anthropogenic organic compounds (AOC) are synthetically made organic chemicals. They range from gasoline components (e.g., benzene, toluene, xylene) to emerging contaminants such as endocrine-disrupting chemicals and personal care products. Because of their widespread use and disposal, AOCs are commonly found in our environments, including in the water we drink, the air we breathe, and the soil in which we grow our food. These compounds are often toxic and can severely deteriorate an ecosystem. They can also bioaccumulate through food chains and cause various diseases (and even death) to organisms, including humans. AOCs behave differently in different environmental media, which vary in their physical, chemical, and biological components and processes. Therefore, a more complete understanding of the biophysico-chemical processes of AOCs in environmental systems is essential to the development of innovative management strategies for sustaining the environment and ecosystem integrity.

Physical, chemical, and biological interfacial interactions and processes govern the fate, transport, availability, exposure, and risk of AOCs. However, the fundamentals of many physicochemical and biological interfacial reactions of AOCs and their impacts on ecosystems largely remain unknown. As a result, predictive models for their fate, transport, and risk in different media are often off target. Advancing knowledge in this area would require a concerted effort of scientists in relevant physical and life sciences, including chemistry, mineralogy, geochemistry, microbiology, ecology, and in the soil, atmospheric, and aquatic sciences.

In contrast to traditional books that largely focus on separate, individual physicochemical and biological aspects, the proposed IUPAC-sponsored book on Biophysico-Chemical Processes of Anthropogenic Organic Compounds in Environmental Systems aims to integrate the frontiers of knowledge related to the fundamentals and the impact of physicochemical and biological interactions and processes of AOCs in soil, sediment, water, and air. The objectives of the book are to address (1) fundamental biophysico-chemical processes of AOCs in the environment, (2) occurrence and distribution of AOCs in air, water, and soil, and their global cycling, (3) state-of-the-art analytical techniques of AOCs, and (4) restoration of natural

environments contaminated by AOCs. The proposed book will also identify gaps in knowledge on the subject matter and, accordingly, suggest future areas of research.

Ideally, this book will bring together world-renowned international scientists to integrate state-of-the-art issues, the latest discoveries, and future prospects related to research on AOCs in the environment. The book will be an important addition to the scientific literature and a valuable source of reference for students, professors, scientists, and engineers.

This book will be coedited by Baoshan Xing, Nicola Senesi, and P. Ming Huang and will be published as Volume III in the IUPAC series on Biophysico-Chemical Processes in Environmental Systems.

For more information and comments, contact Baoshan Xing <[bx@pssci.umass.edu](mailto:bx@pssci.umass.edu)>.



[www.iupac.org/web/ins/2008-001-1-600](http://www.iupac.org/web/ins/2008-001-1-600)

## Applied Thermodynamics of Fluids

The Physical and Biophysical Chemistry Division (I) has endorsed project 2008-014-1-100 for a book entitled *Applied Thermodynamics of Fluids*, proposed by the International Association of Chemical Thermodynamics.<sup>1</sup> This text, which includes contributions from distinguished international experts, is being compiled by the editorial team of A.R.H. Goodwin, J.V. Sengers, and C.J. Peters. It will be the eighth in the series *Experimental Thermodynamics*<sup>2-8</sup> and will be concerned with the measurement and correlation of thermodynamic and transport properties of substances.

The first volume in the series was concerned with calorimetry of nonreacting systems,<sup>2</sup> and the fourth with the calorimetry of reacting fluids.<sup>5</sup> Volume III continued the theme of nonreacting systems with measurements of properties characteristic of the relaxation of a fluid from a nonequilibrium state: the transport properties.<sup>4</sup> The description of noncalorimetric measurement techniques was first recorded in Volume II, published in 1975.<sup>3</sup> Accounts of state-of-the-art experimental methods for the determination of the thermodynamic properties have been presented more recently for single phases in Volume VI,<sup>7</sup> and multiple phases in Volume VII<sup>8</sup>; Volumes VI and VII are also of interest to the data evaluator who needs to assess the reliability of experimental data obtained with specific techniques. The fifth volume presented the theoretical basis for equations of state of both fluids and fluid

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mixtures and has been described as important for engineers and physical chemists.<sup>6,9</sup>

The intent of *Applied Thermodynamics of Fluids* is to revise and update Volume V,<sup>6</sup> albeit with a change in emphasis to the application of theory, without recourse to derivations of the constitutive equations, while retaining the fundamental aspects of the book and including topics omitted previously such as *nano*- and *meso*-scale thermodynamics, associating fluid theory, chemically reacting systems, and nonequilibrium thermodynamics. The new volume, which will be published by the Royal Society of Chemistry in late 2009, is intended to address the needs of practitioners within academia, government, and industry.

### References

1. For further information visit the Web site of the International Association of Chemical Thermodynamics <[www.iactweb.org](http://www.iactweb.org)>.
2. *Experimental Thermodynamics, Volume I, Calorimetry of Non-Reacting Systems*, J.P. McCullough and D.W. Scott, eds., for IUPAC, Butterworths, London, 1968.
3. *Experimental Thermodynamics, Volume II, Experimental Thermodynamics of Non-Reacting Fluids*, B. Le Neindre and B. Vodar, eds., for IUPAC, Butterworths, London, 1975.
4. *Experimental Thermodynamics, Volume III, Measurement of the Transport Properties of Fluids*, W.A. Wakeham, A. Nagashima, and J.V. Sengers, eds., for IUPAC, Blackwell Scientific Publications, Oxford, 1991.
5. *Experimental Thermodynamics, Volume IV, Solution Calorimetry*, K.N. Marsh and P.A.G. O'Hare, eds., for IUPAC, Blackwell Scientific Publications, Oxford, 1994.
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7. *Experimental Thermodynamics, Volume VI, Measurement of the Thermodynamic Properties of Multiple Phases*, A.R.H. Goodwin, K.N. Marsh, and W.A. Wakeham, eds., for IUPAC, Elsevier, Amsterdam, 2003.
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9. L.S. Garcia-Colin and F.J. Uribe. *J. Stat. Phys.* **2002**, *106*, 403-404.

For more information and comments, contact Anthony R.H. Goodwin <[agoodwin@slb.com](mailto:agoodwin@slb.com)>, Jan V. Sengers <[js45@umail.umd.edu](mailto:js45@umail.umd.edu)>, or Cor J. Peters <[c.j.peters@tnw.tudelft.nl](mailto:c.j.peters@tnw.tudelft.nl)>.

 [www.iupac.org/web/ins/2008-014-1-100](http://www.iupac.org/web/ins/2008-014-1-100)

## Analogue and Standalone Drugs

In the book *Analogue-Based Drug Discovery*, published by Wiley-VCH in 2006 under the aegis of IUPAC, we focused first of all on analogue drugs with a double similarity—that is, those that are similar to another drug from both chemical and pharmacological viewpoints. These were referred to as *full analogues*. The book also discussed some examples of *structural analogues*, which have similar chemical structures but different pharmacological properties. We also proposed using the term *pharmacological analogues* to describe drugs that have completely different chemical structures but similar pharmacological properties.

In 2006 a new project of IUPAC's Division VII (Chemistry and Human Health) was started to study the role and the importance of standalone drugs; these are defined as drugs that are neither structural nor pharmacological analogues. The project is chaired by Janos Fischer (Richter Plc) with Robin Ganellin (University College London), Arun Ganesan (University of Southampton), and Dr. John Proudfoot (Boehringer Ingelheim, Ridgefield, United States) as project members.

In this preliminary report, we give a short overview of the top 100 most important drugs worldwide based on the sales data of IMS, a company that provides comparative sales data on the pharmaceutical industry. In 2006 the global sale of drugs amounted to USD 638 billion. The sales of the top 100 drugs represented about 51 percent of global sales (i.e., USD 326 billion). Table 1 shows that 84.4 percent of sales of the top 100 drugs derives from small molecule drugs, whereas macromolecular drugs and biological entities amount to 9.2 percent of sales and vitamins and a hormone amount to 6.4 percent of sales.

**Table 1. Drugs Types of the Top 100 Drugs**

| Drug Types                                   | Sales (2006)<br>USD (billions) | Ratio (%) | Numbers |
|--|--------------------------------|-----------|---------|
| Small Molecule<br>Drugs                      | 275                            | 84.4      | 80      |
| Macromolecules<br>and Biological<br>Entities | 30                             | 9.2       | 10      |
| Vitamins and<br>Hormones                     | 21                             | 6.4       | 10      |

The importance of small molecule drugs remains very high in spite of the increasing role of macromolecular

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drugs (proteins) and biological entities (monoclonal antibodies).

Table 2 lists the small molecule drugs that are among the top 100 drugs according to their analogue status.

**Table 2. Types of Small Molecule Drugs among the Top 100 Drugs**

| Small Molecule Drug Type  | Number |
|---------------------------|--------|
| Pioneer drugs             | 10     |
| Full analogues            | 51     |
| Pharmacological analogues | 8      |
| Structural analogues      | 2      |
| Standalone drugs          | 9      |

It is remarkable how high the number (51) of full analogues is among the top 100 drugs. The analogue drugs among the top 100 belong to 42 different analogue classes of drug action, as defined by the main pharmacological effect (e.g., ACE inhibitors,  $\alpha_1$ -blockers, AT<sub>1</sub> antagonists,  $\beta$ -lactamase inhibitors), and there are only 10 pioneer drugs (“first in class”) among the top 100 drugs from the analogue classes. This is because the pioneer drugs were improved through the making of analogues, and continuous optimization has produced additional analogue drugs that are even better.

The following nine standalone drugs have been identified from among the top 100 drugs: acetaminophen, acetylsalicylic acid, aripiprazole, bupropion, ezetimibe, lamotrigine, metformin, topiramate, and valproate semisodium.

In this project we are focusing on the role of standalone drugs. We will analyze their importance, the need for improvement, and the difficulties in their optimization. The older drugs, such as acetaminophen and acetylsalicylic acid, particularly merit optimization because of their serious side effects.

For more information and comments, contact János Fischer <j.fischer@richter.hu> or C. Robin Ganellin <c.r.ganellin@ucl.ac.uk>.

 [www.iupac.org/web/ins/2008-013-1-700](http://www.iupac.org/web/ins/2008-013-1-700)

## Preparation for the Translation of the “Green Book”

This project will begin the process of using the original computer source files of the IUPAC Green Book,\* in English, for the publication of structurally identical documents in other languages. Initially, the following languages will be involved: German, French, Italian, Turkish, Japanese, Portuguese, and Spanish. In the long run, adherence to the present structure will facilitate generating across-the-languages dictionaries.

The project will consist mainly of a workshop involving all task group members. The aims of this workshop are twofold. First, the participants will learn how to use the LaTeX documents and how to process them, and in particular how to preserve the LaTeX files for formulae and tables to ensure uniform appearance throughout the different language versions. In doing so, we will take advantage of the extensive work performed in the past that can be transferred as such to the translated versions. Second, language-specific technical questions will be discussed related to problems that might arise during the translation of the electronic documents under the constraint of keeping an identical document structure under LaTeX.

\*The IUPAC Green book is titled *Quantities, Units and Symbols in Physical Chemistry* (RSC Publishing, Cambridge 2007 [ISBN 0 85404 433 7; ISBN-13 978 0 85404 433 7]).

For more information and comments, contact Roberto Marquardt <roberto.marquardt@chimie.u-strasbg.fr>.

 [www.iupac.org/web/ins/2008-007-3-100](http://www.iupac.org/web/ins/2008-007-3-100)

## Glossary of Terms Used in Immunotoxicology

The immunotoxicology of both organic and inorganic substances is presently of great interest in occupational and environmental health. A project has been ongoing to explore the immunochemistry of metals. Four technical reports have dealt with the molecular mechanisms of immune sensitization caused by metals [*Pure Appl. Chem.* 76: 1255-1268 (2004)], and critical evaluations of the use of three of the clinical tests potentially available for diagnosing specific metal allergies, namely the lymphocyte proliferation test [*Pure Appl. Chem.* 76: 1269-1281 (2004)], cytokine profiling [*Pure Appl. Chem.* 78: 2155-2168 (2006)], and evaluation of lymphocyte subpopulations [*Pure Appl.*



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*Chem.* 80: 1349-1364 (2008)]. Additional work on the effects of mercury, and particularly dental amalgams, on the immune system is in progress.

In preparing these reports, it became clear that there is an extensive specialized terminology foreign to chemists and not included in the *Glossary of Terms Used in Toxicology* (2nd ed.) [*Pure Appl. Chem.* 79: 1153-1344 (2007)] and *Toxicokinetics* [*Pure Appl. Chem.* 76: 1033-1082 (2004)]. In addition, a number of terms are somewhat ambiguous even within the discipline of immunology. Their careful definition will help to clarify regulatory and legislative discussion. A goal of the Division of Chemistry and Human Health is to incorporate precise chemical terminology into toxicology and risk assessment and, reciprocally

to merge toxicology into the terminology used by chemists. We believe that a *Glossary of Terms Used in Immunotoxicology* will add significantly to the value of the immunochemistry project, as well as serving as an essential addition to the toxicology glossaries referred to above. A projected outcome is a monograph based on the technical reports of the task group dealing with immunochemistry, supplemented by a glossary of correct terminology in this field.

For more information and comments, contact Douglas Templeton <doug.templeton@utoronto.ca>.

 [www.iupac.org/web/ins/2007-053-1-700](http://www.iupac.org/web/ins/2007-053-1-700)

## Provisional Recommendations

*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. Full text is available online.*

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

### Thermochemistry of Chemical Reactions: I. Terminology and Symbols\*

This work, which is presented in two parts, is concerned with the most currently experimental techniques used on the study of the thermochemistry of chemical reactions. The first part of this recommendation deals with the terminology and symbols, discusses the meaning, designation and symbols of the different parameters used in molecular thermodynamic studies. The second part is a brief description of the most important methods used to investigate the thermodynamic stability of molecules and chemical bonds, together with a detailed analysis of its basic assumptions and how thermodynamic quantities are derived.

\*Part II entitled 'Experimental Methods for the Determination of Bond Energies', is to be published as a separate technical report.

#### Comments by 31 December 2008

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### Glossary of Terms Used in Ecotoxicology

The objective of the *Glossary of Terms Used in Ecotoxicology* is to give clear definitions for those who contribute to studies relevant to ecotoxicology but are not themselves ecotoxicologists. This applies especially to chemists who need to understand the ecotoxicological literature without recourse to a multiplicity of dictionaries. The Glossary includes terms related to chemical speciation in the environment, sampling, monitoring and environmental analysis, as well as to adverse ecological effects of chemicals, ecological biomarkers, and the environmental distribution of chemicals. The dictionary consists of about 993 terms. The authors hope that among the groups who will find this glossary helpful, in addition to chemists, are pharmacologists, toxicologists, ecotoxicologists, risk assessors, regulators, medical practitioners, and regulatory authorities. In particular, it should facilitate the use of chemistry in relation to environmental risk assessment.

#### Comments by 31 December 2008

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# Bookworm

## Stop Faking It! Chemistry Basics

William C. Robertson  
NSTA Press, Arlington, Virginia, 2007  
ISBN 978-0-87355-239-4

reviewed by Parker M. Nelson and Hani Morgan

The thought of taking a course in basic chemistry (secondary or collegiate) usually conjures up feelings of dread for most students. Revealing my background as a chemistry instructor to nonscience types is typically met with a strange look or comment: "Yuck! You teach chemistry?" I often reply by attempting to explain some of the most interesting components of chemistry in the simplest terms possible.

So, what's an instructor to do? Throw in the towel or acknowledge the difficulty many students have with understanding basic chemistry? The difficulty is all too real, and what doesn't help matters is the fact that most textbooks explain even simple concepts in a confusing manner. Thus, the need arises for an easy-to-understand guide—one that could serve as a companion volume to basic chemistry textbooks. *Stop Faking It!* fits the bill.

The book is focused on making science fun and on helping students and teachers understand not only formulas and rules, but their underlying implications. It manages to present scientific information simply—while at the same time diving to an impressive depth of knowledge.

This book is divided into six chapters, each broken into two primary sections: "Things to do before you read the science stuff" and "the science stuff." Subsequently, the authors then break the topics down even further: "More things to do before you read the science stuff" and "more science stuff." This pattern usually repeats three to four times per chapter. Each step that the author takes brings the reader deeper and deeper into the presented information without obscuring the basic concepts. The illustrations and examples are designed to develop readers' concep-

tual discernment *without* discouraging them. And lay terminology is used whenever possible, which, paradoxically, seems to enhance the reader's technical comprehension instead of diminish it.

### Chapter Decomposition

Chapter one explains how early Greek philosophers perceived atoms and how their observations were used to explain what atoms are like. This was the time when many scientists believed that four elements existed: fire, earth, air, and water. This depiction of nature was accepted largely because it explained so many observations.

Chapter two shows how an atom's charge and activity relate to its structure and to subatomic particles. The author stresses the fact although no one has ever seen these particles, they can be used to explain scientific observations.

Chapter three describes the way an atom's valence, charge, and configuration determine its location on the periodic table. Readers who may become perplexed by the terminology are directed to the informative glossary at the end of the book.

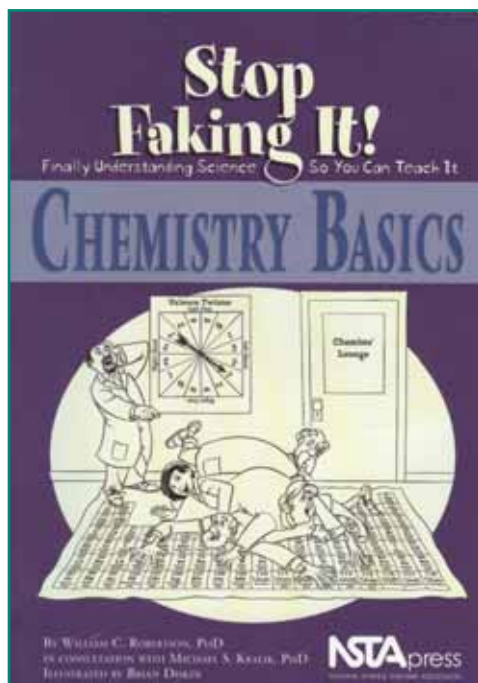
Chapter four reveals why some atoms bond together to form molecules and others do not. The authors explain, for example, why there are two hydrogen atoms and only one oxygen atom in a water molecule.

Chapter five dives into the world of chemical equations. The authors discuss balancing different types of combustion reactions while enlightening

the reader with reference to conservation of mass.

Chapter six explains the basics of organic chemistry by representing carbon atoms as marshmallows; in other words, as sticky atoms that attract other atoms. Using this type of easy-to-grasp analogies facilitates learning and creates a bridge that instructors can use to reach across students' gaps in conceptual knowledge.

From presenting a historical perspective in chapter one to dissecting basic organic chemistry in chapter six, this book does a genuinely fine job of breaking down difficult concepts for students struggling with chemistry. It should be utilized as an additional



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resource or companion guide for any chemistry textbook. *Stop Faking It! Chemistry Basics* is strongly recommended to anyone with an interest in basic chemistry.

Parker M. Nelson, M.Ed. <parker.nelson@usm.edu> is a doctoral candidate in the Department of Curriculum and Instruction at the University of Southern Mississippi,

Hattiesburg. Nelson taught secondary chemistry, physics, and physical science for nearly 12 years and is currently working toward a Ph.D. in secondary education with an emphasis in science. Dr. Hani Morgan <Hani.Morgan@usm.edu> is an assistant professor in the Department of Curriculum and Instruction at the University of Southern Mississippi, Hattiesburg. His areas of study include foundations of education, curriculum, and teaching and international education.

## Environmental Chemistry

### Fundamentals

J.G. Ibanez, M. Hernandez-Esparza, C. Doria-Serrano, A. Fregoso-Infante, M.M. Singh  
Springer, New York, 2007, 334 pp.  
ISBN 978-0-387-26061-7

### Microscale Laboratory Experiments

ibid.

Springer, New York, 2007, 238 pp.  
ISBN 978-0-387-49492-0

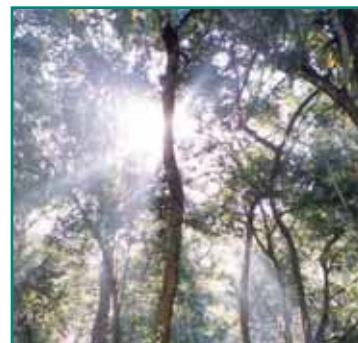
Modern science is not straightforward. Intricate relationships exist among the different disciplines involved in the understanding of virtually every scientific issue and phenomenon. The days of the Renaissance, when a single person could master a large portion of the knowledge available, are long gone. This is not due to a lack of individual capacity, but rather to the explosion of knowledge that is characteristic of our times.

Environmental science—and more specifically, environmental chemistry—finds itself completely immersed in such a scenario. In this context, a book written by several authors with complementary backgrounds and interests is perfectly suited to this challenge.

These books are written with sophomore or junior college students in mind, and students are assumed to have a minimum background in organic chemistry and biochemistry. However, issues are often presented in such a way that general chemistry students—and even graduate students—can find subjects of interest applicable to their level.

The beginning of the first book, *Fundamentals*, presents a general introduction to environmental chemistry (Chapter 1) and a summary of the main background

concepts that a student of environmental chemistry ought to know (Chapters 2 and 3). Subsequent chapters discuss the composition and characteristics of the natural chemical processes that occur in the atmosphere (Chapter 4), the lithosphere (Chapter 5), and the hydrosphere (Chapter 6). This discussion concludes by examining natural biochemical processes and introducing the organisms in the bio-



sphere (Chapter 7). The following chapters analyze the effects of key pollutants (Chapters 8 and 9), their treatment (Chapters 10 and 11), and the minimization and prevention of pollution, with an emphasis on green chemistry (Chapter 12). Each chapter also contains a list of educational experiments in the literature related to its subject and a list of other useful references.

The second book, *Microscale Laboratory Experiments*, presents 24 experiments ranging from the characterization of aqueous media to pollutant-treatment schemes. To increase safety and environmental awareness and to reduce cost, waste, and environmental damage, the authors recommend performing the experiments at the microscale (also called the small-scale) level. Such experiments typically use microliters or micromoles of at least one of the reagents.

All told, the books contain 240 questions, problems, and examples, and more than 150 figures, 70 tables, and 1300 references to the literature (almost 50 percent of these references relate to educational environmental activities and experiments). And 80 additional related projects are suggested in the experimental section.

Because environmental analytical chemistry is of the utmost importance in understanding a large

number of environmental issues, a comprehensive list of environmental chemistry experiments that give prominence to analysis—and that require instrumentation beyond that used in the experimental manual—is given in the Appendix.

Among the most important issues in environmental science are the appreciation and knowledge of the different phenomena involved in our environment, and the ongoing need to participate in its care. Hopefully these books will contribute a grain of sand to such an end.

Names of the authors appear below followed by the institutions where they did graduate work, then by their present affiliations:

- Margarita Hernandez-Esparza (Stanford Research Institute), Universidad Iberoamericana, Mexico City
- Ma. del Carmen Doria-Serrano (Universidad Nacional Autonoma de Mexico), Universidad Iberoamericana, Mexico City
- Arturo Fregoso-Infante (University of Kansas at Missouri), Universidad Iberoamericana, Mexico City
- Mono Mohan Singh (St. Petersburg University), Merrimack College, Massachusetts, United States.
- Jorge G. Ibanez (University of Houston), Universidad Iberoamericana, Mexico City

 [www.springer.com/chemistry/book/978-0-387-26061-7](http://www.springer.com/chemistry/book/978-0-387-26061-7)

### Four Laws That Drive the Universe

Peter Atkins

Oxford University Press, New York, 2007

ISBN 978-0199232369

reviewed by Laurence Lavelle

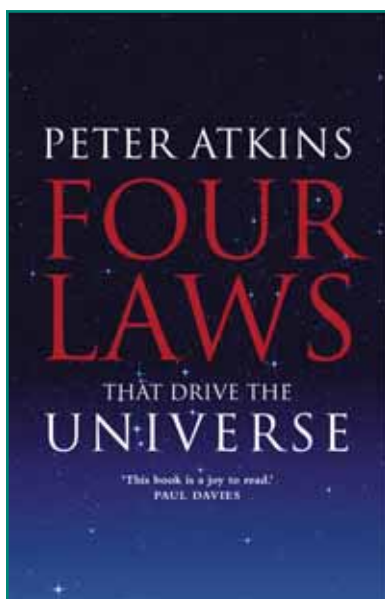
*Four Laws That Drive the Universe* is a delight to read. It is so well written that its 124 small and eloquent pages can be read in a day and its contents enjoyed for a lifetime.

The five chapters (describing the zeroth-, first-, second- and third-laws of thermodynamics and free energy) do far more than cover introductory thermodynamics. They convert what is an often abstract topic of mathematical equations into prose that is logical and easy to read. Atkins explains the concepts behind the equations and develops the equations.

*Four Laws That Drive the Universe* shows that it is possible to construct sentences that are excellent replacements for equations. This aspect of the

book alone will be a great asset to anyone—and in particular any student—who finds it difficult to read equations and comprehend thermodynamics. In addition to making thermodynamics comprehensible to beginners, for specialists, it sets the standard for converting mathematically dense scientific topics into logical text with little lost in translation.

This gem of a book will be helpful to any student hearing about thermodynamics for the first time. Graduate students, who may have already made several attempts at understanding the fundamentals of thermodynamics, will also find this book helpful. Those who teach thermodynamics will find it a useful resource in assisting students understand thermodynamics. This book rewards at many levels, making it an excellent read for beginning students through to specialists in thermodynamics.



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# Conference Call

## Photodynamics

by *Jesús Rubayo-Soneira*

The **Fifth International Meeting on Photodynamics** was held in Havana, 4–8 February 2008. The central theme was the description, both from the experimental and the theoretical point of view, of the physical and chemical processes related to environmental and biological systems. Approximately 110 scientists from 18 countries attended. The meeting featured 37 plenary lectures and 53 poster presentations.

Prior to the conference, a school was held from 30 January to 2 February 2008 focused on the new generation of young researchers, from Cuba and Latin American countries and the rest of the world. Fifty students attended the lectures given by professors with excellence in both teaching and research, who taught short courses on the following topics:

- Non-Adiabatic Transitions in Electronically Excited Molecules (Sergy Yu. Grebenshchikov)
- Structure, Dynamics, and Spectroscopy of Weakly Bounded Molecular Aggregates (Pablo Villarreal)

This school and the meeting took place at the Comodoro Hotel, which is located in the west part of Havana. The purpose of the meeting was to stimulate discussion among scientists working in the chemical physics field related to structure and dynamics of molecular systems. The main topics covered were: Structure and Energetics of Molecular Systems, Dynamics and Reactivity of Isolated Molecular Species, Dynamics of Molecular Species Embedded in Small and Large Clusters, Dynamics of Molecules in the Condensed Phase (liquid, solid) and at Surfaces, Control of Chemical Reactions, Collisions with Surfaces.

Keynote lectures were given by Zamik Rosenwaks (Beer Sheva, Israel), Osman Atabek (Paris, France), Stephen Berry (Chicago, USA), Hiroki Nakamura (Okazaki, Japan), Jeremy Hutson (Durham, England), Joel Bowman (Atlanta, USA), among others.

The conference was sponsored by the Cuban Physical Society, International Union of Pure and Applied Physics, IUPAC, and the Interdivisional Group of Physics for Development from the European Physical Society. The international scientific committee consisted of Vincenzo Aquilanti (Italy), Gerardo Delgado-Barrío (Spain), Antonio Varandas (Portugal), Sylvio Canuto (Brazil), Ramón Hernández-Lamoneda (México), and Jesús Rubayo-Soneira (Cuba, chairman).

The conference was a timely opportunity for scientific exchange among well-known scientists and young researchers from all over the world. Based on the scientific success and interest of this conference, participants agreed that this kind of meeting should be held again in the near future.

More details are available on the conference website <<http://usuarios.lycos.es/photodynamics/>>.

**Jesús Rubayo-Soneira** <[jrs@instec.cu](mailto:jrs@instec.cu)> was chairman of the conference. He is a professor at the Instituto Superior de Tecnologías y Ciencias Aplicadas in Havana, Cuba.

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## Advanced Materials and Polymer Characterization

by *Michael Hess*

The **POLYCHAR 16: World Forum on Advanced Materials**, organized by the University of Lucknow, was held from 17 to 21 February 2008 in the capital of the state of Uttar Pradesh, India. The short course on polymer characterization, a tutorial, was held on 14 February, hosted by the Indian Institute of Technology in Delhi, India.

The events were excellently managed by the local organization committee, headed by Chairman R.P. Singh (former vice chancellor of the University of Lucknow) and assisted by Vice Chairman V.S. Parmar (Delhi University), Executive Secretary-cum-Treasurer P. Tandon (Lucknow University), Secretaries A.K. Gosh (IIT, Delhi) and V. Kumar (CIEPT, Lucknow), and the coordinator of the short course, V. Choudhary (IIT, Delhi). Both events enjoyed the patronage of D. Pental (Delhi University), A.S. Brar (presently vice chancellor at the University of Lucknow), S.K. Dube (IIT Kharagpur), and S. Prasad (IIT, Kharagpur). The venue for the conference was kindly given by the World Unity Convention Centre in Lucknow, through its chairman, J. Gandhi.

The annual POLYCHAR conferences have been sponsored by IUPAC for several years and are known for combining the broad field of materials sciences with a clear focus on polymeric materials (the name "POLYCHAR" is derived from the term "polymer characterization"). The short course is an educational project of the IUPAC Polymer Division (project # 2007-027-1-400).



*Jiasong He (left) of the Chinese Academy of Sciences in Beijing, winner of the Paul J. Flory Research Prize, shakes hands with Rameshvar Adhikari of the Tribhuvan University, Katmandu, Nepal, who was the winner of the International Materials Science Prize.*

### Conference Sessions

The conference was divided into the following non-parallel sessions. The chairperson for each session is shown in parentheses.

- Nanomaterials and Smart Materials I (A.P. Karitonov)
- Natural and Biodegradable Materials and Recycling (D. Berek)
- Materials Synthesis and Characterization (G. Michler)
- Polymers for Energy (J.-M. Saiter)
- Rheology, Solutions, and Processing I (H.W. Siesler)
- Mechanical Properties and Performance (G. Boiteux)
- Rheology, Solutions, and Processing II (A. Pomogradow)
- Characterization and Structure-Properties Relationships I (E.S. Raja Gopal)
- Biomaterials and Tissue Engineering (Y. Chujo)
- Dielectric and Electrical Properties (E.F. Lucas)
- Nanomaterials and Smart Materials II (J. He)
- Characterization and Structure-Properties Relationships II (S.N. Chvalun)
- Synthesis and Characterization I (M. Hess)
- Surfaces, Interfaces, and Tribology (W. Brostow)
- Synthesis and Characterization II (M. Bratychak)
- Predictive Methods (H.-W. Bewersdorff)

At the conference, 292 participants from 35 countries and 4 continents gave 296 presentations, including 28 special and 15 invited lectures and 48 other oral presentations. (A full list of the outstanding oral and

poster contributions from universities, research institutes, and industry can be found at <[www.unt.edu/POLYCHAR/preview16.htm](http://www.unt.edu/POLYCHAR/preview16.htm)>.) Many students attended the presentations, highlighting the conference's goal of attracting young scientists and advanced and graduate students and giving them the opportunity to meet with colleagues and well-known scientists to exchange experiences, make contacts, and present their results to the scientific community. In addition, many student presentations were found in the two poster sessions.

### Awards

The conference is also the platform for the esteemed Paul J. Flory Research Award, given this year to Jiasong He from the Chinese Academy of Sciences in Beijing for his work on polymer blends and composites—in particular, on hybrid materials from polymer liquid crystals and nanoscopic fillers.

The International Materials Science Prize, introduced in 2007, was given to Rameshvar Adhikari from Tribhuvan University in Katmandu, Nepal, for his work in the field of blockcopolymers and his work establishing polymer science and education in Nepal.

In addition, the following students were given IUPAC Student Poster Awards:

- Pooja Chhabra, Centre for Polymer Research and Engineering, Indian Institute of Technology, Delhi, India, for his work on the “Effect of Structure on the Thermal Behavior of Polyamides”
- R. Dhanya, Department of Polymer Science and Rubber Technology, Cochin University of Science and Technology, Cochin, for the poster entitled “Photophysical and Electrochemical Investigation on Photoconducting Polymers”
- Dewyani Patil, Department of Physics North Maharashtra University, Jalgaon, India, for the poster presentation “Organic/Inorganic Hybrid of Poly(o-anisidene) and SiO<sub>2</sub>”

The special “Prof. Brar 60th Birthday Celebration Award” was given to the IUPAC awardees and to D. Vrsaljko, who also received one of the Student Diplomas (see below).

Additional prizes awarded at the conference included:

- Bruce Hartmann Award for Young Scientists, given to Archana Bhaw-Luximon, Department of Chemistry, University of Mauritius, Mauritius, for her contribution “Oligosaccharose-grafted Polymers, Synthesis and Characterization”

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- Jürgen Springer Award for Young Scientists, given to Arote Rohidas, School of Agricultural Biotechnology of the Seoul National University, Seoul, Korea, for his studies on “Novel Biodegradable and Branched Polyesteramines”
- Carl Klason Prize for the Best Student Paper, given to Victor Hugo Orozco, Grupo Ciencia de los Materiales, Instituto de Quimica, Universidad de Antioquia, Medellin, Colombia, for his oral contribution entitled “Preparation and Characterization of Poly(lactic acid-maleic acid-starch) Copolymers”
- Diplomas of Distinction for Student Oral Presentations, given to (1) Jacob Samuel, Department of Chemistry, Kuwait University, Kuwait, for his oral contribution entitled: “Microporous Networks Based on Cobalt Phthalocyanines”; (2) Domago Vrsjalko, Faculty of Chemical Engineering, University of Zagreb, Croatia, for his talk “Effect of Filler Surface Modification on Properties of Filled Polyurethane/Polyvinylacetate Blends”; and (3) L. Barbora, Department of Chemical Engineering, Indian Institute of Technology, Guvahati, India, for an oral presentation on “Composite Polymer Electrolyte Membrane for Direct Ethanol Fuel Cell”
- Diploma of Distinction for a Student Poster Presentation, given to Dustin England, School of Engineering Technology of the Eastern Michigan University, with the title “Reversibly Porating Materials and Coatings”

### Short Course on Polymer Characterization

The Short Course on Polymer Characterization has been an integral part of the conference from the very

beginning and is organized before the conference begins. The idea of the course is to provide basic information on polymer characterization for students and newcomers to the field and to have well-known specialists share popular characterization techniques in a condensed format.

Attending the short course provided an excellent preparation for the conference and allowed the course's 40 participants to follow the subsequent sessions more easily. Even better, the lecturers stayed for the duration of the conference and were available to answer participants' questions throughout the week. In addition, reference materials were provided free of charge to all participants.

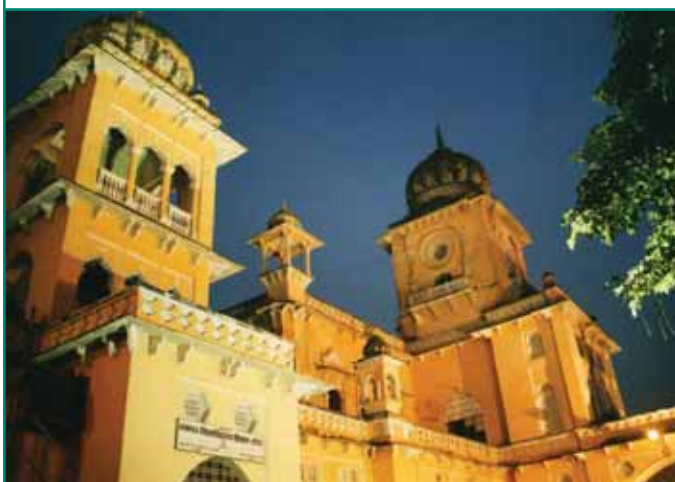
The subjects addressed were:

- Infrared Spectroscopy in Polymer Science (H.-W. Siesler, University Duisburg-Essen, Essen, Germany)
- Liquid Chromatography of Synthetic Polymers (D. Berek, Slovak Academy of Sciences, Bratislava, Slovakia)
- Dynamic-Mechanical Properties of Polymers (M. Hess, University Siegen, Siegen, Germany)
- Light-, Neutron-, and X-Ray Scattering by Polymer Systems (J.-M. Guenet, Institute Charles Sadron, Strasbourg, France)
- Glass Transition in Glassy Polymers and Other Disordered Materials (J.-M. Saiter, University of Rouen, Rouen, France)
- Electron Microscopy of Polymers (G. Michler, Martin-Luther University Halle-Wittenberg, Halle, Germany)
- Tribology of Polymer-Based Materials (W. Brostow, University of North Texas, Denton, United States)
- Hyper-DSC in Materials Characterization (P.S. Jain, Perkin-Elmer India)

In addition to the conference sessions, the awards, and the short course, many fruitful discussions were held during the breaks between sessions and the excursion. The conference truly brought together theorists, individuals from the fields of modelling, synthetic chemistry, and processing, students and newcomers to the field, and some of the most distinguished researchers in polymer science.

Future POLYCHAR Conferences are already being planned:

- POLYCHAR-17, Rouen, France, April 2009; contact: <jean-marc.saiter@univ-rouen.fr>, <www.polychar17.fr>



*Main building at the University of Lucknow.*

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- POLYCHAR-18, Bratislava, Slovakia, 2010
- POLYCHAR-19, Cairo, Egypt, 2011

Michael Hess is a professor at the Department of Macromolecular Chemistry at the University Siegen, in Siegen, Germany. He is secretary of the IUPAC Polymer Division and a member of the subcommittee on polymer terminology, subcommittee on polymer education, and subcommittee on developing polymer materials.

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## Photochemistry

by *Silvia E. Braslavsky*

The XXII IUPAC Symposium on Photochemistry was held 28 July through 1 August 2008 in Göteborg, Sweden. The conference was a real success, with 430 participants from 51 countries.

In spite of the gorgeous weather, all of the sessions at the symposium were well attended. Plenary lectures were given by eight outstanding speakers: Vincenzo Balzani (University of Bologna, Italy), Harry Gray (California Institute of Technology, United States), Leif Hammarström (Uppsala University, Sweden), Stefan Hell (Max-Planck-Institut für Biophysikalische Chemie, Germany), Masahiro Irie (Rikkyo University, Japan), Josef Michl (University of Colorado, United States), Atsuhiko Osuka (Kyoto University, Japan), and Eric Vauthey (University of Geneva, Switzerland). The majority of plenary lectures and many of the invited and selected oral lectures either directly or indirectly addressed the problem of solar energy conversion in view of the climate change and energy crisis confronting the world. In addition, there were 12 invited lectures and 96 selected oral presentations organized by scientific areas, as well as 414 posters that hung throughout the symposium. The discussions after the lectures and during the poster sessions were lively.

A wide range of topics were covered during the week, including the spectroscopy of molecular entities and nanostructures, the photochemistry of drugs, photochemistry in microheterogeneous media, fluorescence markers and sensors of various chemicals, supramolecular units mimicking antennas and reaction centers of photosynthesis, photopolymerizations and photochemistry in solid state, theoretical considerations and calculations of excited states, and spectroscopic studies with biological photosensors. Scientific instruments were also on display at a variety of often-visited booths.

The plenary lecture offered by Stephan Hell was sponsored by the photochemistry and photobiology societies that own the journal *Photochemical and*

*Photobiological Sciences*, which is produced by the Royal Chemical Society. Michael Wasielewski received the prestigious Porter Medal, which was awarded by three photochemistry societies: the Inter-American Photochemical Society, the European Photochemical Association (EPA), and the Asian Photochemical Association. He also gave a plenary lecture on this occasion. EPA Prizes were also given to young photochemists: Maria Abrahamson from Sweden and Alex Fürstenberg from Switzerland.

During the lunch breaks, several committee meetings took place, including that of the presidents of the photochemical societies, IUPAC's Subcommittee on Photochemistry, and the IUPAC project task group on Fluorescence Standards (IUPAC project 2004-021-1-300). In addition, the EPA had its general assembly on Thursday afternoon.

All in all, the conference was well organized and successful, both scientifically and socially. Once more the photochemistry community showed its strength and vitality. Many young fellows enjoyed the scientific discussions and were able to share the results of their research. What's more, the boat trip to the Archipelago was wonderful . . . and the medieval dinner in a dungeon gave us a taste of Sweden's past.

During the conference it was announced that the next IUPAC Symposium on Photochemistry will be held in Ferrara, Italy, in July 2010. The conference's scientific chair is Franco Scandola. It was also suggested that the 2012 Symposium be held in Coimbra, Portugal, and that the scientific chair be Hugh Burrows from Portugal.

Silvia E. Braslavsky <braslavskys@mpi-muelheim.mpg.de> is a member of the Photochemistry Subcommittee of IUPAC's Organic and Biomolecular Chemistry Division (Division III) and the Advisory Committee of the Physical and Biophysical Chemistry Division (Division I). She works at the Max-Planck-Institut für Strahlenchemie, in Mülheim an der Ruhr, Germany.

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## The Role of Chemistry in Sustainable Agriculture and Human Well-Being in Africa: CHEMRAWN XII

by *Piet Steyn and Christoff Pauw*

CHEMRAWN XII: the Role of Chemistry in Sustainable Agriculture and Human Well-Being in Africa, was hosted by Stellenbosch University in the Western Cape Province from 2–5 December 2007. The conference's

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focus was the role of chemistry in improving the quality of life of the peoples of Africa. The objectives of the conference were translated into a number of themes:

- African agriculture in a global context: the role of chemistry
- adequate, safe, and affordable food for Africa
- the safe development and application of biotechnology in agricultural production
- securing and sustaining water and soil quality for agricultural production
- technologies to reduce post-harvest food loss
- the role of chemistry in sustainable agriculture
- value-added and niche chemicals from agricultural produce
- the role of agriculture in building a sustainable energy base



*The rector and vice chancellor of Stellenbosch University, Russel Botman (center) welcomed the delegates, speakers, and guests during the opening ceremony. He is flanked at left by James Martin, opening speaker, and Piet Steyn, conference chair. The CHEMRAWN XII conference was hosted by Stellenbosch University.*

Workshop sessions were also held on applying chemical expertise to the needs of Africa, in keeping with CHEMRAWN's tradition of follow-up and implementation after conferences. The workshops covered the following topics:

- the role of green chemistry in agricultural production in Africa
- chemical and microbiological analyses to ensure safe and wholesome food for Africa
- current biofuel technologies and their application

### Africa's Green Revolution Has Started

According to the UN's Food and Agriculture Organization, Africa is the only region in the world where average per-capita food production has fallen

steadily over the latter half of the 20th century. However, the former secretary general of the United Nations declared in 2004 that, given due national and international support, Africa could start a "Green Revolution" that could potentially end hunger on the continent. This message was amplified at the recent CHEMRAWN XII Conference: Africa's Green Revolution has already begun!

This positive sentiment expressed by the conference's keynote speaker, Pedro Sanchez, was shared by many of the attending scientists from Africa and elsewhere. Sanchez, an agronomist at Columbia University's Earth Institute, referred to the success of the Millennium Villages project, which had demonstrated that by investing in the front end of the food chain rather than the tail end—seed and fertilizer rather than food aid—whole communities could be lifted out of the trap of poverty and malnutrition.

The Millennium Villages project has resulted in increases in maize production of up to 2.6 tonnes per hectare in Malawi, and schemes and logistics were put into place to sell surpluses on local and international markets. These profits were subsequently ploughed back into infrastructure, health clinics, feeding schemes, and the development of human capital.

This encouraging spirit permeated the underlying theme of CHEMRAWN XII—improving the quality of life of the peoples of Africa through the provision of adequate food, with specific attention to the role of chemistry.

### Food Security Challenges

Among the many challenges Africa faces is the fact that the majority of its 25 000 people who die from hunger every day live in sub-Saharan Africa, and that global climate change looks set to worsen this situation. The impact of global climate change was strikingly presented by James Martin, who pointed out the stark implications of current global warming: the earth's breadbaskets will shift northwards to Canada and Russia. If urgent action is not taken, Martin said, global agriculture will be able to provide food for only 500 million people.

And such action is possible. Many of the technologies required to both increase Africa's food production and reduce the impact of global warming are readily available. However, what is lacking is education, science communication, and management. Scientific research dedicated to finding more and better solutions to these challenges remains the key to future agricultural sustainability. However, the mere application of existing knowledge could potentially



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vastly increase food security in Africa.

Currently as much as 60 percent of Africa's produced food is lost as a result of post-harvest spoilage and unsafe food quality. Optimal irrigation of crops and better post-harvest technologies, including proper storage of produce, could greatly reduce this loss, said Leopoldt van Huyssteen, former dean of the Faculty of Agriculture at Stellenbosch University. Given that as much as 70 percent of Africa's workforce is involved in the agricultural sector and that the agricultural industry contributes a reported 40 percent to the continent's GDP, such improvements could have major benefits for Africa's entire population, particularly now that global food stocks are under pressure.

### Measures to Promote Sustainable Agriculture

Numerous other technologies that could be implemented were presented in papers and posters at the conference. Salome Guchu from the International Centre of Insect Physiology and Ecology (ICIPE) in Kenya reported how interspersing maize with *Desmodium* legumes, commonly grown for fodder, prevents witch weed (*Striga hermonthica*), a parasitic plant that cripples maize production, from taking hold in maize plantations.

Wilhelm Holzapfel from the University of Karlsruhe in Germany explained how fermentation prevents the growth of dangerous mycotoxins on food. A study on fermented porridge produced markedly lower occurrences of diarrhea in children and increased their immunity.

CHEMRAWN XII dovetailed with the South African National Energy Research Institute Biofuels Conference hosted from 5 to 6 December at the same venue. The CHEMRAWN XII workshop on biofuels was scheduled as the opening session of the Biofuels conference, and thus CHEMRAWN XII delegates were able to take part in the opening session and to register for the Biofuels Conference. The theme was "Sustainable Biofuels for the Future," and six international and 15 national speakers discussed the current world trends and future biochemical and thermochemical technologies for cellulosic biomass conversion to biofuels and their application to the Southern African scenario.



*Pedro Sanchez, from Columbia University's Earth Institute, delivering the keynote lecture on Africa's Green Revolution.*

Apart from technologies that could support sustainable agriculture in Africa, a number of presentations focused on policies and science communication. In a presentation on the implementation of widely applicable, robust technologies for increasing agriculture's role in the development of Africa, Leopoldt van Huyssteen illustrated how a logical systems approach could ensure the effective application of chemistry to soils, water, plant protection, readiness for harvest, post-harvest processes, seed treatments, traceability/falsification, barriers to entry into the market, and biodiversity.

In a keynote presentation entitled "Grand Challenges for African Universities and Research Institutions," Sospeter Muhongo, director of the International Council for Science's (ICSU) Regional Office for Africa, highlighted the importance of quality human capital production and development in Africa. This is an achievable goal when scientific knowledge and data are allowed to influence policy- and decision-making processes and a community of practice is established that focuses on science, technology, and innovation across academia, industry, and the public.

In a similar vein, Shem Wandiga from Kenya's Centre for Science and Technology Innovations reported on measures taken in Kenya to mobilize the interface between science and policy, while including farmer groups in the process. These projects aim to strengthen and diversify production systems through the promotion of rainwater-harvesting technologies,



*Keynote speakers and conference organizers during the opening ceremony, from left: Emile van Zyl, James Martin, Piet Steyn, John Malin, Pedro Sanchez, and Leopoldt van Huyssteen.*

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agroforestry systems for soil and water conservation, minimum tillage to conserve soil moisture, revegetation of degraded areas, and increased agricultural production using locally available manure and other farm inputs.

### Supporting Africa's Scientists

In addition to its scientific contribution, CHEMRAWN XII also witnessed the announcement of a new Royal Society of Chemistry (RSC) initiative, the Pan African Chemistry Network. This network follows the success

of the Archives for Africa program, which made all of the RSC's journal content free to scientists from African universities. The new network, with funding from Syngenta, aims to increase connections

between scientists, researchers, schools, and libraries across the continent.

The conference was attended by more than 200 delegates, 58 of them from 18 African countries outside South Africa. From an initial 160 abstracts received, over 40 papers and almost 60 posters were presented. The poster sessions ensured that the poster presenters received adequate exposure, and four prizes were awarded to the best presenters, two of which went to young scientists.

The keynote addresses were delivered by:

- Pedro Sanchez (Earth Institute, Columbia University, New York)
- James Martin (21st Century School, Oxford University, United Kingdom)
- Pol Coppin (Catholic University of Leuven, Belgium)
- Jens Kossmann (Stellenbosch University, South Africa)
- Sospeter Muhongo (ICSU-Africa)
- Linus Opara (Sultan Qaboos University, Oman)
- James Simon (Rutgers University, New Jersey, United States)
- Leopoldt van Huyssteen (Stellenbosch University, South Africa)

Piet Steyn and Christoff Pauw were, respectively, chair and secretary of the Conference Organizing Committee. Piet Steyn <psst@sun.ac.za> is director of research of the Division of Research Development at Stellenbosch University, South Africa. He has been involved with IUPAC for many years and was IUPAC president from 2002-2003. Christoff Pauw <cpauw@sun.ac.za> is with the International Office at Stellenbosch University.

## Chemistry in a Changing World—New Possibilities within the IUPAC Family

by Michael Droescher



IUPAC is strongly based on academia and national organizations. The links to industry are not as tight, although IUPAC is also the International Union of *Applied Chemistry*. Among the membership of IUPAC there are about 80 company associates (CAs): 25 from Europe, 35 from Japan, and 4 from the USA. Clearly, Japan is the leading country in terms of IUPAC-industry interaction. COCI, the Committee on Chemistry and Industry, wants to strengthen the rather weak links between chemical companies and the Union. To move forward in this direction, COCI supports the move to increase the number of CAs and to improve the cooperation between IUPAC and the chemical industry on a global scale.

Improvement only comes with contacts and exchange of ideas. Therefore, COCI started a series of workshops to engage chemical industry directly and through industrial federations. The first workshop was held 25 April 2008 in Marl, Germany, together with the annual COCI meeting. The events were hosted by Evonik Industries.

About 25 representatives from IUPAC, COCI, the European Chemical Industry Council (Cefic), the German Chemical Industry Association (VCI), the German Chemical Society (GDCh), the Royal Society of Chemistry (RSC), and some industrial companies met for one day to discuss the topic "Chemistry in a Changing World—New Possibilities within the IUPAC Family."

The workshop started with a dinner on the 24th, where Gernot Klotz from Cefic kicked off the discussion with a presentation about the potential for cooperation between industry and IUPAC. In the morning, Michael Droescher welcomed participants and introduced Evonik to the audience. Evonik is a newly formed company whose chemical division is the former Degussa. Then, IUPAC President Jung-Il Jin, who personally took part in the workshop because of the importance of the topic, extended a warm welcome to all participants and introduced IUPAC to the audience. Mark Cesa, the chair of COCI, reviewed COCI's priorities, including the sharing of best practices, knowledge transfer to developing countries, capacity building, and building public appreciation of chemistry. Rene van Sloten from Cefic reported on the activities of

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Europe's High Level Group on Competitiveness of the European Chemical Industry. Marian Mours, also from Cefic, talked about innovation in the chemical industry, and Rodney Townsend, from RSC and chair of the European Technology Platform Sustainable Chemistry, discussed the international strategy of the RSC.

After lunch, the workshop broke into three parallel sessions in which participants exchanged views and discussed opportunities for future activities. The first session focused on "Innovation—Turning Chemistry into Practical Value" and was moderated by Colin Humphris, the second on "Objective Chemical Regulations," moderated by Mike Booth, and the third on "Reputation and Public Appreciation of Applied Chemistry," moderated by Bernard West.

In the context of innovation, an obvious starting point is the realization that chemistry alone is not enough, and that the discipline needs to reach applications, customers, and other disciplines. During the discussion, the importance of educating people with the right skill sets for industry was raised: Aside from a general science education, individuals should acquire an ability to discuss science, and an emphasis on seminars, communications, team work, and business awareness should be included in their training. Consultation with experienced people (including retired professionals) could be valuable, especially during transition phases to commercial development (pilot plants, etc.). To foster innovation, the right infrastructures are necessary. Various industries have adapted different strategies; some are providing "seed funds," others are creating strategic alliances with academic institutions. The role and place of science in such a framework is evolving, and the question was asked "What role can IUPAC play in facilitating industry/academia interaction?"

In terms of regulations and policies, it is recognized that Cefic in Europe is well set to help the chemical industry respond to regulations such as REACH. What IUPAC/COCI could add is assistance in spreading this information to the rest of the world. It could also assist chemists by informing them of the basic scientific facts that are important in, and relevant to, regulations. IUPAC can add the global perspective that is needed. For example, European regulations are impacting business globally because companies from countries exporting to Europe, such as South Africa, Australia, and Russia, have to comply with specific regulations.

To conclude the workshop, the plenum met to hear reports from the break-out sessions by Carolyn Ribes,



*Members of COCI and invited guests at the annual meeting and workshop in Marl, Germany, in April 2008.*

Aldo Bologna Alles, and Davis Evans and to discuss future actions. In summary, it was concluded that IUPAC has the power to contribute strongly to the positioning of the global chemical industry. Two examples include promoting and sponsoring the Year of Chemistry in 2011 or by transferring knowledge gained from the European Technology Platform Sustainable Chemistry to the developing part of the world. To make this work, IUPAC needs to attract more chemists in the chemical and pharmaceutical industry to take part in IUPAC's activities. IUPAC should also attract more companies as Company Associates.

To be a stronger voice as the global scientific organization on chemistry, IUPAC should be recognized as an official scientific Non Governmental Organization with other relevant NGOs. Based on IUPAC's excellent global reputation in the fields of nomenclature and standards, this goal should be easily achievable if IUPAC improves its communication outside of the organization.

IUPAC's focus should be more in the developing world than in Europe or other regions, where national or regional organizations like GDCh, RSC, or EuCheMS make sure that chemistry is represented. Focus is meant here as the direct transfer of knowledge, such as through training of safety measures, by developing innovative fields, or by improving teaching methods. On a global scale, IUPAC should work more closely together with the International Council of Chemical Associations.

A second workshop is being planned for the Asian region in Japan in April 2009.

**Michael Droescher** <michael.droescher@evonik.com> works for Evonik Industries, Innovation Management Chemicals, in Essen, Germany. He has been a member of the IUPAC Committee on Chemistry and Industry since 2004.

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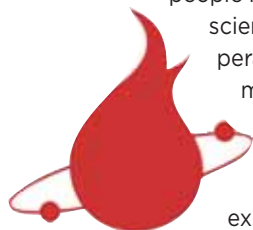
## High Temperature Materials

14-18 September 2009, Davis, CA, USA

The **High Temperature Materials Chemistry Conference-XIII (HTMC-XIII)** will be the next in a series of conferences that are held every three years, the last occurring in Vienna, Austria. The conference will be held 14-18 September 2008 at the University of California-Davis, USA.

The conference's goal will be to bring together people from chemistry, geology, and materials science who are working with high-temperature phenomena in solid and liquid materials. Selected conference topics include high-temperature thermodynamic measurements, the interplay of theory and modeling with experiment in high-temperature materials, earth and planetary materials at high pressure and temperature, materials for aerospace applications, materials for nuclear energy applications, transport, ionic and electronic conduction, densification, grain boundaries, interfaces and surfaces, and melts, glasses, and amorphous materials.

Contributions to the meeting are being solicited as talks and posters. The scientific committee will review



the submitted abstracts and decide which will be accepted for which type of presentation. The conference language, and thus the language of the abstracts, will be English.

The meeting is being jointly organized by UC-Davis's Nanomaterials in the Environment, Agriculture, and Technology Organized Research Unit and the Peter A. Rock Thermochemistry Laboratory and is sponsored by IUPAC and several partners from industry. The meeting chair is Alexandra Navrotsky. Confirmed speakers include Masaki Azuma, Ricardo Castro, Yingwei Fei, Susana Fries, Jonathan Stebbins, and Sharon Webb. The international advisory committee members are Masaki Akaogi, Giovanni Balducci, Ricardo Castro, Yingwei Fei, Sophie Guillemet-Fritsch, Adolf Mikula, Hans Seifert, and Sharon Webb. The national organizing committee members are Steve Amundson, Sangtae Kim, Charles Lesher, Sabyasachi Sen.

For additional and up-to-date information, please see the conference website.

See **Mark Your Calendar** on page 37 for contact information.

 <http://neat.ucdavis.edu/HTMC-13>

## Trace Elements in Food

1-3 April 2009, Rome, Italy

Diet is the main source of trace elements, and exposure to dietary trace elements has a direct impact on the health of hundreds of millions of people worldwide. Insufficient intake of essential trace elements is a global issue. Deficiencies in iron, zinc, iodine, and selenium result in millions of people being affected by various diseases, with very serious consequences in those countries where malnutrition is widespread. At the same time, the impact of toxic element species such as inorganic arsenic and methylmercury on whole populations has become a priority for both the scientific community and health authorities.

The **3rd International IUPAC Symposium on Trace Elements in Food (TEF-3)** will be held 1-3 April 2009 in Rome, Italy, organized by the Istituto Superiore di

Sanità. The meeting will consist of two and a half days of oral and poster presentations. Plenary lectures will be given by invited speakers in the following areas:

- advances in trace element analysis in food matrices
- sources and transfer of trace elements in the food chain
- toxicology and risk assessment
- trace element nutrition and human health

The different facets of trace elements will be addressed throughout the symposium, with special emphasis on the biological effects of elements. Advances in the different areas will be discussed and special attention paid to ways of preventing adverse health effects on those individuals and populations most vulnerable to trace-element inadequacies, excesses, or imbalances.

Topics covered will include essentiality, toxicity, bioaccessibility, bioavailability, speciation,



sources and transfer in the food chain, effects of processing, food fortification, supplementation, international legislation and standards, analytical developments, analytical quality assurance, and reference materials. Special emphasis will be placed on research and development efforts that have taken place in the past few years as well as on emerging issues in the area.

This meeting follows previous ones held in Warsaw, Poland in 2000 and in Brussels, Belgium in 2004. Like these meetings, TEF-3 aims at providing a forum for the exchange of new ideas and experiences among researchers in the trace element area with a view to

give an evidence base for policy, advice on the development of improved foods, and information on risk-management tools to protect public health.

The deadline for submission of abstracts is 1 December 2008, and the deadline for reduced fee payment is 15 January. Further details are available on the symposium website.

See **Mark Your Calendar** on page 36 for contact information.

 [www.tef3-2009.it](http://www.tef3-2009.it)

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

## 2008 (later than 1 October)

 IUPAC poster prizes to be awarded

### 12-17 October 2008 • Biotechnology • Dalian, China

*13th International Biotechnology Symposium (ISB 2008): "Biotechnology for the Sustainability of Human Society"*  
Prof. Fengwu Bai, Dept. of Bioscience & Bioengineering, Dalian University of Technology, 2 Linggong road, Dalian 116023, China, Tel.: +86 411 84706329, Fax: +86 411 84708083, E-mail: [fwbai@dlut.edu.cn](mailto:fwbai@dlut.edu.cn)

### 15-18 October 2008 • Novel Materials and Synthesis • Zhenjiang, China

*International Symposium on Novel Materials and their Synthesis (NMS-IV)*  
Prof. Yuping Wu, Fudan University, Department of Chemistry, Shanghai, 200433, China  
Tel.: +86 21 55 664 223, Fax: +86 21 55 664 223, E-mail: [wuyup@fudan.edu.cn](mailto:wuyup@fudan.edu.cn)

### 26-30 November 2008 • Soil Science • Pucon, Chile

*International Symposium of Interactions of Soil Minerals with Organic Components and Microorganisms*  
Dra. Maria de La Luz Mora, Universidad de La Frontera, Ciencias de Recursos Naturales, Temuco, Chile,  
Tel: +56 45 325479, Fax: +56 45 325053, E-mail: [mariluz@ufro.cl](mailto:mariluz@ufro.cl)

## 2009

 IUPAC poster prizes to be awarded

### 15-17 February 2009 • Radical Polymerization • Melbourne, Australia

*Materials of the Future-Science of Today: Radical Polymerization*  
Dr. Graeme Moad, CSIRO Molecular Science, Bag 10, Clayton South, Victoria, 3787, Australia  
Tel.: +61 3 9545 2509, Fax: +61 3 9545 2446, E-mail: [graeme.moad@csiro.au](mailto:graeme.moad@csiro.au)

### 8-11 March 2009 • Heterocyclic Chemistry • Gainesville, FL

*10th Florida Heterocyclic Conference*  
Prof. Alan R. Katritzky, University of Florida, Department of Chemistry, Gainesville, FL 32611-7200, USA, Tel: +1 352-392-0554, Fax: +1 352-392-9199, E-mail: [katritzky@chem.ufl.edu](mailto:katritzky@chem.ufl.edu)

### 1-3 April 2009 • Trace Elements in Food • Rome, Italy

*3rd International Symposium on Trace Elements in Food (TEF-3)*  
Dr. Francesco Cubadda, National Centre for Food Quality and Risk Assessment, Istituto Superiore di Sanità, Viale Regina Elena 299, I-00161 Rome, Italy  
Tel.: +39 06 4990 3643, Fax: +39 06 4990 2540, E-mail: [francesco.cubadda@iss.it](mailto:francesco.cubadda@iss.it)

### 16-17 April 2009 • Clinical Laboratory Diagnostics • Barcelona, Spain

*5th European Symposium on Clinical Laboratory and Diagnostic Industry: Standardization and Tumor Markers*  
Dr. Xavier Filella, Hospital Clínic, Department of Biochemistry & Molecular Genetics, C/ Villarroel 170, E-08036 Barcelona, Spain, Tel: +34 93 227 54 00 x 3141, Fax: +34 93 337 93 76, E-mail: [xfilella@clinic.ub.es](mailto:xfilella@clinic.ub.es)

## Visas

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

## How to Apply for IUPAC Sponsorship

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

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

**29 June–3 July 2009 • Chemical Thermodynamics • Moscow, Russia**

*XVII International Conference on Chemical Thermodynamics in Russia (RCCT 2009)*

Prof. J. D. Tretjakov, Moscow State University, Department of Inorganic Chemistry, Leninskiy Gory, GSP-2, RF-119991 Moscow, Russia, Tel.: +7 8 495 939 2074, Fax: +7 8 495 939 0998, E-mail: rcct2009@kstu.ru

**5–9 July 2009 • Polymers and Organic Chemistry • Montréal, Canada**

*13th International IUPAC Conference on Polymers & Organic Chemistry (POC-'09)*

Prof. Will Skene, Université de Montréal, CP 6128, Succ. Centreville, Montréal, QC H3C 3J7, Canada  
Tel.: +1 514 340-5174, Fax: +1 514 340-5290, E-mail: wskene@umontreal.ca

**19–24 July 2009 • Novel Aromatic Compounds • Luxembourg City, Grand Duchy of Luxembourg**

*International Symposium on Novel Aromatic Compounds (ISNA-13)*

Prof. Carlo Thilgen, ETH Zürich, Laboratorium für Organische Chemie, Wolfgang-Pauli-Strasse 10, CH-8093 Zürich, Switzerland, Tel.: +41 1 632 2935, Fax: +41 1 6321109, E-mail: thilgen@org.chem.ethz.ch

**26–31 July 2009 • Ionic Polymerization • Lodz, Poland**

*19th IUPAC International Symposium on Ionic Polymerization (IP '09)*

Prof. Stanislaw Penczek, Polish Academy of Sciences, Centre of Molecular and Macromolecular Chemistry, Sienkiewicza 1123, PL-90 363 Lodz, Poland, Tel.: +48-42-681 9815, Fax: +48-42-684 7126, E-mail: ip09@bilbo.cbmm.lodz.pl

**26–31 July 2009 • Organometallic Chemistry • Glasgow, UK**

*15th International IUPAC Conference on Organometallic Chemistry Directed Towards Organic Synthesis*

Prof. Pavel Kocovsky, University of Glasgow, Department of Chemistry, Glasgow, G12 8QQ, United Kingdom, Tel.: +44 141 330 4199, Fax: +44 141 330 4888, E-mail: pavelk@chem.gla.ac.uk

**1–9 August 2009 • IUPAC 45th General Assembly • Glasgow, UK**

*Chemistry Solutions*

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

**2–7 August 2009 • IUPAC 42nd Congress • Glasgow, UK**

IUPAC 2009, Royal Society of Chemistry, Thomas Graham House, Science Park, Milton Road, Cambridge, CB4 0WF, UK, Tel.: +44 (0) 1223 432380, Fax: +44 (0) 1223 423623, E-mail: iupac2009@rsc.org  
<www.iupac2009.org>

**14–18 September 2009 • High Temperature Materials • Davis, CA, USA**

*High Temperature Materials Chemistry Conference–XIII (HTMC–XIII)*

Alexandra Navrotsky, University of California at Davis, One Shields Avenue, Davis, CA 95616 USA  
Tel.: +1 530 752-3292, Fax: +1 530 752-9307, E-mail: ANavrotsky@UCDavis.edu

**10–14 October 2009 • Molecular Environmental Soil Science • Hangzhou, China**

*International Symposium of Molecular Environmental Soil Science at the Interfaces in the Earth's Critical Zone*

Prof. Jianming Xu, Zhejiang University, College of Environmental & Resource Sciences, Hangzhou, 310029, China, Tel.: +86 571-8697-1955, Fax: +86 571-8697-1955, E-mail: jmxu@zju.edu.cn

**2010**

 IUPAC poster prizes to be awarded

**4–8 July 2010 • Pesticide Chemistry • Melbourne, Australia**

*12th IUPAC International Congress of Pesticide Chemistry*

Dr. Elizabeth Gibson, RACI, 1/21 Vale Street, North Melbourne, VIC 3051, Australia, Tel.: +[61] 0 3 9328 2033, Fax: +[61] 0 3 9328 2670, E-mail: elizabeth@raci.org.au