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

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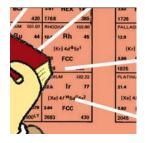






















Mendeleev



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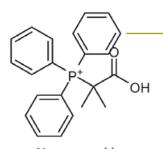
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# Vice President's Column

# Adding a Stone to the IUPAC Edifice

by Nicole J. Moreau



t has been eight years already since I began to take an active part in IUPAC. That period coincided with the beginning of the project system in its present form. The high effectiveness of the system and the general high standards of our organization make me very happy

and proud to belong to the Executive Committee and to be one of the five officers. To be honest, I feel somewhat anxious to be as successful as my predecessors. When I look at the work of some recent presidents, I need to be very optimistic to be up to the task! However, without challenges life would be somewhat monotonous.

I am fully aware of the huge potential and the tremendous strength of the IUPAC membership, working with so much willingness and determination for the benefit of science worldwide. Thanks to their efforts, chemists in scientifically emerging countries are having a far easier time learning and practicing chemistry. I sincerely hope to bring my stone to this edifice. As I begin my term as vice president of IUPAC, it is still the moment to express wishes. But before that I will tell a story.

Each year since 1951, Nobel Prize winners in chemistry, physics, physiology, or medicine accept an invitation to a unique meeting in Lindau, Germany, on Lake Constance, to discuss issues of importance to their fields with students from around the world. The meetings include lectures by, and informal discussions with, the Nobel Laureates. Back at the end of the '60s, three young French chemists close to finishing their Ph.D.s were chosen to represent their country at the event. It was their first scientific travel out of their country. As I was one of them, I recall how it turned out to be a wonderful experience.

Just imagine hearing Harold Urey describe his investigations into the origin of the planets, and the chemical problems of the origin of the earth. Or picture Leopold Ruzicka teaching—in German!—about isoprene annelation and steroid hormones, and then, because he had just referred to Adolph Butenandt, with whom he shared the Nobel Prize, stopping, look-

ing at the audience, and saying "Wo bis du, Butenandt" (Where are you, Butenandt?), and Butenandt coming up on the platform to have a discussion with him. For the audience of young scientists, it was almost a miracle to see such celebrities having such conversations in front of them. The meeting included a reception on the island of Mainau, hosted by Count Bernadotte, to increase personal contact between the junior participants and the Nobel Prize winners. The most striking thing was how we, as young students from all over the world, were proud to be chemists, how science looked beautiful to us. Perhaps it was a period in which young people were less concerned about their future than they are nowadays, but we were very enthusiastic and full of dreams and imagination.

Why are these memories so strong? Because for a young person, it is fantastic to be proud of and to believe in what one does, to admire great chemists, to read the literature in order to recognize the ingenuity of others, and to think of chemistry as such a smart science.

I wish that young people would find the enthusiasm of their predecessors and pursue the path of science, especially of chemistry. However, in doing so, they should be proud of their membership in the community of chemists. Why does a chemist, when asked what he/she does for a living, shyly admit that he/she works in chemistry? Because his/her interlocutor-by that I mean the public-does not know what chemistry is. The public often thinks of our science in relation to pollution, as a hindrance to sustainable development, or as a field that contributes to the detriment of human health. It is this same distorted vision that leads some to think of a drug not as a matter of chemistry, but of medicine; to regard synthetic vanillin as a poison compared to natural vanilla; or to believe that the abuse of pesticides or fertilizers is the fault of chemistry, and not of the farmers who perhaps use them thoughtlessly.

So, who can best help convey a less dubious, more correct image of chemistry? This may not be so easy for industry, which will be suspected of bias; perhaps the teachers, but generally they do not seem overly concerned with the image of chemistry; and not the politicians, since they appear to be poorly informed about chemistry issues and they might hesitate to upset their electorate. What remains then are the national chemical societies, and, on the international level, IUPAC, because of its status as an international, unbiased organization that is not industry driven. However, how can people trust something they do not

know? The prerequisite is therefore to make IUPAC known. This same argument has been put forth in many of these columns. We all know that IUPAC effectively serves the worldwide chemistry community, and that among IUPAC's missions, the one of communicating the right image of chemistry is very important. But how to do this efficiently? It seems to me that a bottom-up approach might be a good one.

The work of IUPAC's numerous volunteers is considerable, and as I discover its span and its multiple facets, I am more and more proud of our organization. Its internal communication is good, even if it is not so easy to achieve and maintain. The problem is not IUPAC's itself, it is that in most countries, IUPAC and its many roles are very poorly known, even among the chemical societies. It is unusual that a chemist in one of these countries would use the IUPAC website to research a particular fact or to locate information about a particular conference.

IUPAC cannot be fully effective without communicating well with the global chemical community. We must not forget that since its inception in 1919, IUPAC "has fostered worldwide communications in the chemical sciences, uniting the academic, industrial, and public sectors of chemistry in a common language." This should not be a boring notion for chemists, but on the contrary should be an object of pride, of satisfaction: We can immediately communicate with colleagues from other countries and languages, thanks to this universal language. When things are so easy, one tends to find it quite normal and to forget who is at the origin of the convenience. Anyway, we must not confine us to this sole merit, but show that IUPAC actually does other things.

If one looks at IUPAC's vision statement, it reads "advancing worldwide chemistry." In this case, worldwide not only means from IUPAC towards the world community of chemists, but it also means from the bottom up, from the regional and national levels. It seems that if we want to make IUPAC known, it is less the role of IUPAC as a whole than the role of each IUPAC member in his or her country or sphere of influence. What we ought to do is to each make a resolution to play such a role in our own country or sphere of influence, in addition to our specific responsibilities within a division or a committee. It is up to each of us, as individual members of IUPAC, to explain the Union's purpose when attending a meeting or a congress, to write about IUPAC in a national publication of our chemical society or in our university's journal, to take advantage of a science festival to show an IUPAC

poster or presentation.

Can we be successful? In communicating about IUPAC, let's not only target accomplished scientists, but also young scientists as well-and here is where my story about young chemists is relevant. For instance, we might expand on our efforts to encourage young chemists to attend the biennial IUPAC Congress. They might argue that our congress is not convenient for them because there are too many thematics involved, that their interest is, for example, the chemistry of fluorine compounds, and that they should not waste their time attending lectures about other topics. Then we ought to tell them that if they want to progress and go outside the small niche in which they performed their Ph.D. or their post-doc, they have to broaden their minds to other disciplines. If they attend a general congress, they may well discover domains they didn't know existed or have discussions about research that can supplement what they are doing, thus giving more originality to their own work. And in any case, it can be very fruitful to meet people with different interests. We can show them that eminent chemists such as Nobel Prize winners attend IUPAC congresses. Aren't recent conference themes such as "Chemistry at the Interfaces," "Innovation in Chemistry," "Chemistry Protecting Health, Natural Environment and Cultural Heritage" attractive ones? and how about the 2009 IUPAC Congress for which "Chemistry Solutions" is key theme?

Another argument for chemists to speak up is that in this period in which ecological problems (pollution, climate change, evaluation of risks, toxicity, greenhouse gases, and the protection and restoration of our environment) are major issues in every country, IUPAC should not be shy to play some political role. Chemistry is at the heart of sustainable development, not to hinder it, but to help to ensure it. As chemists, we have to make IUPAC known, not only to the general public, but also to stakeholders, leaders, and politicians. And each of us can do that in his or her own country, under the guarantee and behind the nongovernmental status of our organization, its independence, and objectivity. Then we could help IUPAC to create a platform for influencing decisions, based upon its expertise and reputation. 🦃

Nicole J. Moreau <nj.moreau@free.fr> has been vice-president of IUPAC since January 2008. She has been an elected member of the Bureau since 2000 and a member of the Executive Committee since 2006. She is also general secretary of the French National Committee for Chemistry.



Large version of the Periodic Table shown in the stamp
Tabla Periódica de Elementos de Mendeléiev on the wall
of the Experimental Science Department (Facultad de
Ciencias Experimentales) at the University of Jaén, Spain,
on the day of its unveiling: 22 November 2007. Each element is made of an individual ceramic tile (20 x 30 cm).

Chemistry weeks are wonderful opportunities to promote and raise public awareness about, and appreciation for, chemistry. In some countries, they are guite popular, some even have been institutionalized and are on our calendar every fall. In general, they prove to be quite successful. Sometimes, the events provide children with their first exposure to science and for many they are a good occasion for remembering a science studied a long time ago. Based on such experience, and following the International and World Years of Mathematics (2000), Physics (2005), and Astronomy (2009), IUPAC endorsed, at its last Council (11-12 August 2007, Torino, Italy), a plan to obtain United Nations approval of 2011 as an International Year of Chemistry. In 2007, Spain celebrated its National Year of Science with many activities to celebrate and promote chemistry on the occasion of the centenary of Dimitri Ivanovich Mendeleev's death (1834-1907). Herein, we share our experience in the hope we can all celebrate again in 2011.

# by Javier García-Martínez and Pascual Román Polo

he winter of 1907 was particularly cold in St. Petersburg, Russia, Mendeleev had suffered a bad flu since December. Despite this, he had to go to the Office of Weights and Measures, as the Minister of Trade and Industry had a visit scheduled for that day. That was a bad decision, since the effort further deteriorated his precarious health. Shortly thereafter, on 2 February, Mendeleev died at his home while his wife, Ana Popova, was reading to him a passage from one of his favorite books, A Journey to the North Pole by Jules Verne. A few days later, he was buried at the Volkovo cemetery, next to the tomb of his mother. Maria Dmitrievna. Those days, the cold was so intense that the workers could only write his name on the tombstone. There, even today, is only his name. Someone commented: "on a tomb as it could not be put otherwise." His former students of the University of St. Pertersburg carried a large banner at his funeral with the Periodic Table in which Dmitri Ivanovich Mendeleev lives forever.1

A hundred years later, Spain celebrated a Year of Science with a large number of activities. This was an excellent opportunity to raise public awareness and promote chemistry on the occasion of the centenary of Mendeleev's death.

# The Periodic Table as a Tool to Promote Chemistry

The Periodic Table is perhaps one of the most popular icons of science. It is hung in our chemistry classrooms, found in many science books, in most laboratories throughout the world, and even in advertisements, logos, and T-shirts. It summarizes, not in an equation, but in a powerful image, the order and periodicity in which all matter is organized. Its construction, still going on, is a team effort and one of the best examples of international collaboration since at least 13 countries have contributed with the discovery of elements. The Periodic Table is also one of the best known activities of IUPAC, which standardizes and organizes it as new elements are discovered. We had very little doubt when we decided that the Periodic Table, the great legacy of Mendeleev to future genera-

tions, should be the official image of activities organized to promote chemistry in 2007 in Spain.

### A Stamp to Celebrate Mendeleev's Great Legacy

Mendeleev's Year began formally on 2 February 2007 with the launch of a very special stamp entitled *Tabla Periódica de Elementos de Mendeléiev* (Mendeleev's Periodic Table of Elements)—see box below. Surprisingly, this is the only stamp that has been dedicated to the Periodic Table to date and the second ever devoted to Mendeleev by a non-Soviet country.<sup>2</sup> Djibouti issued a Mendeleev stamp in 2006.

Although the Periodic Table (or some portions of it) is shown in some stamps, including stamps related to

Mendeleev,<sup>2</sup> the stamp described here is probably the only one ever dedicated solely to the Periodic Table. Although there have been many stamps featuring famous chemists issued by countries like Germany, UK, France, Sweden, and the USA, only the USSR (1934, 1951, 1957 and 1969), Poland (1959), Bulgaria (1984), and the The Democratic People's Republic of Korea (1984) issued stamps on Mendeleev until recently. Although Mendeleev died well before the October Revolution (October 25, 1917), politics excluded him from Western philatelia until 100 years after his death.

The General Post Office of Spain issued the first copies of *Tabla Periódica de Elementos de Mendeléiev* 

# Designing the Periodic Table Stamp

When the Spanish General Post Office (Correos) proposed, through my friend Roman Polo, that I (Javier García-Martínez) design this stamp, I was writing a review article about philately dedicated to Mendeleey, recently published in Anales de Química—the official journal of the Spanish Royal Society of Chemistry. Spain has relatively few stamps on science and technology. In fact, until the creation of the stamp dedicated to Mendeleev's Periodic Table, there was only one Spanish stamp clearly related to chemistry, although at least 15 stamps are devoted to related subjects. This is the 1983 stamp *Bicentenario del* Descubrimiento del Wolframio that celebrates the 200th anniversary of the discovery of the element wolfram by Juan José Delhuyar (1754–1796) and his brother Fausto (1755–1833).<sup>2</sup>

From the beginning, it was clear to me that this would be a great opportunity to present a modern and positive image of chemistry. I wanted my design to be radically different from the more traditional stamps previously issued. Piet Mondrian's (1872–1944) *Neo-Plasticism* served as my inspiration. The colorful box-like designs of his paintings are very suitable to a

new version of the Periodic Table, with bright plain colors, thick black borders, and simplified forms. I chose the colors of each block from the ones used on the webelements webpage<sup>3</sup> as a tribute to a modern, online periodic table that receives thousands of hits per day. This new version of the Periodic Table features four void spaces corresponding to the elements predicted by Mendeleev: ekaboron (scandium), ekaaluminum (gallium), ekasilicon (germanium), and ekamanganese (technetium). These have been included to celebrate Mendeleev's genius; he not only ordered the known elements, but predicted the existence of new elements, and even their properties with amazing accuracy; something that allowed for an early confirmation of his Periodic Law. A recent issue of Philatelia Chimica et Physica, which has on its cover this new stamp, includes an article in which I describe in detail some relevant aspects of this stamp. For those interested, this is a good source of additional information.4

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- 2. a) J. J. de Luyart, y F. de Luyart "Analisis Quimico del Volfram, y Exàmen de un Nuevo Metal, que Entra en



su Composicion," Extractos de las Juntas Generales Celebradas por la Real Sociedad Bascongada de los Amigos del País, Vitoria, September 1783, pp. 46–88. b) J. J. D'Elhuyar, F. D'Elhuyar "Chemical Analysis of Wolframite and Examination of a New Metal Entering into its Composition," Extracts of General Meetings, Academy of the Sciences, Inscriptions and Belles Letters of Toulouse (1784), b) J. A. Schufle "Juan Jose D'Elhuyar, Discovery of Tungsten," *J. Chem. Educ.* 52, 325, 1975; c) P. Román Polo, Los Hermanos Delhuyar, la Bascongada y el Wolframio, Ed. Real Sociedad Bascongada de los Amigos del País. Comisión de Vizcaya. Bilbao. 2000.

- a) Webelements webpage <www.webelements.com>.
   b)A note on this stamp in the news site of the webelements webpage <www.webelements.com/nexus/node/1169>.
- J. García-Martínez, "Remembering Mendeleev's Centenary: Spain Issues the First Stamp Dedicated to the Periodic Table," *Philatelia Chimica et Physica* 29(3), 132–139, 2007.

exactly a century after Mendeleev's death, at the price of 0.30 euros (first class) in a limitless edition. On the eve of its release, 1 February 2007, the stamp was officially presented at the Residencia de Estudiantes (Madrid, Spain). The minister of Home Affairs (Ministro del Interior), Dr. Alfredo Pérez Rubalcaba; the president of the General Post Office, Dr. José Damián Santiago Martín; and the president of the Spanish Royal Society of Chemistry, Prof. Nazario Martín León, attended the crowded presentation of the Mendeleev stamp. For this occasion, the Spanish General Post Office issued a special postmark that was used during the ceremony to cancel 3 000 first-day envelopes. On 2 February, over 45 million Periodic Tables-in the form of 40.9 x 28.8 mm stamps—were issued. This was probably the largest dissemination ever of the Periodic Table and it was an efficient and smart way to promote chemistry.

Recently, Daniel Rabinovich wrote an excellent column about this stamp in *Stamps International*, which appears in this magazine.<sup>3</sup> The stamp also contains hidden codes to be discovered, teaching lessons, and, above all, a profound tribute to Mendeleev. The use of this stamp as a didactic tool to introduce students to the Periodic Table, Mendeleev's life, and the history of chemistry has been nicely highlighted by Gabriel Pinto in *Education in Chemistry* and the *Journal of Chemical Education*.<sup>4,5</sup> He uses this stamp in the activities described in those articles in his classes at the Polytechnic University of Madrid. Many other news outlets, more or less related to chemistry and/or philately, have covered the issuance of this new stamp.

A few months ago, the University of Jaén decided

to decorate the wall of its Experimental Science Department with a large version of the Periodic Table of this stamp. The photo on page 4 shows this beautiful Periodic Table, which is made of ceramic tiles, on its inauguration day of 22 November 2007. We were impressed to see such a large version of the periodic table (3.80  $\times$  2.70 m) compared to the usual stamp size.

### A Design Competition to Spark the Imagination

The Periodic Table is not only the fixed organization of elements hanging on the chemistry classroom, but a living creature that grows and changes over time. There are literally hundreds of versions of the Periodic Table, each one emphasizing a different aspect of the Periodic Law. So, why not give everyone the opportunity to have his or her own version? With this objective, the First Periodic Table Design Competition was launched in June 2007 to promote science and art, especially among the young. Once again, young people showed they are full of creativity and excitement about chemistry when given the opportunity.

All the Periodic Tables received were put on display at the University of La Rioja, where students, faculty, and the public were amazed by their beauty and creativity. The entries were organized according to their various properties, electronic configuration, dates of discovery, or even their names. The awards were presented on 13 July at the closing ceremony of the History of Chemistry Summer School in Logroño, Spain (see photo below). The first prize went to Luis Otaño. He designed a beautiful and very original Periodic

Table in which each element was represented by a portrait of its discoverer. Some elements shared the same person, elements 94-98 have Seaborg as their discoverer; others did not have any portrait since they have been known since antiquity, such as copper, silver, and gold. Jorge García received second prize for a Periodic Table organized by the electronic configuration of each element, and the third prize went to Alberto Soldevilla.



Participants of the First Summer School on the History of Chemistry held at the University of La Rioja, Logroño (July 11-13, 2007).

### RSEQ Prize for the Best Comic on Mendeleev

On October 2007, the Spanish Royal Society of Chemistry (RSEQ, Real Sociedad Española de Química) launched a competition for high school and college students for the best comic about Mendeleev's life. Twenty-four comics were received from Spain, Mexico, and Argentina from students with ages ranging from 14 to 25 years old. The comics show some of the best known moments of Mendeleev's life. We were amazed by the beauty and detail of the comics received, as can be observed in the samples shown on the cover of this issue. So, we decided to make them available, as well as selected periodic tables from the First Periodic Table Design Competition, at the official RSEQ website <www.rseq.org/comics>. It is hoped that this site can be used by teachers and students to learn more about Mendeleev and the Periodic Table.

At the RSEQ Council meeting in Madrid on 23 November 2007, the president of the RSEQ presented prizes to the following students: María de la Cueva León Merino for her comic *Mendeléiev* (1834-1907), Aysha Zreika for *Vida y Obra de Dimitri Mendeleyev*, and to Sergi Segura Font who presented a very original black and white comic entitled *Dimitri Mendeleyev*.

# First Summer School on the History of Chemistry Dedicated to Mendeleev

On many occasions, chemistry students get the impression from their well-organized text books and planned lessons that chemistry has been developed in the same way, from its solid principles to the complexity of the modern branches of chemistry. The history of chemistry helps them (and us) discover the creativity, intuition, and effort that great chemists relied upon to unfold a relatively new science hidden between layers of magic and secrecy. On 11 July 2007, students of the First Summer School on the History of Chemistry gathered at the University

of La Rioja to begin what were most likely their first lessons on the principles and techniques of medieval alchemy. Over the following days they discovered how chemistry grew as an independent science, how some theories were discarded whereas others, thanks to careful observation, measurement, and the scientific method, were confirmed.

The students learned that in the middle of the 19th century there was not a clear understanding of how chemical elements were organized, although some similarities among them had been known for a long time. Prof. Fernández Garbayo described how



Mendeleev (an actual-size-cardboard model) with some participants in the Science Week at Murcia, Spain, during the presentation of the stamp "Tabla Periódica de elementos de Mendeléiev" on November 2007. Javier García-Martínez is standing to the left and Pascual Román Polo is next to him.

the chemical elements were discovered, emphasizing those isolated by Spaniards (platinum: Antonio de

Ulloa, 1735; wolfram: Juan José and Fausto Delhuyar, 1783; vanadium: Andrés Manuel del Río, 1801). One of us (PRP) presented the contributions of Mendeleev in organizing the chemical elements, his Periodic Law, and some relevant moments of his fascinating life. The students were amazed to learn the details of Mendeleev's great love, and second wife, Ana Popova, or his solo ascent using a balloon—with no previous experience—to measure a solar eclipse. The summer school showed once again how useful the history of chemistry is for engaging students, and raising public awareness

and appreciation about a subject usually considered difficult.

## Mendeleev: Main Character at Science Week

Every fall, around the first week of November, towns in Spain, as in many other countries, become full of activities promoting science, especially among the young. At that time of year, it is common to see science fairs in parks, hands-on exhibitions in museums, and lectures by famous scientists to children. During recent years, many people who usually are not exposed to science have had the opportunity to

actively participate in literally hundreds of activities. Science Week is one of the most successful initiatives for raising public awareness and appreciation about science and technology.

Since 2007 was the National Year of Science in Spain, last year's Science Week (actually extended over several weeks in November) was especially extensive and ambitious. Almost all the major scientific institutions took part in an attractive and diverse program. Many of the activities, especially those organized to promote chemistry, had Mendeleev as their main character. He made an attractive and easy-to-recognize symbol, with his long disorganized hair and beard. The photo on page 7 shows an actual-size cardboard model of him holding his Periodic Table surrounded by students and the activity organizers.

At least 20 lectures about Mendeleev, his life, and the Periodic Table were organized last year at high schools, universities, parks, and museums. Local and national newspapers echoed these activities. For example, *El País*, with a circulation of half a million, included an extensive article on 27 June 2007 about Mendeleev.<sup>6</sup>

One of us (JGM) had the opportunity to attend the XVIII Mendeleev's Congress on General and Applied Chemistry held in Moscow (23–28 September 2007) to celebrate the 100th anniversary of these conferences and share with some of our Russian colleagues the activities that we have been carrying out in Spain. Some of them were surprised about the number of activities that Spain organized to celebrate Mendeleev and to learn that he actually spent time in Spain. He visited Toledo, Madrid, and Seville during his (second) honeymoon after (finally) getting married to Ana Popova. Probably, one of the happiest times of his life.

Looking back at 2007, we have to admit that it was a lot of hard work that took much of our time, but it was also an enjoyable year. Not only because of the personal fulfilment from organizing so many activities to promote an admired chemist, but mainly because of the impact of those activities on other peoples' lives. Now, we receive letters from all around the world from people who want to share stamps with us from their respective countries. Chemistry is usually defined as the study of matter, its properties, and transformations. Last year, we learned that it is much more. It is also history—as there are stories behind every discovery and the men and women that make them, art—as we use graphical schemes to represent

molecules, chemical reactions, and even the periodic law in a table, and even a great way to make new lasting friends with similar interests. We hope our experience, as well as previous events (Germany, 2003; South Korea, 2006) will be useful to others organizing similar initiatives, such as the 2009 National Year of Chemistry in Russia and the 2011 IUPAC International Year of Chemistry.

# Acknowledgements

The authors thank the many people that helped with the organization, dissemination, and activities related to Mendeleev's centenary in Spain and with reviewing this contribution for *Chemistry International*.

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### For More Information

Correos (General Post Office in Spain) <www.correos.es>
Philatelia Chimica et Physica <www.cpossu.org>

www.ciencia2007.es

# Physical and Biophysical Chemistry

# Where Does IUPAC Stand with Regard to this Discipline?

by Christopher Brett and Michel Rossi

he aim of the Physical and Biophysical Chemistry Division (PBCD), Division 1, is to organize and promote the international collaboration between scientists in physical and biophysical chemistry and related fields in accordance with the strategic goals and aims of IUPAC. More specifically it seeks to:

- address problems and formulate recommendations on nomenclature, symbols, units, terminology, and conventions in physical and biophysical chemistry, disseminate the recommendations, and encourage their translation as well as monitor their acceptance by the chemical community
- establish and stimulate the use of methodologies, standards, and reference materials in physical and biophysical chemistry
- encourage the compilation and documentation of critically evaluated physical chemical data
- recognize new developments in physical and biophysical chemistry and the fields in which they are applied
- promote future-oriented projects that contribute to science and technology and to the needs of the world community

These activities are carried out through PBCD projects and interdivisional projects, some of them involving the organization of special symposia. The Division Committee is currently composed of 10 titular members, 6 associate members, and 8 national representatives. The division committee meets every year, at the General Assembly in odd-numbered years and at a

convenient location in even or "off" years, with regular contact between committee members by e-mail. The purpose of these meetings is to discuss current and completed projects, and to discuss strategy and possible new projects involving emerging themes of research on which consensus is needed, and that

might be appropriate for the division. The membership of the committee is composed to ensure global diversity and expertise in most areas of knowledge and current activity within physical and biophysical chemistry, including thermodynamics, kinetics, theoretical



Christopher Brett (left) and Michel Rossi.

chemistry, electrochemistry, surface and interfacial chemistry, and spectroscopy and all of its biophysical implications. Topics are addressed at the molecular level, in nanoscience, nanotechnology, and materials, and with links to energy, environment, and health.

The division is also home to the Commission on Physicochemical Symbols, Terminology, and Units, whose primary role is producing the "Green Book" (more details below). In addition, the division's Advisory Subcommittee, consisting of 44 distinguished scientists, helps to review project proposals and suggests themes for new projects. It has been very valuable in furthering division activities.

Twenty-one PBCD projects are currently under way, including four interdivisional projects and three that are nearing completion; the division is also participating in nine interdivisional projects led by other divisions. The large number of interdivisional projects testifies to the high importance given to the interdisciplinary nature of chemistry and to the strong links between physical and biophysical chemistry and other areas of chemistry. The traditional frontiers between the different "classical" areas of chemistry seem to become more fuzzy as we have recently seen an increasing number of project proposals that are addressed to several divisions at the same time. New materials, chemical appli-



cations directed to energy generation and storage, and the physical chemistry of nanoscience are just three examples of a possible paradigm change, perhaps at the expense of "traditional" biophysical or molecular/biochemical aspects in physical chemistry. We certainly will

Physical and Biophysical Chemistry

critically and continuously observe such developments in order to monitor subtle changes in the interest of the physical chemistry community at large.

Many of the division's projects have resulted in publications even before completion of the project, and new and ongoing projects have been described in articles in *Chemistry International*. Projects leading to technical reports on different topics, recommendations on the use of techniques and data analysis, and reporting and databases of critically-evaluated data have been produced. Each project has a member of the division committee attributed as a project monitor who acts as a liaison between the task group leader and the Division Committee.

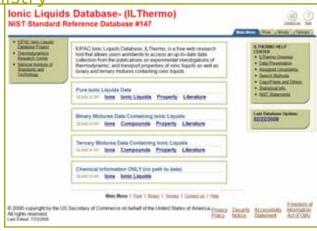
Four examples are presented below that illustrate some of the current division activities, which, it is hoped, have a positive impact for chemists worldwide.

Over the last 10 years, an evaluated kinetic database with data relevant to atmospheric kinetics has been produced (see Tools of the Trade, Jan 07 *Cl*, p. 15), together with a website <www.iupac.org/projects/2007/2007-001-2-100.html> and <www.iupac-kinetic. ch.cam.ac.uk>. This database has been highly successful, with a very large number of accesses, probably because of its impact on the simulations of climate change that take into account modifications of the composition of the atmosphere owing to chemical or photolytic reactions. In addition, selected rate

constants also control the multiphase sulphur chemistry, simultaneously taking place both in the gas, as well as in the aqueous phase, of the ocean. Continuous updating is necessary and the protocols for future updating and addition of new reactions have been recently decided. Expansion of the atmospheric degradation reactions of

organic compounds to include higher alkanes, aromatics, and perfluoro-compounds is being undertaken.

The division's projects involving ionic liquids arose as a result of the perceived need by the chemical community for better understanding of the thermodynamic and thermophysical properties for applications in industrial processes. In addition, there was interest in creating an open-access, free, and comprehensive online database for the storage and retrieval of metadata and numerical data in this new area, including the syntheses, structure, properties, and uses of this data.



Industrial applications are already emerging from this work. Details on the projects can be found at <www.iupac.org/projects/2002/2002-005-1-100.html> and <www.iupac.org/projects/2003/2003-020-2-100.html>. The ILThermo website (screen shot above) with ionic liquid data was officially launched in March 2006. It can be accessed at <ilthermo.boulder.nist.gov>. The site is divided into pure ionic liquids, binary and ternary mixtures, and further chemical information.

Another recent, important division activity was the publication of the third edition of *Quantities, Units and Symbols in Physical Chemistry* (Green Book) in July 2007 (see Nov-Dec 2007 *CI*, p.28). A project has just been approved to produce an abridged version of the Green Book in order to reach a wider audience,

particularly students. Such an abridged version is necessary given the crucial importance of standardized nomenclature to enable proper communication of comparative data and to ensure standardized links between nomenclature and concepts. Translations of the Green Book into several other languages are planned, which attests to the great popular-

ity of previous editions among students and professionals alike. Following IUPAC policy in this matter, management of the project and financial support will arise mainly from the concerned national chemical societies .

A final example concerns an innovative type of project with an educational slant that has just commenced. In conjunction with the Committee on Chemistry Education, this "test case" project seeks to reach out to parts of the world where resources are limited. The project involves promoting the application of



# Where Does IUPAC Stand with Regard to this Discipline?

wet surface vibrational spectroscopies to problems in interfacial chemistry by selecting, documenting, testing, and disseminating to universities a collection of experiments, suitable for undergraduate teaching laboratories, that can be performed with inexpensive equipment. More details can be found at <www.iupac.org/projects/2006/2006-050-3-100.html>.

The increasingly interdisciplinary nature of chemistry, among its branches and between chemistry and other sciences and with engineering, is reflected in the division's close contacts with other IUPAC divisions and with Standing Committees. Such collaborations are expected to increase.

Last year's meeting of the Physical and Biophysical Division took place at the General Assembly in Torino in August 2007 with 11 members of the Division Committee present and three Young Observers who played an active part in the proceedings. One of the Young Observers has since submitted a project that is now underway. The Division Committee's 2008 meet-

ing took place in April in Switzerland.

We are always seeking to identify and encourage project proposals, which should reflect the needs of chemistry today. These needs are in constant change, reflecting the needs of the chemistry community. For this reason, it is important that the Advisory Subcommittee advises us on new directions that members of the Division Committee may be unaware of.

If you feel that you can make a positive contribution to the work of the division and have an idea for an appropriate project, or have any other comments, please contact us via email at the addresses below.

Christopher Brett <a href="mailto:specification: np. 2006-2007">because from the University of Coimbra in Portugal. Michel Rossi <a href="mailto:smichel.rossi@">michel.rossi@</a> epfl.ch> is currently president of the division (2008-2009); he is a professor at the Federal Polytechnic School in Lausanne, Switzerland.

# Stamps International Stamps.html

# Triads, Triads, Everywhere

Johann Wolfgang Döbereiner (1780-1849), a professor of chemistry at the University of Jena, was the first to recognize that several groups of three elements, such as lithium, sodium, and potassium, or chlorine, bromine, and iodine, had similar chemical properties. In addition, he noticed that the atomic weight of the middle element in these triads was roughly the average of those of the other two. These observations led to his Law of Triads (1829), which firmly established his reputation as a pioneer in the development of the modern periodic table some 40 years before Mendeleev's masterpiece was published.

However, the stamp illustrated in this note, issued in East Germany (DDR) on 26 February 1980 to commemorate the 200th anniversary of Döbereiner's birth (which was actually on 13 December 1780), does not mention his seminal contribution to the organization of the elements but features instead his "other" claim to fame. The stamp shows a schematic drawing of his renowned lighter, in which a stream of hydrogen gas, generated from zinc and sulfuric acid, spontaneously ignites upon contact with finely divided platinum. This



novel chemical reaction received a lot of attention since it was first described by Döbereiner in the summer of 1823 and was swiftly reproduced by others. Within months the discovery was reported in multiple European scientific journals, which ushered in an era of interest in catalysis that continues to this day.

For a recent discussion of triads in the periodic table, see: Scerri, E. *J. Chem. Educ.* 2008, **85**, 585-589.

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

# Chemistry in the Information and Communications Technology Age

# On the 20th Conference on Chemical Education, 3-8 August 2008, Mauritius

nformation and communications technologies are transforming chemistry education. Experience and research have demonstrated that when technologies such as computers and the Internet are available to teachers and students the following often occurs:

- students are more engaged and more motivated to learn
- time schedules for learning are more flexible
- the amount of resource materials for learning are vastly increased
- multimedia presentations enhance the learning pro-
- students can more easily exchange information and ideas in virtual meetings and forums
- teachers can find more opportunities to educate themselves

The Internet alone has enabled a whole new world for chemistry education. Following are just a few of the chemistry resources available through the Internet:

- online chemistry books and journals, such as the DIDAC project <a href="http://didac.kvcv.be/didac-eng/">http://didac.kvcv.be/didac-eng/</a> didac1.htm>
- online chemical education conferences, where there is no registration fee, such as the CONFCHEM <www.ched-ccce.org/confchem>
- regular, free webinars, or online lectures, about chemistry

In view of these developments. the 20th International Conference on Chemical Education (20th ICCE) will be held on the theme of "Chemistry

the Information and Communications Technology Age." It will be held in Mauritius at Le Méridien hotel, from 3-8 August 2008. As part of the 20th ICCE, there will be an online conference one month before the main confer-

ence (no registration fee), which

will be followed by a satellite symposium in Nairobi. The conference is sponsored by IUPAC.

One of the main objectives of the conference is to encourage participants to exchange ideas and concepts about chemistry education. This is very important since many countries face the challenge of how to encourage students to study chemis-

try. Additionally, many of the worlds great challenges, including climate change, food and water shortages, and energy conservation will require chemistry expertise to solve.

The Organizing Committee is looking forward to gathering many participants for the 20th ICCE. Attendees will undoubtedly enjoy all that the island of Mauritius has to offer, especially its sun, sea, and sand. The conference Organizing Committee is comprise of president Henri Li Kam Wah, chairman Ponnadurai Ramasami, and secretaries Minu Gupta Bhowon and Sabina Jhaumeer-Laulloo.

Dr. Ponnadurai Ramasami is a theoretical chemist. He is currently working in the Department of Chemistry at the University of Mauritius.

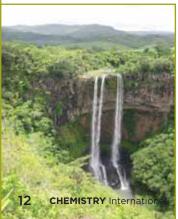
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# Tools of the Trade

# Analytical Terminology and the Orange Book—The Resources at the End of the Rainbow

by Roger M. Smith

ow do you describe an analytical method, or name the new chemical that you have just assayed, or report the units of the measurement? Where do you turn for the definitions? You need to use *terms* and *names* that are clear and unambiguous and can be understood worldwide. In other words, you need the resources of the IUPAC "Color Books": Gold, Orange, Blue, Red, Green, Purple, White, and Silver—not quite a rainbow leading to a pot of gold, but in this case the compendia of the accumulated agreements of the world's chemists, providing the *terminology* and *nomenclature* of chemistry.

For analytical chemists, the principal tool of the trade, or source of terms, is the *Compendium of Analytical Nomenclature*, the so-called Orange Book, named because of the color of its cover. Originating in 1978, it was most recently updated with a third edition in 1997,<sup>1</sup> and was subsequently converted (and updated with additional terms) to an online version by David Moore in 2002.<sup>2</sup> Strictly speaking, the title should now be updated to *Compendium of Analytical Terminology*, not nomenclature, since the latter term is now reserved for the rules for naming chemical structures. In addition to definitions and terms, the Orange

Book also describes the different meanings of terms and expands on basic expressions.

As a test, ask yourself if you can readily define the following terms in the context of analytical chemistry; if you cannot then check the Orange Book online.<sup>2</sup> Some are more obvious than others.

- Stokes shift
- supercritical fluid
- selective
- stripping
- difference between a spectrograph, spectrometer, and spectroscope
- when to use a chiral selector

The process of defining a term is a major and continuing part of the activity of the Analytical Chemistry Division Committee of IUPAC and its task groups. The process usually starts with the need to stabilize the terminology for a new and expanding area, or to clarify ambiguities that have arisen over time in an established field, typically because of conflicting usages by different research groups.

A task group of experts in the field is formed by the division. This group will meet (often on numerous occasions) and prepare a draft proposal, which is acceptable to all the members. They then take this draft through a sequence of consultations with representatives of all interested parties, including journal editors and the chemical community at large. The various comments and suggestions are used to generate a provisional recommendation, which is then submitted via the IUPAC website for public review<sup>3</sup> (such as the recent review of Metrological Traceability of Measurement Results in Chemistry). At the same time, the recommendations are assessed by the Interdivisional Committee on Terminology, Nomenclature and Symbols. Finally, when all parties are in agreement, the approved, revised, or new terminology is published as IUPAC Recommendations in the official journal of IUPAC Pure and Applied Chemistry.



# **Feature Articles Wanted**

*CI* is currently seeking feature articles

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

# Tools of the Trade

These newly approved terms and descriptions are then available and ready to be added to a future updating of the online Orange Book. In many cases, the terms will also be added to the *Compendium of Chemical Terminology* (the Gold Book), which is now also available in an online version.<sup>4</sup> Analytical chemists also need to be aware of the content of other color books, especially *Quantities, Units, and Symbols in Physical Chemistry*<sup>5</sup> to ensure the correct usage of units and abbreviations.

The most important step is for the analytical community to adopt and then use the IUPAC recommended terms in everyday practice, in publications, journal articles, books, lectures, and other presentations. Journal editors, referees, and editorial boards play an important role in ensuring that contributors employ the correct terminology and avoid older, superseded, or ambiguous expressions. When changes are recommended, general acceptance is often rapid. For example, when, in 1993, the terminology of chromatography replaced "capacity factor (k')" by "retention factor (k)"

and standardized the definition of "plate number" as N (not n), the new terms were adopted rapidly and, except in older textbooks, the archaic terms are now rarely seen.

### References

- Compendium of Analytical Nomenclature (definitive rules 1997), 3rd edition Inczedy, J.; Lengyel, T. and Ure, A.M (Editors) Blackwell Science, 1998 [ISBN 0-86542-6155]
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- Quantities, Units, and Symbols in Physical Chemistry, 3rd edition, Cohen, E.R., Cvitaš, T., Frey, J.G., Holmström, B., Kuchitsu, K., Marquardt, R., Mills, I., Pavese, F., Quack, M., Stohner, J., Strauss, H.L., Takami, M. and Thor, A.J. RSC Publishing, Cambridge 2007

Roger M. Smith <r.m.smith@lboro.ac.uk> is a professor at Loughborough University, UK. Until December 2007, Smith was secretary of the IUPAC Analytical Chemistry Division: he is now the U.K. national representative on the division.

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# **IUPAC** Wire

# Peter Mahaffy Awarded 3M Canada **Teaching Fellowship**

ing's University College chemistry professor Peter Mahaffy has been awarded the 3M Canada Teaching Fellowship, which honors educational leadership and excellence in undergraduate teaching. The 3M Fellowship is regarded as Canada's top teaching award.

Mahaffy was recognized for his contributions to the learning community at King's University College and

> for his leadership in international science education.

> "It is gratifying to see Mahaffy's teaching excellence recognized with such a celebrated award," said King's President Harry Fernhout. "His contributions at both the national and international level are a reflection of the amazing work he does right here at King's. His approach to teaching both inspires our students and serves as



Peter Mahaffy.

a model for university professors far and wide. We are privileged to have him as part of our team."

"Professor Mahaffy's passion for chemistry has made him a visionary science educator," noted King's Vice-President Academic, Dr. Harry Spaling. "Mahaffy uses a wide range of teaching techniques to connect with learners. Even more importantly, he is such a gifted teacher because he authentically values his relationship with students. He has an unsurpassed ability to inspire all students, including nonscience majors, to articulate an understanding of the scientific world."

Mahaffy works both with chemistry majors in the nationally accredited chemistry program at King's, and has developed innovative approaches to teaching chemistry to arts and science students. As one of the early adaptors of molecular modeling for teaching purposes, he continues to collaborate with colleagues at the King's Centre for Visualization in Science to develop eye-catching visualizations and other teaching aids now used around the world.

One of Mahaffy's significant contributions is a new metaphor for chemistry education. His tetrahedral model incorporates the existing triangle metaphor that learners encounter in their chemistry textbooks, but extends the triangle in a third dimension, representing the human contexts for chemistry. Chemical educators have embraced this new metaphor, and organizers of major international conferences have

invited Mahaffy to describe this new approach to chemistry education.

Mahaffy's roles as chair of IUPAC's Committee on Chemistry Education and as a member of the International Council on Science's Committee on Freedom and Responsibility in the Conduct of Science place him in global leadership positions in science education and science policy. During his 28-year career as a chemistry professor, Dr. Mahaffy has been described as "Mister Chemical Educator."

"If there is any area of professional success that is by definition never an individual achievement, it is in the rewarding world of teaching and learning," says Mahaffy. "It is such a privilege to work with inspirational students and colleagues in our supportive learning community at King's, and with international collaborators to use the tools of science and science education to help make the world a better place."



www.kingsu.net/page.aspx?ID=97209

# Pieter S. Steyn Receives Science for Society Gold Medal

ormer IUPAC President Piet Steyn (2002-2003) was awarded the 2007 Science for Society Gold Medal from the Academy of Science of South Africa (ASSAf) at a ceremony held 26 November 2007 in Pretoria, South Africa. Two medals are awarded annually to individuals from South Africa who apply



Piet Steyn (left), holding his ASSAf 2007 Science for Society Gold Medal, Naledi Pandor (minister of Education), Robin Crewe (president of ASSAf), and Wieland Gevers (chief executive officer of ASSAf).

scientific thinking in the service of society. Steyn was honored for his many scientific accomplishments, but especially for his role in furthering science education.

While president of IUPAC, Steyn played a decisive role in raising the profile of the teaching and public understanding of chemistry, culminating in the formation of the Committee on Chemistry Education to address these matters. Further evidence of his commitment to science education is SEDIBA (the Tswana word for a fountain), a project created while he was at the University of the North West in Potchefstroom, which works to upgrade the scientific and pedagogical skills of science and mathematics educators in disadvantaged communities. At Stellenbosch University, Steyn played a prime role in procuring USD 1 million from the Mellon Foundation to create postgraduate and postdoctoral scholarships for students from previously disadvantaged communities, some of whom have subsequently joined faculties at Stellenbosch and other South African universities.

Steyn has always placed a high premium on building the capacity of young researchers and sought to create opportunities for colleagues to improve their qualifications through advanced study or research positions at South African or international universities. In addition, he has been supervisor, co-supervisor or external examiner to numerous masters and doctoral students, both locally and at the Imperial College of Science, Technology and Medicine in London.

Steyn's research has been devoted to the isolation, analysis, structure elucidation, synthesis, and biosynthesis of mycotoxins and, to a lesser extent, other toxic and medicinal substances from plants. As a mycotoxin expert, Steyn has consistently been called upon to advise the food industry. His expertise on mycotoxins was also sought for a joint project in the 4th Framework Programme of the European Union, called "Biological degradation of aflatoxins in fermented maize and sorghum products". This successful project involved collaboration with researchers in Germany, Denmark, Nigeria and Ghana, and was acknowledged by the EU as a "model project." Their research findings later led to a patent on the selective and mild degradation of aflatoxin. Steyn received several awards from the South African Chemical Institute for his research contributions.

www.assaf.co.za

# Chemical Heritage Foundation Produces *Distillations*, a Weekly Podcast

n December 2007, the Chemical Heritage Foundation (CHF), based in Philadelphia, Pennsylvania, USA, launched a new weekly podcast. Distillations: Extracts from the Past, Present, and Future of Chemistry offers entertaining reports on subjects ranging from alchemy to the contents of your kitchen cupboard to the chemistry of space exploration. It makes the wonders of chemistry available to listeners around the world.

Distillations airs every Friday and features host Robert D. Hicks, director of the Roy Eddleman Institute for Interpretation and Education at CHF, and guests. Recorded in Philadelphia and produced in San Francisco, Distillations



has a radio-quality sound that you can listen to wherever your iPod takes you.

In the premier episode of *Distillations*, "Communicating Chemistry," listeners can hear Paul Smith, a Michael Faraday reenactor from Purdue University, explain how public chemistry lectures enchanted Londoners in the early decades of the nineteenth century. In this episode's installation of "The Element of the Week," a recurring segment, you'll hear how phlogiston was discovered and subsequently discarded in favor of the element we now call oxygen.

Episode 4, titled "Measurement," includes a brief interview with Norman Holden, Brookhaven National Laboratories, on changing atomic weights and the valuable work done under the IUPAC Commission on Isotopic Abundance and Atomic Weights (II.1). On a different issue related to measurements, a brief account of the debates over how to fix the standard kilogram is also included in that podcast. <a href="http://distillations.chemheritage.org/?p=55">http://distillations.chemheritage.org/?p=55></a>.

Each show lasts 6 to 10 minutes. *Distillations* is available free of charge through the iTunes store and at its website <a href="http://distillations.chemheritage.org">http://distillations.chemheritage.org</a>>.

Show topics are varied and have included the following: Wonder Drug, Color, Electronic, and Cleaning Up. *Distillations* is a presentation of CHF and is made possible by the generous support of the Richard Lounsbery Foundation.

# The Project Place

# **Mechanistic Aspects of Chemical Vapor Generation of Volatile Hydrides for Trace Element Determination**

Aqueous phase chemical vapor generation (CVG) by derivatization with borane complexes, coupled with atomic and mass spectrometric detection techniques, is one of the most powerful and widely employed methods for determination and speciation analysis of trace and ultratrace elements (viz. Ge, Sn, Pb, As, Sb, Bi, Se, Te, Hg, Cd and, more recently, several transition and noble metals). Thousands of research papers and many regulated analytical methods are based on CVG. However, since its inception more than 35 years ago, the application and validation of CVG to many different analytical targets has been the prevailing focus of "research," whereas only limited efforts have been dedicated to clarification of the mechanistic aspects of the reactions. Analytical CVG is still dominated by erroneous concepts, which have been disseminated and consolidated within the analytical scientific community over the course of many years. The overall approach to CVG has thus remained completely empirical, which hinders possibilities for further development.

A rationalization of the field based on a more rigorous scientific approach appears to be necessary. The aspects requiring rationalization, which form the objectives of this project, can be classified as follows: mechanism of hydrolysis of borane complexes, mechanism of hydrogen transfer from the borane complex to the analytical substrate, and mechanism of action of additives commonly employed in analytical applications of CVG. Enhanced comprehension of these three different mechanisms and their mutual influence will provide the tools to explain the reactivity of a CVG

At present, there are essentially two main sources of information useful for comprehension of the mechanistic aspects of CVG. The first is represented by the fundamental data and experimental evidence relating to the chemistry of borane complexes that has been collected and reported in the literature in past years (1950-1980); regrettably, the analytical community has disregarded most of this fundamental literature. The second source is represented by the most recent experimental evidence specifically devoted to clarification of the mechanism of CVG (the past 10 years of work). The combination of these two major sources of information should make possible the rationalization of the mechanistic aspects of CVG, and will hopefully provide an impulse for further development in the field.

For more information and comments, please contact the Task Group Chair Alessandro D'Ulivo <dulivo@ipcf.cnr.it>.



www.iupac.org/projects/2007/2007-041-1-500.html

# **Assessment of Theoretical Methods** for the Study of Reactions Involving **Global Warming Gas Species Degradation and Byproduct Formation**

Experimental techniques have always been used to study the thermodynamics and kinetics of chemical reactions. However, due to the explosive growth of computational power, quantum mechanical methods (semiempirical, ab initio, and density functional) have been found to be useful for these studies. Some researchers have also developed more adapted procedures using ab initio and density functional methods for studies.

Since global warming is a major concern, various studies are exploring the reactions involving global warming gas species degradation and byproduct formation. The aim of this new project is to carry out a critical analysis of the theoretical methods used to investigate these reactions and to assess to what extent the methods used are suitable in the predictions of thermodynamical parameters such as standard enthalpies, entropies, and heat capacities, and kinetics parameters such as activation energies and rate constants.

One of the outcomes of this project is to help researchers decide about the most promising method/ methods in their future investigations.

The objectives of this project are as follows:

- to review the quantum mechanical methods that have been used to investigate reactions involving global warming gas species degradation and byproduct formation
- to assess the performance of the methods used by comparison with experimental data

For more information and comments, please contact the Task Group Chair Ponnadurai Ramasami <ramchemi@intnet.mu>.



www.iupac.org/projects/2007/2007-048-2-100.html

# The Project Place

# Analysis of the Usage of Nanoscience and Technology in Chemistry

The last few years have observed a wide proliferation of the terminology related to nanotechnology and nanoscience in chemistry. Today, all high-impact chemistry journals contain a large number of papers devoted to this growing area, as many conferences include specific sessions on nanotechnology.

The objective of this new project is to map and critically study the use of the prefix nano in various fields of chemistry. For this purpose, we will use the different search engines available to compare the usage of nano-containing terms. We will map the evolution and usage of nano-containing descriptive terms according to different criteria, and critically analyze their validity in scientific (chemical) language. This project is the first step towards recommendations on the use of chemistry terminology related to nanoscience and nanotechnology.

The methodology proposed is the following. First, we will use widely available and popular chemistry search engines, such as Sci Finder, and others provided by the CAS and RSC. The hits on "nano\*" will be analyzed according to criteria, such as time, country, and source. Secondly, we will repeat the process by restricting the search to some of the most highly cited journals of each chemistry discipline, to learn if "nano-" terminology has impacted all the areas of chemistry and if so, to what extent and at what rate.

For more information and comments, please contact the Task Group Chair Javier Garcia Martinez <j.garcia@ua.es> or Sanjay Mathur <smathur@inm-gmbh.de>.

www.iupac.org/projects/2007/2007-040-2-200.html

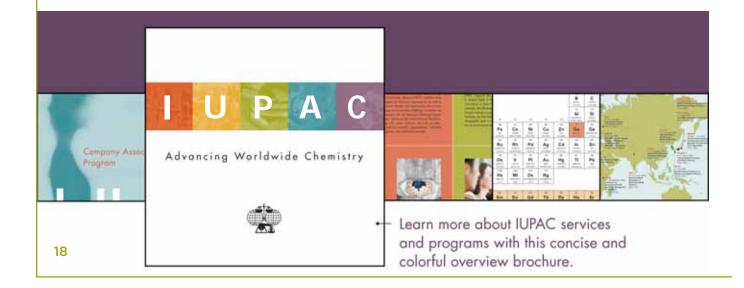
# Extension of ThermoML—The IUPAC Standard for Thermodynamic Data Communications

This project is an extension of project 2002-055-3-024, XML-Based IUPAC Standard for Experimental and Critically Evaluated Thermodynamic Property Data Storage and Capture, which was successfully completed in 2006. From that project, a new XML-based IUPAC standard (ThermoML) was established for thermodynamic data communications (Pure Appl. Chem., 2006, 78, 541-612). Initially, ThermoML provided support of communications for experimental, critically evaluated, and predicted data for thermodynamic properties of pure and multi-component mixtures of molecular compounds with comprehensive representation of uncertainties (J. Chem. Eng. Data, 2003, 48, 2-13; 2003, 48, 1344-1359; and 2004, 49, 160-174). Prior to the standard release, enhancements for aqueous electrolyte solutions and ionic liquids were included. The current project will broaden the scope of ThermoML to support storage and exchange of thermodynamic property data for speciation and complex equilibria in aqueous and non-aqueous solvents, and thermodynamic properties of biomaterials.

For more information and comments, please contact the Task Group Chair Michael Frenkel <frenkel@boulder.nist.gov>.



www.iupac.org/projects/2007/2007-039-1-024.html



# 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.

www.iupac.org/reports/provisional

# **Explanatory Glossary of Terms Used** in Expression of Relative Isotope Ratios and Gas Ratios

To minimize confusion in the expression of measurements of isotope and gas ratios, a glossary based on recommendation by the Commission on Isotopic Abundances and Atomic Weights of the IUPAC is presented. Entries in the glossary are consistent with the SI system of units or with recommendations of the Commission. The recommendations presented herein are designed to clarify expression of quantities related to measurement of isotope and gas ratios by ensuring that quantity equations and not numerical-value equations are used to define quantities. Examples of column headings consistent with SI recommendations and examples of various deprecated usages connected with the terms recommended are presented herein.

# Comments by 31 May 2008

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www.iupac.org/reports/provisional/abstract08/coplen\_310508.html

# Glossary of Class Names of **Polymers Based on Chemical** Structure and Molecular Architecture

This document defines class names of polymers based on the class names of starting monomers and characteristic features of the chemical constitution of polymer molecules (macromolecules), i.e., class names that have gained general acceptance in the polymer and material literature, science and technology as well as in public.

The glossary is divided into three parts:

- Source-based class names, which identify common classes of starting monomers such as "acrylic", "diene", "phenolic", "vinylic".
- Class names based on chemical structure, which identify characteristic groups in the main chains (backbones) of the polymer molecules such as (i) inter-unit groups derived from functional groups, e.g., "amide", "ester", "ether"; (ii) a specific group of atoms, e.g., "alkenylene", "siloxane", "sulfone"; (iii) ring structures, e.g., "benzimidazole", "benzoxazole", "quinoxaline".

Class names based on molecular architecture, which identify mainly the overall shapes of polymer molecules through the type of their graphical representation such as "linear", "branched", "dendritic", "comb".

Each part of the glossary is arranged in a non-hierarchical alphabetical order. Each entry provides: a) the polymer class name; b) its definition; c) specific or generic examples including IUPAC names and a structure or graphical representation; d) relations to other polymer classes and subclasses; e) notes on the inclusion or exclusion of borderline cases. Alphabetical index of all class names is included.

## Comments by 30 June 2008

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www.iupac.org/reports/provisional/abstract08/vohlidal\_300608.html

# Making an imPACt

# **Further Conventions for NMR Shielding and Chemical Shifts** (IUPAC Recommendations 2008)

Robin K. Harris, Edwin D. Becker, Sonia M. Cabral de Menezes, Pierre Granger, Roy E. Hoffman, and Kurt W. Zilm

Pure and Applied Chemistry, 2008 Vol. 80, No. 1, pp. 59-84 doi:10.1351/pac200880010059

IUPAC has published a number of recommendations regarding the reporting of nuclear magnetic resonance (NMR) data, especially chemical shifts. The most recent publication [PAC 73, 1795 (2001)] recommended that tetramethylsilane (TMS) serve as a universal reference for reporting the shifts of all nuclides, but it deferred recommendations for several aspects of this subject. This document first examines the extent to which the <sup>1</sup>H shielding in TMS itself is subject to change by variation in temperature, concentration, and solvent. On the basis of recently published

results, it has been established that the shielding of TMS in solution [along with that of sodium-3-(trimet hylsilyl)propanesulfonate, DSS, often used as a reference for aqueous solutions] varies only slightly with temperature but is subject to solvent perturbations of a few tenths of a parts per million. Recommendations are given for reporting chemical shifts under most routine experimental conditions and for quantifying effects of temperature and solvent variation, including the use of magnetic susceptibility corrections and of magic-angle spinning (MAS). This document provides the first IUPAC recommendations for referencing and reporting chemical shifts in solids, based on high-resolution MAS studies. Procedures are given for relating <sup>13</sup>C NMR chemical shifts in solids to the scales used for high-resolution studies in the liquid phase. The notation and terminology used for describing chemical shift and shielding tensors in solids is reviewed in some detail, and recommendations are given for best practice.



www.iupac.org/publications/pac/80/1/0059

# Transport of Pesticides via **Macropores (IUPAC Technical** Report)

Werner Kördel, Hans Egli, and Michael Klein Pure and Applied Chemistry, 2008 Vol. 80, No. 1, pp. 105-160 doi:10.1351/pac200880010105

This report provides an overview of the transport of solutes via macropores, focusing on the practical relevance of the phenomenon. After a description of matrix flow and preferential flow in soil, information related to macropores, including their formation and measurement techniques, is briefly presented. Then, the influence of experimental conditions and of environmental and agricultural factors and pesticide properties is discussed, based on a statistical evaluation of all published studies offering sufficient quantitative information.

Most of the analyzed parameters do not significantly influence the experimental pesticide losses. The

groundwater ubiquity score index turned out to be the most important compound property to describe substance losses through macropore flow. In a third section, tools for modeling pesticide transport through macropores are presented and critically evaluated. Results of the computer model MACRO, which is also used in the European Union pesticide registration process, are compared with experimental losses. For five out of seven investigated pesticides, the simulated losses are in agreement with the experimental data. However, for two compounds with very low soil adsorbtion values, MACRO overestimated the losses. Finally, the significance of pesticide transport via macropores for contamination of ground and surface water is assessed. Losses caused by macropore transport may considerably exceed losses caused by matrix transport at a specific site. Therefore, a site-specific assessment of pesticide leaching is needed.



www.iupac.org/publications/pac/80/1/0105

# Performance Evaluation Criteria for Preparation and Measurement of Macro- and Microfabricated Ion-Selective Electrodes (IUPAC Technical Report)

Ernö Lindner and Yoshio Umezawa Pure and Applied Chemistry, 2008 Vol. 80, No. 1, pp. 85-104 doi:10.1351/pac200880010085

Over the last 30 years, IUPAC published several documents with the goal of achieving standardized nomenclature and methodology for potentiometric ion-selective electrodes (ISEs). The ISE vocabulary was formulated, measurement protocols were suggested, and the selectivity coefficients were compiled.

However, in light of new discoveries and experimental possibilities in the field of ISEs, some of the IUPAC recommendations have become outdated. The goal of this technical report is to direct attention to ISE practices and the striking need for updated or refined IUPAC recommendations that are consistent with the state of the art of using macro- and microfabricated planar microelectrodes. Some of these ISE practices have never been addressed by IUPAC but have gained importance with the technological and theoretical developments of recent years. In spite of its recognized importance, a generally acceptable revision of the current IUPAC recommendations is far beyond the scope of this work.



www.iupac.org/publications/pac/80/1/0085

# Chemists and "The Public": **IUPAC's Role in Achieving Mutual Understanding (IUPAC Technical** Report)

Peter Mahaffy, Anthony Ashmore, Bob Bucat, Choon Do, and Megan Rosborough

Pure and Applied Chemistry, 2008 Vol. 80, No. 1, pp. 161-174 doi:10.1351/pac200880010161

This report informs IUPAC's efforts to enhance the public understanding of and appreciation for chemistry by evaluating IUPAC's mandate, strengths, and weaknesses, and providing insights from a substantial review of the relevant science communication literature. It summarizes the recommendations of an IUPAC project whose overall goal is to provide a framework that will bring the same level of intellectual rigor to IUPAC's science communication activities as to its scientific activities. This implies that careful attention must be paid to the terminology used to describe these activities, to clear articulation of goals and motives for public understanding of chemistry initiatives, and to inclusion of rigorous evaluations of outcomes from the outset in the design of projects on the public understanding of chemistry.

Informed by our analysis of best practices for science communication, this report provides the following conclusions and recommendations:

1. IUPAC has an important role to play in enhancing

- public understanding of chemistry.
- 2. Public understanding of chemistry activities aimed at supporting teachers and students within the formal school system are more effective than those aimed at the general public.
- 3. IUPAC's primary targeted public should be IUPAC chemists and educators, and IUPAC's most important role is to help them understand and work with a variety of other publics.
- 4. It is proposed that IUPAC's niche be to focus on activities that indirectly enhance public understanding, such as:
  - (a) helping scientists identify and understand their publics
  - (b) influencing international organizations
  - (c) supporting science education systems, particularly in countries in transition
  - (d) supporting scientists and educators by communicating relevant findings from IUPAC projects, conferences, and activities at an appropriate level
  - (e) supporting national chemical societies and other organizations
- Recommendations are presented for steps to be undertaken by IUPAC to implement these recommendations and to develop a clearer strategy for public understanding of chemistry initiatives and activities.



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# Making an imPACt

# Glossary of Terms Related to Solubility (IUPAC Recommendations 2008)

Heinz Gamsjäger, John W. Lorimer, Pirketta Scharlin, and David G. Shaw

Pure and Applied Chemistry, 2008 Vol. 80, No. 2, pp. 233-276 doi:10.1351/pac200880020233

Phenomena related to the solubility of solids, liquids. and gases with one another are of interest to scientists and technologists in an array of disciplines. The diversity of backgrounds of individuals concerned with solubility creates a potential for confusion and miscommunication and heightens the need for an authoritative glossary of terms related to solubility. This glossary defines 166 terms used to describe solubility and related phenomena. The definitions are consistent with one another and with IUPAC recommendations for terminology and nomenclature.



www.iupac.org/publications/pac/80/2/0233

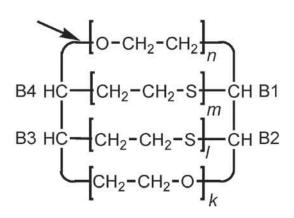
# Structure-Based Nomenclature for Cyclic Organic Macromolecules (IUPAC Recommendations 2008)

## W. Mormann and K.-H. Hellwich

Pure and Applied Chemistry, 2008 Vol. 80, No. 2, pp. 201-232 doi:10.1351/pac200880020201

A structure-based nomenclature system for monocyclic and polycyclic organic macromolecules is presented. Single-strand mono- and polycyclic macromolecules, as well as spiro macrocyclic compounds, are covered. However, rotaxanes and catenanes, which contain interlocked rings, and rings or ring systems formed by noncovalent bonds are excluded. Also, polypeptides and carbohydrate polymers are not included. The nomenclature of cyclic macromolecules is based on the existing nomenclature of regular and irregular macromolecules, which in turn is based on the nomenclature of organic chemistry, also published by IUPAC.

The procedure for naming a cyclic macromolecule consists of transforming it to an open-chain regular or irregular macromolecule in such a way that naming of units proceeds in descending order of seniority but otherwise follows the rules established for these types of macromolecules. For polycyclic macromolecules, the same principles are followed after the main ring, bridges, and branch units are identified and locants for branch units as well as bridges are assigned. The complete names are assembled by citing the component



# Example 39

Name: [B1],[B4]-[poly(sulfanediylethylene)]-[B2],[B3]-

> [poly(sulfanediylethylene)]-cyclo[poly(oxyethylene)-[1:B1][2:B2]ethylene-poly(oxyethylene)-[1:B3][2:

[B1],[B4]:[B2],[B3]-bis[poly(sulfanediylethylene)

]-cyclo[poly(oxyethylene)-[1:B1][2:B2]ethylenepoly(oxyethylene)-[1:B3][2:B4]ethylene]

names and locants in the appropriate order according to the rules in this document. Wherever possible. examples for illustration of the naming procedure have been chosen from the literature.



www.iupac.org/publications/pac/80/2/0201

# Making an imPACt

# Impact of Scientific Developments on the Chemical Weapons Convention (IUPAC Technical Report)

Mahdi Balali-Mood, Pieter S. Steyn, Leiv K. Sydnes, and Ralf Trapp

Pure and Applied Chemistry, 2008 Vol. 80, No. 1, pp. 175-200 doi:10.1351/pac200880010175

This report summarizes the findings and recommendations of an international workshop that was organized jointly by IUPAC and the Organisation for the Prohibition of Chemical Weapons (OPCW), and held in Zagreb, Croatia, from 22 to 25 April 2007. It was held to assist with preparation for the Second Review Conference of the Chemical Weapons Convention (CWC), which will commence in April 2008. The CWC has been in force since 29 April 1997, and today 182 States have joined the Convention.

The CWC aims at the total prohibition of all chemi-

cal weapons (CW) and the destruction of all CW stockpiles and production facilities by 2007. Extensions have been agreed upon and, for some CW stockpiles, the deadline is now 2012. This disarmament is subject to strict international verification by the OPCW. The CWC also prohibits the development, production, acquisition, stockpiling, and retention of CW and requires national implementation measures, including legislation, together with the international verification of chemical industry facilities. Furthermore, the CWC aims to strengthen States Parties' capacities in the field of protection against CW, and encourages international cooperation in the peaceful application of chemistry.

The CWC requires that reviews of the operation of the Convention are carried out at five-year intervals and specifies that such reviews "shall take into account any relevant scientific and technological developments," so as to ensure the continued effectiveness of the treaty and of its verification and implementation systems. This report has been prepared to assist the parties of the CWC with that review.



www.iupac.org/publications/pac/80/1/0175

# **Graphical Representation Standards** for Chemical Structure Diagrams (IUPAC Recommendations 2008)

# Jonathan Brecher

Pure and Applied Chemistry, 2008 Vol. 80, No. 2, pp. 277-410 doi:10.1351/pac200880020277

The purpose of a chemical structure diagram is to convey information-typically the identity of a molecule—to another human reader or as input to a computer program. Any form of communication, however, requires that all participants understand each other. Recommendations are provided for the display of twodimensional chemical structure diagrams in ways that avoid ambiguity and are likely to be understood correctly by all viewers. Examples are provided in many areas, ranging from issues of typography and color selection to the relative positioning of portions of a diagram and the rotational alignment of the diagram as a whole. Explanations describe which styles are preferred and which should be avoided. Principal recommendations include: 1) Know your audience: Diagrams that have a wide audience should be drawn as simply as possible; 2) Avoid ambiguous drawing styles; 3) Avoid inconsistent drawing styles.



www.iupac.org/publications/pac/80/2/0277

# Internet Connection

# The Periodic Table: Database or XML?

by Daniel Tofan

n the July-August 2004 issue of *Chemistry International*, I suggested the idea of an XML specification dedicated to exchanging scholarly data among course management systems and, in general, applications dealing with learning general chemistry. The project, under the proposed name Chemical Education Markup Language (ChEdML), is a major undertaking and its success is highly dependent on the willingness of software developers to implement a new standard. While building such consensus may not be entirely feasible, smaller projects that can demonstrate the usefulness of data structuring in chemical education are easier to implement and publish.

The main goal of the Periodic Table Database/XML project is to provide an open source of data about the elements in various formats. The project came to life during the past few months as a group project in a graduate-level course I taught titled "Computers in Chemical Education." The idea was inspired from the myriad of periodic tables that are now available on the internet. Students needed a way of extracting the data about the elements and putting it in some user friendly electronic format as part of the course requirements. They found no structured way of extracting all such data at once without navigating multiple web pages and filtering out ads. A web search was conducted, looking for a database or an XML specification that would provide properties of the chemical elements in a structured, computer readable form. Very few web-

bondLenath superconducting Elements thermalConduction ectronBindinaEner.. thermalExpansio atomicNumbe 00 atomicNumber atomicMass label symbol ThermoProperties orbital elementName atomicNumber bindingEnergy periodNumber state groupNumber enthalpyFormatio dationStates groupOldNumber freeEnergyForma atomicNumber groupCommonName oxidationState specificHeat block common molarSpecificHea elementType casID enthalpyFusion otopes discoveryYear enthalpyVaporiza atomicNumber enthalpyAtomiza discoveryPlace massNumber discoveredBy atomicMass CrystalStructure description abundance atomicNumber biologicalRole nuclearSpin spaceGroup healthHazards magneticMoment spaceGroupNur history radioactive structure trivia halfLife halfLifeUnits

sites were found to be significantly helpful, and there are scarce attempts to organize the periodic table in XML. The ones that we were able to identify were rather lacking—only a few properties were included for each element. We did not find a complete representation of the periodic table in XML.

While searching for databases, we noticed that many people call "database" a collection of web pages that display information about a subject, in this case the periodic table. What was sought was an actual database product that can be gueried in order to extract meaningful information. The only serious product that we found that uses a database was the Periodic Table of Data, a project of the Royal Society of Chemistry.<sup>1</sup> A close inspection of this Access 2003 database file (available for free download from the RCS) reveals much redundancy in the construction of the database tables. The database was not an actual relational database but merely a collection of tables having the same field structure, which were apparently being populated in different ways. It is important for a database to be well designed from the start in order to eliminate redundancy, to minimize storage space, and maximize search capabilities. Thus, we decided to implement our own version of the periodic table data in comprehensive form.

The main decision to be made was whether to use a database format or an XML format to store the periodic table in a structured fashion. In an attempt to expand on the ChEdML project, XML was our first choice, and students taking the course were given the task of creating the XML structure and populating it with the most important data about the elements. WebElements<sup>2</sup> was chosen as the main source of information. Once a template for the XML structure was agreed upon, students worked in small groups and populated the skeleton with data about the elements. XmlShell<sup>3</sup> was used to edit, duplicate, and move the XML fragments in order to expand the common template to include the entire table. The goal of the work was to merge all individual XML files (each representing a group of elements) into one master document that would be subsequently subjected to data validation. Unfortunately, but perhaps to be expected when several different students inexperienced in XML work on a common project, the end result had many inconsistencies. A very basic DTD (document type definition) was created to check the final product, and the data validation step failed. Clearly, we had been using the wrong approach to creating a consistent, accurate representation of the periodic table in XML.

The project was started over and we had the

same dilemma of using XML versus a database. XML has the advantage that it is plain text and thus readable by humans as well as computers. However, building and editing XML files, even when using a dedicated editor, proved to be very tedious and error prone. The main reason to use XML is to export data in a structured. open-source format that can be read by other applications. From the point of view of creating the structure and entering the data, we soon realized that a database is by far the PDF Relational XML database

| Continue | Co

better approach. A relational database offers many advantages over XML: it is fast, compact, can enforce data integrity, can be queried in complex ways, offers user friendly forms for data input, and has extensive export capabilities. Careful design of the tables and relationships between tables offer advanced querying capabilities and the ability of grouping data into meaningful categories. More importantly, exporting the data from the database in XML format is possible in a very elegant fashion, through software, thus guaranteeing that the data is XML-valid.

We chose Microsoft Access 2007 as our database product. Access has a very user friendly interface, and thus creation of tables, relationships, and forms was straightforward. The main table, called "Elements," contains the most basic information about each element (nomenclature, position in table, description, and other factual information). With the exception of atomic number and mass, all other numerical data about the elements were stored in separate tables, grouped by category (bulk properties, thermodynamic properties, electronic properties, etc.). Relationships were built between the main tables and the additional tables using the atomic number (primary key in the "Elements" table) as a foreign key in all tables except one that stores units of measurement for various properties reported. Referential integrity was enforced, thus ensuring that each record is linked to a valid element. No duplicates were allowed for information that is inherently unique, such as atomic number, symbol, or name. Field sizes were restricted to meaningful values in order to save space (for example, "state" was allowed to take one value from the set "s", "l", or "g", thus using only 1 byte instead of 255, the default for a "text" field type). When multiple records were needed per element for one subset of data, but not for the entire table (such as isotopes, which share most elemental properties except nuclear ones), a separate table was created and a *one-to-many* relationship was built between the main table and the new table. This strategy eliminates data redundancy and complies with modern database design principles.

The database is populated with almost all properties available for the elements. We used the most recent atomic masses published by IUPAC and compiled everything else from data provided by the WebElements site. Using Java programming and XML code libraries such as JDOM,4 we can generate the entire table in XML by running a simple command. The only condition needed is accuracy of the data inside the database. The generated XML is guaranteed to be well formed and valid. This is a tremendous advantage over creating the XML from scratch. In addition, applications can be built to display data on demand and take advantage of the querying capabilities of the database to show only information of interest to the user. The XML exporting capabilities of Access 2007 are also being investigated. Exporting to other formats such as HTML or PDF is a definite possibility.

The project currently maintains a website<sup>5</sup> displaying a periodic table that has links for all elements. Each link is a PDF file that displays one element, with a picture of an element sample if available, basic data about the element, crystal structure representations in JMol, and a list of facts and trivia about the element. All element sheets were combined together in one poster representing the periodic table and displayed in our school. Our next step is the implementation of a Java application that will display the periodic table

continued on page 26

# Bookworm

# The Investigation of Organic Reactions and their Mechanisms

edited by Howard Maskill Blackwell Publishing, Oxford, 2006

### reviewed by Tadeusz Marek Krygowski

This 370-page volume consists of 12 monograph reviews dealing with modern-but classical in origin-physical organic chemistry. The first chapter by H. Maskill is a valuable introduction to problems of the relations between the kinetics and mechanisms of organic reactions, providing a perspective for the issues presented in the whole volume. Then, T.W. Bentley discusses how to investigate mechanism reactions by studies of their products. The next chapter by L.M. Canle, H. Maskill, and J.A. Santaballa presents a wide spectrum of experimental methods for investigating kinetics. Important problems of relationships between the mechanism and rate law are presented by the same authors in the next chapter. Kinetics in the multiphase systems is also an important field of current research and is reviewed by J.H. Atherton.

O. Hammerich reviews electrochemical methods for investigating the organic reaction mechanism with a presentation of specific features of these methods in experimental practice. P.R. Schreiner answers the question: How can computational chemistry help to elucidate the reaction mechanisms? He covers funda-

mental ideas and basic approximations employed in quantum chemistry, the methods of which are a theoretical basis for most approaches in this field. Recent developments in calorimetry and IR-ATR spectroscopy for investigating the reaction kinetics are reviewed by U. Fischer and K. Hungerbuehler.

Detection of intermediates in the chemical reaction is a very important research problem, particularly as it concerns their structure. C.I.F. Watt presents an expert opinion on this problem by answering the question What is an intermediate? and by providing the reader with a systematic approach to the description of the mechanism of chemical reaction. Another important review deals with the investigation of catalysis by acids, bases, and enzymes written by A. Williams.

All review articles are well referenced in two ways: they refer the reader to some other, earlier review articles and monographs, and they provide references to the most important original papers. This volume is a very valuable source of comprehensively presented knowledge in the field kinetics and mechanisms of organic reactions. It is recommended to all researchers involved in the kinetics and mechanical studies of chemical reactions in chemistry, chemical technology, biochemistry, and materials science.

Tadeusz Marek Krygowski is a professor in the Department of Chemistry at the University of Warsaw.

### continued from page 25

# **Internet Connection**

in various ways depending on what information is requested and will generate the data in XML, PDF, or other formats upon demand.

We believe that a project blending database, XML, HTML, and PDF formats in one place is unique and represents a useful source of information about the elements, readily available to the chemistry community.

## Acknowledgments

Many people contributed to this project. The bulk of the data entry and the Periodic Table poster was the responsibility of Jennifer Imel, a senior B.A. Chemistry student at Eastern Kentucky University. The original XML fragments were populated by nine undergraduate and graduate students who took my course. Most element slides available now on our website were completed by students in General Chemistry I as part

of our initial project titled "Learn About the Elements." Images displayed on the slides were provided by Fred Bayer.<sup>6</sup> I am grateful to all who participated and continue to work on this useful project.

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# **Modern Physical Chemistry** for Advanced Materials

by Yuriy Kholin and Nikolay Mchedlov-Petrossyan

On 26-30 June 2007, V. Karazin Kharkiv National University (Kharkiv, Ukraine) hosted the international conference Modern Physical Chemistry for Advanced Materials (MPC'07). The conference celebrated the 100th birthday of Soviet chemist Nikolai Izmailov (1907-1961). The conference was organized under the auspices of IUPAC by V. Karazin Kharkiv National University in cooperation with the L.M. Litvinenko Institute of Physico-Organic Chemistry and Coal Chemistry of the National Academy of Sciences of Ukraine (Donetsk, Ukraine) and the Physical Chemistry Department of the Ukrainian Chemical Society.

Christian Amatore, a member of the French Academy of Sciences, acted as chairman of the International Scientific Committee and as IUPAC representative. Nikolay Mchedlov-Petrossyan (V. Karazin Kharkiv National University) was cochairman. Anatoliy Popov, a member of the National Academy of Sciences of Ukraine and director of the L.M. Litvinenko Institute of Physico-Organic Chemistry and Coal Chemistry, was chairman, and Vil Bakirov, Rector of V. Karazin Kharkiv National University, served as cochairman of the International Organizing Committee.

Altogether, 170 participants from 23 countries took part in the conference, representing Austria, Belarus, Brazil, Bulgaria, Denmark, France, Japan, Hungary, Germany, Greece, Iran, Korea, Romania, Norway, Russia, Slovakia, Slovenia, Spain, Sweden, Taiwan, Ukraine, the United Kingdom, and the United States. Both well-known experts and young researchers were present.

The conference started with the presentation of the book Scientific Heritage of N.A. Izmailov and Topical Problems of Physical Chemistry, (V. Lebed, N. Mchedlov-Petrossyan, and Yu. Kholin, eds.; V. Karazin Kharkiv National University, 2007, 675 p.) to the academic community and mass media. The book contains reminiscences about Izmailov's life and scientific activity, several papers and reviews



Christian Amatore, chairman of the International Scientific Committee.

in relevant fields of physical chemistry written by contemporary authors, and the second edition of the monograph V. Aleksandrov "Acidity of Non-Aqueous Solutions."

The conference program included 65 plenary, keynote, and oral papers and 111 poster presentations. The main emphasis was on the contribution of physical chemistry to modern materials science. The presentations were organized around the following main

- supramolecular chemistry, nanochemistry, hybrid materials, microreactors, and sensors
- physical chemistry of true and organized solutions (thermodynamics, physico-organic chemistry, electrochemistry, and spectroscopic methods)
- physical chemistry of interfaces, catalysis, and chromatography
- theoretical methods in modeling molecules and molecular assemblies; computer synthesis and design of materials



Conference participants in front of the main entry to V. Karazin Kharkiv National University.

The chairpersons of plenary sessions and conference symposia were V. Berezkin (Russia); N. Funasaki, M. Hojo, and E. Osawa (all from Japan); C. Reichardt and W. Schröer (Germany); E. Tyihak (Hungary); A. Walcarius (France); and V. Cheranovskii, A. Doroshenko, O. Gryzodub, V. Kalchenko, G. Kamalov, A. Korobov, L. Loginova, A. Popov, and V. Zaitsev (all from Ukraine).

During the oral and poster sessions there were many fruitful discussions and exchanges of opinions and papers. New contacts were established, and plans for cooperation were designed.

Information about the conference was published on the internet <a href="http://izmailov2007.univer.kharkov">http://izmailov2007.univer.kharkov</a>. ua> and in local mass media. In addition, the proceedings will appear in special issues of the journals Pure and Applied Chemistry, Molecular Liquids, the Russian Journal of Physical Chemistry, and Functional Materials (Ukraine).

During the conference, the mantle of Doctor Honoris Causa was delivered to Yoshitaka Gushikem of Brazil, a member of the International Scientific Committee of the conference. It is appropriate to mention that the senate of V. Karazin Kharkiv National University on 29 November 2007 gave the same award to another out-

> standing chemist and a member of the International Scientific Committee, Christian Reichardt (Germany).

> The conference's social events included a classical music concert, a welcome party, a conference reception, sightseeing tours of Kharkiv, an excursion to Chuguev (native city of the great Russian painter II'ya Repin), and an all-day excursion to the typical Ukrainian city of Poltava.

The conference would not the European

have been possible without the generous help of IUPAC, V. Karazin Kharkiv National University, Association for Chemical and Molecular Sciences, the Alumni Association of V. Karazin Kharkiv

National University, the State Scientific Institution "Institute of Single Crystals" (Kharkiv), the Scientific Council of Analytical Chemistry of the National Academy of Sciences of Ukraine, AllConferences.Com, Kharkiv University graduate S.N. Goncharov, the companies SAGMEL, Inc. (United States) and Zdorovye (Ukraine), and an anonymous sponsor from Russia.

After the conference, the organizing committee received many letters from participants congratulating it on this successful international event.

Yuriy Kholin <kholin@univer.kharkov.ua> was the chairman of the Local Organizing Committee and was a member of the International Organizing Committee. He is vice-rector and the head of the Materials Chemistry Department of V. Karazin Kharkiv National University.

Nikolay Mchedlov-Petrossyan <Nikolay.O.Mchedlov@univer.kharkov.ua> was the cochairman of the International Scientific Committee for this conference. He is the head of the Physical Chemistry Department of V. Karazin Kharkiv National University.

# **Physical Organic Chemistry in** Latin America

by Adriana B. Pierini

The Ninth Latin American Conference on Physical Organic Chemistry (CLAFQO9), held 30 September-5 October 2007 in Los Cocos in the province of Córdoba, Argentina, was locally organized by researchers from the faculty of Chemical Sciences at the Universidad Nacional de Córdoba (UNC) and from the faculty of Exact, Physical, and Natural Sciences from the Universidad Nacional de Río Cuarto (UNRC).

CLAFQO9 was the ninth in a series of conferences held several times in Brazil (1991, 1995, 1997, 2003, 2005) and also in Argentina (1993), Chile (1999), and Venezuela (2001).

The opening ceremony included speeches by Eduardo Humeres (Universidade Federal de Santa Catarina, Florianópolis, Brazil), a member of the Latin American Committee; Norma Nudelman (Universidad Nacional de Buenos Aires, Faculty of Exact and Natural Sciences) representing IUPAC; and Adriana B. Pierini (Faculty of Chemical Sciences, UNC), chair of the organizing committee. In addition, a message by Ambassador Kalimi Mworia, director of the International Cooperation and Assistance Division of the Technical Secretariat of the Organisation for the Prohibition of Chemical Weapons was delivered.

Attendees had the opportunity to participate in a comprehensive program that included 15 plenary lectures, 6 invited lectures, 31 oral presentations, and 2 poster sessions with 117 posters. To promote the participation of attendants in all activities, the conference was not divided into individual or parallel sessions. Instead, its scientific program was designed to cover



Anatoliy Popov, chairman of the International Organizing Committee.

most of the different areas in modern physical organic chemistry, including:

- theoretical and experimental interpretation of reaction mechanisms in solution and in the gas phase
- reaction dynamics
- electron transfer in redox enzymes
- development of bioinspired electron-transfer systems and their applications to renewable and clean energy resources
- photocatalysis as an environmentally friendly synthetic path to chemicals
- photobehavior of protein-bound drugs and drug phototoxicity
- design and development of new materials from gels to nanostructured blocks
- generation of metal and semiconductor nanoparticles by organic photochemistry
- design of nanoparticles and small molecules as probes for cellular function
- radical chemistry
- reactions in organized systems
- mimicking of biological processes
- enzymatic catalyses
- enzymes reactions
- oxidative DNA damage

A list of plenary and invited lectures can be found on the conference website listed below. In total, 176 registered participants joined the conference from 16 countries: Argentina, Brazil, Canada, Colombia, Costa Rica, Chile, France, Germany, Italy, Israel, Japan, Pakistan, Spain, the United States, the United Kingdom, and Venezuela. Peru, Uruguay, Taiwan, Hungary, Poland, and Romania participated through joint contributions. Conference abstracts are available at <www.fcg.unc. edu.ar/claf9>.

Of the registered participants, 68 were Ph.D. stu-

dents, reflecting CLAFQO9's emphasis on providing an international forum for young researchers and advanced students to present their scientific work. As part of this effort, 29 fellowships were awarded by the local organizing committee to partially cover the costs of the Ph.D. students' registration and hotel accommodations. Two poster prizes were also



Participants in the opening ceremony of CLAFQ09 (from left): Roberto A. Rossi, Adriana B. Pierini, Gladys B. Mori de Moro, and Norma Nudelman.

awarded to young researchers (doctoral candidates and/or recently graduated Ph.D.s). The poster quality was assessed by an academic committee led by Rita H. de Rossi (Argentina), Juana Chessa de Silber (Argentina), Julio Mata Segreda (Costa Rica), Oswaldo Núñez (Venezuela), and Eduardo Humeres (Brazil). The following CLAFQO9 poster prizes were awarded at the conference:

- Photolysis of Asymmetric Diazenes. From Solid State to Supercritical Fluids: A Cage Effect Study, Pablo A. Hoijemberg, et al.
- Physical Characterization of Spin-Coated Films of Luminescent 2,1,3-Benzothiadiazole-Based Liquid Crystalline Compounds, André A. Vieira, et al.



Participants in the Ninth Latin American Conference on Physical Organic Chemistry (CLAFQ09).

The conference provided an ideal opportunity for Latin American participants to attend lectures by prominent researchers, giving them valuable insights into current and future trends in the field. In addition, many Latin American scientists had the opportunity to exhibit their works to a prestigious audience of international scientists. All told, the conference promoted the exchange of ideas in both formal and informal ways, allowed for the renewal of personal contacts among friends and colleagues from Latin America and all over the world, and encouraged the development of new joint projects.

In sum, the following objectives for the conference were fully met:

- the promotion of physical organic chemistry in Argentina, Latin America, and the world at large
- the enhancement of scientific interactive relationships among groups from Latin America and group leaders from other countries
- the fostering of physical organic chemistry in the new generations of graduate students
- the promotion of peaceful uses of physical organic chemistry

It is important to mention the large number of representatives from different institutions who attended the conference, especially from Argentina. It was the first time that scientists from such varied universities and research centers from throughout Argentina were able to participate in CLAFQO. This coming together has paved the way for further intercommunication and integration of research groups and institutions, as well as for the future of physical organic chemistry in Argentina, Latin America, and many other nations.

In the closing ceremony, C. Dale Poulter (University of Utah, United States) outlined the importance and main contributions of the physical organic chemistry to the advance of science.

The organizers wish to thank the Universidad Nacional de Córdoba and Río Cuarto, CONICET, the National Agency for the Promotion of Science and Technology, the Argentine Association for Physical Chemistry Research, and the Argentine Society for Research in Organic Chemistry for their invaluable sponsorship and financial assistance.

The conference also received financial support from the Organisation for the Prohibition of Chemical Weapons and the *Journal of Organic Chemistry*, a publication of the American Chemical Society. IUPAC's sponsorship is greatly appreciated; it allowed the conference to earn IUPAC's academic recognition and gave it international scope. A special issue of

the Journal of Physical Organic Chemistry is being devoted to CLAFQO9, and participants have been invited to submit manuscripts containing original unpublished work.

CLAFQ010 is to be held in Florianópolis, Brazil, 2009. It will be organized by Faruk Nome from the Federal University of Santa Catarina, Florianópolis, Brazil.

Adriana B. Pierini <adriana@fcq.unc.edu.ar> is a professor and CONICET researcher in the Department of Organic Chemistry, Faculty of Chemical Sciences, Universidad Nacional de Córdoba, Argentina.

# Infrared Spectroscopy Applied to Biological and Biomimetic Systems

# by Andrea Gómez-Zavaglia

The International Workshop on Infrared Spectroscopy Applied to Biological and Biomimetic Systems: From the Isolated Molecule to the Cell (FTIR 2007) was held 5–7 November 2007 at the Goethe Institute, Buenos Aires, Argentina.

As the conference demonstrated, the versatility of infrared spectroscopy has stimulated a substantial number of new developments in experimental techniques and instrumentation as well as in theoretical methods, specialized software, and computational equipment. Nowadays, the combination of experimental and computational spectroscopic approaches has become the new methodological paradigm to undertake advanced research on biologically relevant problems.

For this reason, the main purpose of FTIR 2007 was to facilitate discussion about all aspects of infrared-spectroscopy-based methodologies and their applications in physics, chemistry, biology, biochemistry, biophysics, and medicine. To fulfill this aim, topics such as Infrared Spectroscopy of Cells and Tissues, Low Temperature Infrared Spectroscopy, Infrared Spectroscopy of Lipids and Proteins, and Infrared Spectroscopy in Molecular Diagnostics and in Biomimetic Systems were discussed.

In summary, the aim of FTIR 2007 was to cover the most outstanding breakthrough of FTIR (Fourier Transform InfraRed) spectroscopy methodology (from isolated-molecules to cells) and diffuse it among young researchers. The meeting helped elucidate the applications of FTIR in different, but still intercon-

nected fields: from the isolated molecule to whole cellular systems, from the structure and reactivity of simple biological molecules to the investigation of the functionality of enzymes, nucleic acids, and membranes, from looking at the fundamental physics underlying simple molecular processes to uses in clinical biochemistry.

The participation of well-known specialists in different domains of infrared spectroscopy provided a complete overview about the full potential of the technology. In this sense, it is worth mentioning the interesting lectures of Henry Mantsch, Dieter Naumann, Jürgen Schmitt, Rui Fausto, Ronald Birke, Urs Peter Fringeli, José Luis Arrondo, Jean-Marie Ruysschaert, and Klaus Brandenburg among many others, which provided different points of views on the potential of FTIR. These perspectives definitely enriched the discussions after each session.

At the same time, the informal ambience of this event also helped stimulate the interaction among participants. This is particularly important for encouraging open-minded younger scientists.

The decision to hold the meeting in a "far away" city such as Buenos Aires represented a big challenge. For this reason, it was gratifying to have spectroscopists from Asia, Africa, Europe, and America take part in the meeting. This created a valuable human richness that was much appreciated by the participants.

During this three-day meeting, 9 plenary lectures, 10 semiplenary lectures and 10 short talks took place. The first day was dedicated to the biomedical applications of vibrational spectroscopy. The second day, to the physicochemical characterization of biologically relevant compounds, and the third day, to the infrared spectroscopy of lipids and proteins.

IUPAC's financial support enabled the conference organizers to cover some of the travel costs of the plenary lecturers and also to provide grants to younger participants, which constituted one of the most fundamental objectives of this meeting (to provide an opportunity for young scientists to meet internationally recognized scientists in this field and to learn from them and develop their chosen professions).

The success of the meeting encouraged the organizers to consider FTIR 2007 as the first in a series of meetings. After the event, the idea of organizing a meeting in approximately two years was accepted by everyone.

Andrea Gómez-Zavaglia <angoza@interar.com.ar> is a professor at the Universidad de Buenos Aires, Argentina.

# Malta III—Research and Education in the Middle East

by John M. Malin

Known as "Malta III," the third conference in the series, Frontiers of Chemical Sciences: Research and Education in the Middle East, was held in Istanbul, Turkey, from 8-13 December 2007. This remarkable series of meetings continues to bring scientists from Middle Eastern countries and other nations together to discuss common problems and encourage collaborative research in the fields of energy, materials science, natural products, green chemistry, education, and environment.

Middle Eastern participation in Malta III was the largest yet of the three conferences, named for the island of Malta where the first two meetings were held. Of the 90 participants, 67 were from Middle Eastern countries: Bahrain (1) Egypt (9), Iran (8), Iraq (3), Israel—both Arabs and Jews (12), Jordan (9), Kuwait (2), Lebanon (4), Palestinian Authority (10), Saudi Arabia (1), Turkey (4), United Arab Emirates (4). Other nations represented included Canada, Germany, Norway, Switzerland, UK, and USA.

As in Malta I and II, a multinational organizing committee chaired by Zafra M. Lerman from Columbia College Chicago produced the event. Cosponsoring organizations were the United National Educational, Scientific, and Cultural Organization (UNESCO); IUPAC; Columbia College Chicago; American Chemical Society (ACS), Royal Society of Chemistry (RSC), and Gesellschaft Deutscher Chemiker (GDCh).

## **Plenary Sessions and Workshops**

A special feature of the conference was a series of six plenary lectures by Nobel Laureates Aaron Ciechanover (Israel), Richard Ernst (Switzerland), Roald Hoffmann (USA), Tim Hunt (UK), Walter Kohn (USA), and F. Sherwood Rowland (USA).

The first plenary session was chaired by Hasan Salah Dweik of Al Quds University (Palestinian Authority). In his address, entitled "The Nature of Energy," Peter Atkins (Oxford University, UK) presented an enlightening overview of how the qualitative concepts of energy, entropy, temperature, space, and time have lead to development of the quantitative tools of thermodynamics.

Ameen Farouk M. Fahmy, Ain Shams University (Egypt), chaired the second plenary session in which Richard Ernst (Nobel Laureate, E.T.H., Switzerland)

discussed development of an important spectroscopic technique, "The Importance of the Fourier Transformation in Spectroscopy: From Monsieur Fourier's Calculus to Medical Imaging." In the third plenary session, chaired by Mehdi Jalali-Heravi, Sharif University of Technology (Iran), Tim Hunt (Nobel Laureate, Imperial Cancer Research Fund, UK), discussed "The Cell Cycle and Cancer," reviewing the genetic components of carcinogenesis and the current limits of chemotherapy.

The chair of the fourth plenary session was Hanan Malkawi of Yarmouk University (Jordan) who introduced Nobel laureate F. Sherwood Rowland (Nobel Laureate, University of California at Irvine, USA), who spoke on "Greenhouse Gases and Global Climate Change." Plenary session five was called to order by Venice Gouda, Former Minister of Research (Egypt). He introduced Roald Hoffmann (Nobel Laureate,



Cornell University, USA) who spoke on "Chemistry Bonds: Three intensive workshops for young scientists in the Middle East," detailing three workshops he has organized in the Middle East for younger scientists.

Plenary session six was opened by session chair Sultan Abu-Orabi, Tafila Technical University (Jordan). He introduced plenary speaker Walter Kohn (Nobel Laureate, University of California Santa Barbara, USA), who spoke on "The Power of the Sun" and screened his recently produced video on the uses and importance of solar cells. Alfred Abed Rabbo, Bethlehem University (Palestinian Authority) began plenary session seven

by introducing Aaron Ciechanover, (Nobel Laureate, Technion-Israel Institute of Technology, Israel), who presented "On the Middle East and Converting the Ubiquitin System Into a Drug Platform."

The organizers ensured that Malta III would provide significant opportunities for interpersonal interactions. A poster session featuring some 42 presentations was carried on throughout the conference. Discussions centered on the posters during morning and afternoon coffee breaks as well as before and after dinner. One evening, Roald Hoffmann led an informal session of Middle Eastern dancing.

Middle Eastern and other scientists presented their results in workshops that were held throughout the conference and which served to develop conference recommendations. The Workshop on Environment: Air and Water Quality was co-chaired by Charles Kolb (USA), Hanan Malkawi (Jordan), and Abdallah Al-Zoubi (Jordan). Catherine Costello (USA), Samira Islam (Saudi Arabia), and Stanley Langer (UK) chaired the Workshop on Medicinal and Natural Products. The Workshop on Nanotechnology and Materials Science was chaired by Mukhles Sowwan (Palestinian Authority) and Zehra Sayers (Turkey). The workshop on Science Education and Green Chemistry was co-chaired by Boshra Awad (Egypt), Farouk Fahmy (Egypt), and Ann Nalley (USA), while the workshop on Alternative Energy Sources was co-chaired by Hani Khouri (Jordan) and Hassan Zohoor (Iran).

### **Conference Recommendations**

Workshop participants urged that the conference recommendations should be carried forward to the appropriate agencies and authorities. An especially urgent need for action was identified during the Environmental Workshop when Yousef Abu-Mayla, director of the Water Research Center at Al-Azhar University in the Gaza Strip, described widespread degradation of water quality in Gaza. Malta III attendees unanimously adopted a communiqué to urge action on this issue (see Mar-Apr 2008 *Cl*, page 18) to be addressed to regional and world leaders. The document has been delivered to Tony Blair, envoy to the Middle East working on behalf of the USA, Russia, the United Nations, and the European Union.

Other important recommendations from the workshops are summarized as follows:

 A project to build a canal from the Red Sea to the Dead Sea to generate hydroelectric power and also to replace water lost by evaporation from the Dead Sea should be carried forward. Middle

Eastern scientists will be looking for help from the world community in analyzing, evaluating, and potentially planning and executing this bold project. In general, large collaborative projects should commit a significant fraction of the project's budget to support active graduate and postdoctoral student participation in the project.

- Regional alliances of scientists and engineers with environmental skills should be established to evaluate regional environmental issues and to advise policy makers and other stakeholders on management strategy and technological development systems.
- Innovative, efficient desalinization technologies should be developed, including more efficient separation filters and/or membranes; solar-powered water purification/desalinization systems, and improved analyses of potential environmental impacts and opportunities for more efficient utilization of desalinization byproducts.
- Better methods should be developed for collecting, cleaning, treating, and appropriately reusing domestic, agricultural, and industrial waste and grey water.
- Regional drinking and wastewater treatment and testing methods should be standardized.
- Water use strategies must be greatly improved for Palestinian areas. For example, an isotopic ratio analysis of lead in Gaza waters should be carried out to determine sources of lead pollution.
- Energy problems for Middle Eastern nations should be addressed by vigorous pursuit of solar energy options tied in with global efforts to develop alternative energy sources. Energy development should be continued in Jordan to extract oil by retorting bituminous rocks.
- Workshops and other educational programs are needed to foster development of alternative energy R&D, sustainability and Green Chemistry, disposal of chemical waste, discussion of scientific method and ethics of science in the Middle East, strategic plans to attract students to scientific careers, and to educate scientists from multiple disciplines in the areas of pharmacology. toxicology, pharmacy and clinical chemistry.
- Centers of excellence should be developed for chemical analysis and structure determination of natural products. Programs should be instituted to enable short-term exchange visits by faculty, students and postdoctorals.
- A Middle East Virtual Campus should be estab-

- lished to facilitate exchanges of ideas among Middle East scientists. Web-based resources are needed, including a directory of laboratory equipment and expertise plus weblinks connecting to freely available databases and software.
- Newly-developed theories in chemical education should be integrated into Middle East curricula. Green chemistry, energy, nanotechnology, medicinal chemistry should be combined with the Systematic Approach in Teaching and Learning Chemistry for assessing secondary and tertiary students' skills. Newly developed curricula should be made available to secondary schools.
- Commercial pharmaceutical companies should be encouraged to perform R&D onsite in the relevant countries.
- Kuwait and Saudi Arabia should be encouraged to join the SESAME project. Individual scientists need to be made aware of how they can participate.

### **Concluding Observations**

As Zafra Lerman, chair of the Organizing Committee, noted, "Science can be a powerful force for bringing together cultures, and the Malta conference series is a powerful example." The organizers met their principal goals by raising the necessary funds, then bringing an increased number of Middle East chemical scientists together safely. Discussions took place among Israeli, Arab, Persian, and Western participants, which, as with Malta I and II, can be expected to lead to fruitful bi-national interactions. Malta III was successful for the following reasons:

- Chemists from the Middle East contributed strongly to the sessions. Workshops were an important activity designed to stimulate future research cooperation. A substantial number of women scientists from the Middle East participated.
- According to participants surveyed at the close of Malta III, the topics addressed were relevant to twenty-first century chemistry in the region. Middle East scientists chaired all sessions.
- Participants stated that the opportunity for interaction with other Middle East scientists was the most important aspect of the conference. They were pleased to meet colleagues from Saudi Arabia, Kuwait and Iran, and they called for greater participation by scientists from Syria, Turkey, Iraq, Qatar, and Yemen.
- The poster session stimulated informal discussion

- by inviting all conferees to present research.
- Participants were enthusiastic. They voted overwhelmingly that a "Malta IV" conference should be held in 2009 and said that they would recommend it to their colleagues.

### **Acknowledgements**

In addition to the sponsoring organizations, financial support was provided by the Camille and Henry Dreyfus Foundation, Humboldt Foundation, ChemRAWN XIV—ACS Green Chemistry Institute, the U.S. Civilian Research and Development Foundation (CRDF), the U.S. Department of Energy, the U.K. Government, the University of Mainz, the Chemistry Division of the American Association for the Advancement of Science, and some 39 individual donors. The conference organizing committee led by Zafra M. Lerman, thanks the distinguished lecturers and six Nobel Laureates for their participation. The help of many others is acknowledged with gratitude.

John M. Malin < jmalin023@verizon.net> was the chair of the CHEMRAWN committee in 2007: he has been involved with the committee since 1998.

# The Future of Science Is through Its Students

by Laure Joumel

Every year, the Chemical Heritage Foundation, based in Philadelphia, Pennsylvania, USA, holds the Ullyot Public Affairs Lecture, which emphasizes to the general public the positive role that the chemical and molecular sciences play in our lives. In November 2007, Shirley Tilghman, president of Princeton University spoke on "Strategy or Happenstance: Science Policy in the USA." Tilghman chose the topic, she said, "because I believe in the profound importance of scientific discovery and innovation as an engine for economic and social progress."

To make her point, Tilghman enumerated the remarkable impact that science had in the 20th century: the dramatic increase in life expectancy, particularly in infants; the reduction in infant mortality; the virtual eradication of some diseases, such as small pox through systematic world-wide vaccinations; the invention of household conveniences that have freed us from manual labor; safe drinking water and sanitation; the power of television, radio, and film to foster greater understanding among peoples of dif-

ferent cultures; and in the development of the Internet. She added: "It's been estimated by economists that upwards of 40 percent of the growth in the U.S. economy over the last 50 years has come from investments in fundamental research. What is remarkable is that most of these advances grew out of research in university laboratories and, often as not, research conducted by students and faculty pursuing knowledge for its own sake with no commercial application in mind. This remarkable progress did not happen by chance, so not happenstance."

Next, Tilghman discussed the Program for International Student Assessment's (PISA) 2006 survey, which revealed a pessimistic picture for science in the USA. PISA is an evaluation of 400 000 15-year-old students from 57 countries. It is the result of collaboration between participating countries and the Organization for Economic Co-operation and Development (OECD). The survey revealed that for 93 percent of students, science is important for understanding the natural world, but only 37 percent said they would like to work in a career involving science. The survey's science

performance measurement showed that USA is in the 21st position out of 30, while Finland is number one, Belgium 13, and France 19.

While young people's motivations for science achievement goes down, paradoxically, the scientific budget follows. For the first time in 25 years, overall federal spending in the USA for academic research and development, after adjusting



Shirley Tilghman, president of Princeton University, delivers the 2007 Ullyot Public Affairs Lecture at the Chemical Heritage Foundation.

for inflation, fell in Fiscal Year 2006. In Fiscal Year 2004, federal funding in the physical sciences, as a fraction of GDP, was 54 percent less than in 1970. In engineering, it was 51 percent less. And although the total national R&D budget has been growing steadily

for many years, the ratio of government-to-privatesector investing has reversed itself, from the government providing two-thirds of the total budget 45 ago to one-third today.

Tilghman said, "This retrenchment in the support of science and engineering could not come at a worse time, there are dangerous signs that America's dominance in scientific competitiveness is at risk from newly rising economic powers, particularly in Asia." She added, "Nearly 60 percent of patents filed in the USA in information technology now originate in Asia. We are not only losing our edge in what could be considered old manufacturing industries, such as textiles, steel, and automobiles, we are losing ground in areas that are considered the 'new' thing. Darwin famously said that it is not the strongest who survives, or even the most intelligent, but the individual who is most responsive to change. And, to change we have to be investing in innovation and creativity."

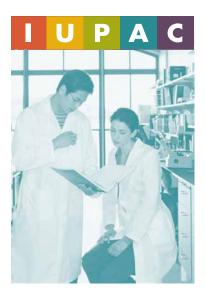
Then Tilghman also shared a worried feeling on a completely different—but just as important—matter: the age of scientists when they get their jobs. In the 1950s and 1960s, the research enterprise expanded and created the next generation of scientists and faculty members. Eventually the problem became how to produce fewer students without having a negative effect on scientific productivity. In physics, there was a nationwide effort on the part of the American Physical Society to decrease graduate admissions from the

1980s to 1990s to adjust to the fact that there were no longer jobs for its graduates.

"In my own field of life sciences" she explained, "no such agreement could be reached and the number of students didn't simply remain constant but, fueled by the National Institutes of Health (NIH) funding, continued to grow faster than the number of available jobs. Something had to give, and what gave was the length of time that students spend in training. This has resulted in young scientists who are in training well into their 30s, while their classmates from college are settling down, raising families, and adding to their pension plans. The average age of a first-time principal investigator at NIH is now 42.9 years. The age when you receive your first NIH grant. Aside from the personal cost to individual students, should we be worried that the late 30-somethings are still in training?"

In front of the large audience in Ullyot Meeting Hall at CHF, Tilghman concluded her talk with a warning: "There's a pressing need for intelligent and openminded discourse among scientists and policy makers so that together we can craft sound science policy for the United States at a time when its scientific preeminence is being challenged."

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# Where 2B & Y

# Physical Organic Chemistry

13-18 July 2008, Santiago de Compostela and A Coruña, Spain

The 19th IUPAC Conference on Physical Organic **Chemistry** will be held at the Universities of Santiago de Compostela and A Coruña, Spain, between 13-18 July 2008. The ICPOC series is dedicated to scientists active in the area of physical organic chemistry and reactivity and will cover the diversity of modern research in this area, emphasizing its interactions with other fields. The program will include plenary and invited lectures, oral communications, and poster presentations.

See Mark Your Calendar on page 39 for contact information.



www.icpoc2008.org

# Safe Food

# 24-27 September 2008, Novi Sad, Serbia

The significance of safe food production and consumption is becoming more widely recognized as the risks increase that industrial production food production will reduce its nutritive value. Even in highly developed countries, industrial food production



brings about new threats to human health. Although this issue is receiving more attention in developed countries, from scientists and the general public, the countries of the former Soviet Union are lagging far behind.

Since 2000, the **Ecological** Conference on Safe Food has been held in even years with the general aim of communi-

cating valid knowledge, supporting the exchange of opinions and experiences, and making such knowledge actionable. Conference organizers hope to accomplish the following:

- address, on a scientific-expert level, a wide range of key issues concerning safe food production and environmental consciousness
- discuss and assess the causes of ecological imbalance in conventional agricultural production, and the impact of various pollution sources on agricultural production at present

- offer practical solutions, based on scientific indicators and expert opinions, to help meet actual challenges and those that lie ahead
- give relevant proposals and suggestions for longterm strategic programs in food production (in industrialized, controlled, integral, alternative, and sustainable agriculture) without negative effects on human health and the environment

The conference is open to all issues concerning safe food, from the point of its production, to the point of consumption. Contributions are most welcome that point out good or bad practices, while validating factors affecting food safety and quality in the following subject areas:

- ecological factors and food production
- correct choice of seed (genetic) material
- status and preparation of soil as the basic substrate for the production of food and feed
- use of fertilizers and pesticides in integrated plant protection
- use of biologicals
- food processing technology
- economic aspects, marketing and packaging of safe food

For more information contact <ekopokret@eunet.yu>.



www.ekopokret.org.yu

# Macro- and Supra-Molecular **Architectures and Materials**

7-11 September 2008, Düsseldorf, Germany

Novel and functional polymer materials will play a key role in science and technology in the 21st century. As functional properties of polymers, which are crucial for controlled molecular architectures and systems, depend on a wide variety of parameters, a discussion of the actual knowledge and state-of-the-art approaches is very important.

The 4th International Symposium on Macro- and Supramolecular Architectures and Materials (MAM-08) will be held in Düsseldorf, Germany, from 7-11 September 2008. The objective of the symposium is to provide an interdisciplinary forum for scientists engaged in the full spectrum of research, development, and application. Furthermore, the current status and recent developments of new polymer materials and their applications will be discussed, particularly with respect to their macro- and supramolecularity. The meeting will provide an opportunity to overview the field by covering a wide range of topics. Themes have been selected to cover the whole area of research to facilitate interdisciplinary interactions in academic fields and industrial technology. The impact of the meeting is indicated by the number of prominent speakers from industry.

The symposium will bring together scientists from all over the world to present scientific and technological findings related to the areas of polymer chemistry (macromolecular) and extended molecular networks (supramolecular). By gathering engineers, material scientists, and inorganic, organic, and physical chemists, this event will offer a diversified view on these fascinating and versatile issues of science.

See Mark Your Calendar on page 40 for contact information.



www.chemie.uni-duesseldorf.de/Faecher/Organische\_Chemie/ OC2/ritter/MAM 08

# Challenges in Organic and **Bioorganic Chemistry**

22-25 July 2008, Berkeley, California, USA

The Ninth Tetrahedron Symposium will take place in Berkeley, California, USA, 22-25 July 2008. Eighteen renowned international speakers will present at the event (see website for list). The symposium is organized and hosted by Elsevier, publisher of Tetrahedron, Tetrahedron Letters, Tetrahedron: Asymmetry, Bioorganic & Medicinal Chemistry, and Bioorganic & Medicinal Chemistry Letters.

The organizing committee is composed of Stephen Martin (chair), University of Texas, USA; Dale Boger, Scripps Research Institute, USA; Bruce Ganem, Cornell University, USA; Jim Thomas, University of Manchester, UK: and Yoshi Yamamoto, Sendai University, Japan.

The purpose of the event is to promote the Tetrahedron series of journals to the international community, and to provide an opportunity for scientists to meet and interact with the editors in a scientific setting.

### Comments from delegates at Tetrahedron 2007

"All the presentations were really good and interesting. The speakers were of a really high level. The conference was great."

"I found the line-up of speakers very impressive, and they were my single motivation to attend the conference. It was a good mix from very established speakers, whom I admire for their life-time achievement, and speakers from a younger generation whose talks were scientifically more informative."

"The quality was superb and the chemistry inspiring—I went back to work very enthusiastically and was full of great new ideas to try out-Thanks!"

"This reunion of so many great chemists was a total success and was extremely encouraging for chemistry's future."

www.tetrahedron-symposium.elsevier.com

# Nano-Bio & Clean Tech

27-30 October 2008 Burlingame, California, USA

The International Association of Nanotechnology is now accepting abstracts to be presented at the upcoming 5th International Congress of Nano-Bio & Clean Tech 2008. The conference will gather world class researchers, business executives, and engineers from over 30 countries and cover the following topics:

- nanomaterials
- nanoparticles
- nanodevices
- nanoelectronics
- nanofabrication
- MEMS & NEMS
- nanobiotechnology
- nano scale characterization
- standards & nomenclature
- nano tools
- molecular engineering
- nano manufacturing
- nanoparticles toxicology
- heath safety implications
- renewable energy
- biofuels
- photovoltaic
- hydrogen
- electric car



- sustainable energy public policy
- direct thermal energy conversion
- electrochemical conversion and storage
- nanostructured solar cell manufacturing
- intellectual property
- commercialization
- venture capital investment and other related
- intellectual property and technology transfer
- education & workforce training
- societal & environmental impacts
- capital funding and grants for start-up ventures

# Featured Session: Emerging Tech Investment Forum

This session will provide a unique opportunity for start-up companies to present their products, services, and business models to an audience of venture capitalists and private investors.



# **Chemistry Industry and Environment**

20-23 November 2008, Principality of Monaco

World CIA 2008, Chemistry, Industry, and Environment, is dedicated to the world of chemistry and its wide range of products. This international conference will showcase industrial chemical applications, products, and technologies for the environment. This vear, the event moves outside Italian borders to the Montecarlo's new multifunctional Grimaldi Forum. The conference will focus on the best technologies and will offer a favorable context within which to develop new ideas and opportunities, new research, materials. and manufacturing techniques.



# Mark Your Calendar

# 2008

IUPAC poster prizes to be awarded

### 2-6 June 2008 • Molecular Order and Mobility in Polymer Systems • Saint-Petersburg, Russia

6th International Symposium on Molecular Order and Mobility in Polymer Systems Prof. T.M. Birshtein, Institute of Macromolecular Compounds, Russian Academy of Sciences (IMC RAS), Bolshoi pr. 31, Saint-Petersburg, RU-199004 Russia, E-mail: birshtein@imc.macro.ru

# 22-27 June 2008 • Organic Synthesis • Daejeon, Korea 🛣

International Conference on Organic Synthesis (ICOS-17)

Prof. Sung Ho Kang, Department of Chemistry, KAIST, Daejeon 305-701, Korea, Tel.: +82-42-869-2825, Fax: +82-42-869-2810, E-mail: shkang@kaist.ac.kr

## 29 June-4 July 2008 • Macro 2008 • Taipei, China 😓

Polymers at Frontiers of Science and Technology

Conference Secretariat, MACRO 2008, Department of Chemical Engineering, National Tsing-Hua University, 101, Section 2, Kuang-Fu Road, Hsinchu, 30013 Taiwan, Tel.: (03) 5713131 ext. 33683, Fax: (03) 5715408, E-mail: acsu@mx.nthu.edu.tw

# 6-11 July 2008 • Solid State Chemistry • Bratislava, Slovakia

8th Conference on Solid State Chemistry

Dr. Milan Drabik, Ceramics Department, Institute of Inorganic Chemistry, Slovak Academy of Sciences, SK-84536 Bratislava, Slovakia, E-mail: uachmdra@savba.sk, Tel.: +421 (7) 5941-0474, Fax: +421 (7) 5941-0444

## 13-18 July 2008 • Biodiversity and Natural Products • Charlottetown, Prince Edward Island, Canada 🛣

International Conference on Biodiversity and Natural Products (ICOB-6 & ISCNP-26)

Prof. Russell Kerr, Department of Chemistry, University of Prince Edward Island, 550 University Avenue Charlottetown, PEI C1A 4P3, Canada, Tel.: + 1 902 566 0565, Fax: +1 902 566 0632,

E-mail: rkerr@upei.ca. Ann Worth, Conference Manager, E-mail: info@iupac-icbnp2008.com

# 13-18 July 2008 • Physical Organic Chemistry • Santiago de Compostela, Spain 🛣

19th International Conference on Physical Organic Chemistry (ICPOC-19)

Prof. J. Ramón Leis. Faculty of Chemistry. Universidad de Santiago de Compostela. E-15782 Santiago de Compostela, Spain, E-mail: qfirleis@usc.es, Tel.: +34-98-156-3100, Fax: +34-98-159-5012

# 17-19 July 2008 • Chemistry of Vanadium • Lisbon, Portugal

6th International Symposium on Chemistry and Biological Chemistry of Vanadium

Prof. João Costa Pessoa, Centro de Química Estrutural, Instituto Superior Técnico-TU Lisboa, Av. Rovisco Pais P-1049-001 Lisboa, Portugal, Tel.: +[351] 218 419 268, Fax: +[351] 218 464 455, E-mail: joao.pessoa@ist.utl.pt

# 20-24 July 2008 • Polymer Colloids • Prague, Czech Republic

2008 Prague Meetings on Macromolecules—48th Microsymposium "Polymer Colloids: From Design to Biomedical and Industrial Applications"

Dr. Daniel Horák, Institute of Macromolecular Chemistry, Heyrovský Sq. 2, CZ-162 06 Prague 6, Czech Republic, Tel.: + 42 029 680 9260, Fax: +42 029 680 9410, E-mail: horak@imc.cas.cz

### 27-31 July 2008 • Solubility Phenomena • Dublin, Ireland 🛣

13th International Symposium on Solubility Phenomena Including Equilibrium Process (ISSP-13)

Prof. Earle W. Waghorne, Chairman, School of Chemistry & Chemical Biology, University College, Belfield, Dublin 4, Ireland, Tel.: +353 1 716 2132, Fax: +353 1 716 2127, E-mail: earle.waghorne@ucd.ie

# 27 July-1 August 2008 • Carbohydrates • Oslo, Norway

24th International Carbohydrate Symposium (ICS 2008)

Prof. Berit Smestad Paulsen, School of Pharmacy, University of Oslo, P.O. Box 1068 Blindern, N-0316 Oslo, Norway, Tel.: +47 22 856 572, Fax: +47 22 854 402, E-mail: b.s.paulsen@farmasi.uio.no

### 27 July-2 August 2008 • Bioanalytical and Biochemistry • San Juan, Puerto Rico

XXVIII Latin American Chemistry Congress and PRCHEM 2008 (FLAQ-2008)—Bioanalytical and Biochemistry: Their Role in Bioscience and Biotechnology

Dr. Ethel Rios-Orlandi, Chairman of the Scientific Program, Colegio de Quimicos de Puerto Rico, 52 Hatillo Street, San Juan 00918, Puerto Rico, Tel.: +1 787-763-6070, Fax: +1 787-758-2615, E-mail: cqpr@cqpr1941.org or flaq2008@cqpr1941.org

# Mark Your Calendar

# 28 July-1 August 2008 • Photochemistry • Gothenburg, Sweden 🏶

XXII IUPAC Symposium on Photochemistry

Prof. Devens Gust, Department of Chemistry and Biochemistry, Arizona State University, Tempe, AZ, USA, 85287-1604, USA, Tel.: +1 602 965 4547, Fax: +1 602 965 2747, E-mail: gust@asu.edu

# 3-8 August 2008 • Chemical Education • Pointe aux Piments, Mauritius 🎡

20th International Conference on Chemical Education: Chemistry in the Information & Communications Technologies Age, (20th ICCE)

Dr. Ponnadurai Ramasami, Department of Chemistry, University of Mauritius, Reduit, Mauritius, E-mail: p.ramasami@uom.ac.mu

# 3-8 August 2008 • Chemical Thermodynamics • Warsaw, Poland 👺

20th International Conference on Chemical Thermodynamics

Questions should be addressed to E-mail: info@icct2008.org. Comments, concerns, proposals, etc., should be addressed to E-mail: secretariat@icct2008.org.

# 7-11 September 2008 • Macromolecular Chemistry • Düsseldorf, Germany

Macro- and Supra-Molecular Architectures and Materials

Prof. Dr. D. H. Ritter, Institute of Organic Chemistry & Macromolecular Chemistry, Universität Düsseldorf, Universitätsstrasse 1, D-40225 Düsseldorf, Germany, Phone: + [49] 211 811 4760, Fax: + [49] 211 811 4788, E-mail: mam08@uni-duesseldorf.de

# 8-11 September 2008 • Macromolecules & Materials • Kruger National Park, Mpumalanga, South Africa 🛣

10th Annual UNESCO/IUPAC Conference on Macromolecules & Materials

Prof. Ronald D. Sanderson, Department of Chemistry & Polymer Science, University of Stellenbosch, Stellenbosch 7602, South Africa, Tel.: +27 (21) 808-3172, Fax: +27 (21) 808-4967, E-mail: rds@sun.ac.za

# 14-20 September 2008 • Green Chemistry • Moscow, Russia 🏶

2nd IUPAC Conference on Green Chemistry

Prof. Valery V. Lunin, Chairman Russia Chemistry Department, M.V. Lomonosov Moscow State University, Leninskiye Gory 1, build. 3, 119992 Moscow Russia, Tel.: +7-495-9394575, Fax +7-495-9394575, E-mail: vvlunin@kge.msu.ru

### 14-20 September 2008 • Humic Substances • Moscow, Russia

14th Meeting of the International Humic Substances Society (IHSS-14)

Prof. Irina V. Perminova, Department of Chemistry, Moscow State University, 119992 Moscow, Russia, E-mail: jperm@org.chem.msu.ru, Tel: +7 495 939 5546, Fax: +7 495 932 8846

### 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

### 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

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- Professor Peter G Bruce
   University of St Andrews, UK
- Professor Dr Ben L Feringa
   University of Groningen, The Netherlands
- Professor Sir Harold Kroto
   Florida State University, USA
- Professor Sir J Fraser Stoddart Northwestern University, USA
- Professor Vivian W W Yam
   The University of Hong Kong, Hong Kong
- Professor Richard N Zare Stanford University, USA

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