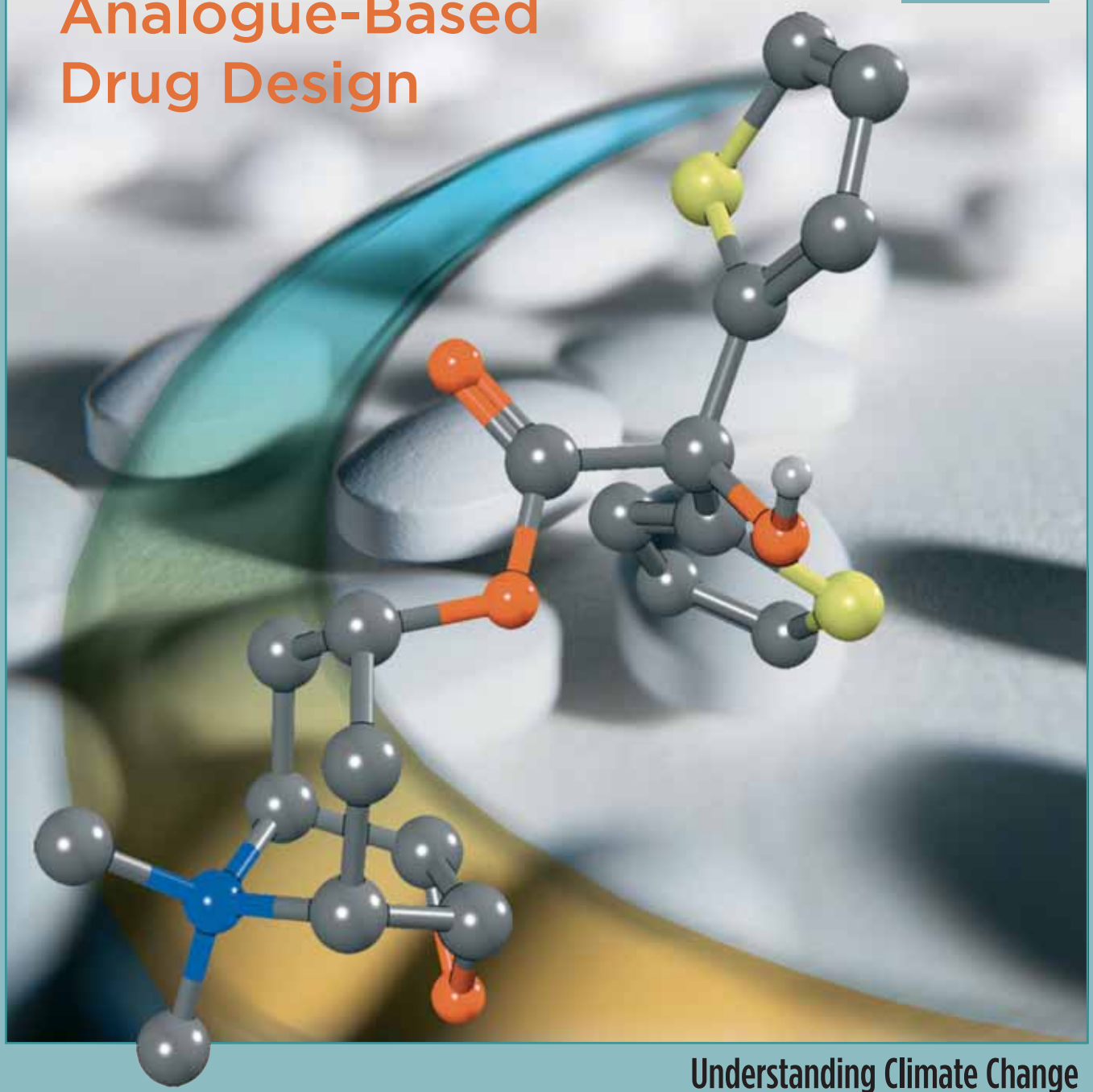
The News Magazine of the
International Union of Pure and
Applied Chemistry (IUPAC)

CHEMISTRY International

July-August 2010
Volume 32 No. 4

Analogue-Based Drug Design



Understanding Climate Change

Chemistry 2.0

CHEMISTRY International

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www.iupac.org/publications/ci

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Printed by:
Cadmus Communications, Easton, PA, USA

Subscriptions
Six issues of *Chemistry International* (ISSN 0193-6484) will be published bimonthly in 2010 (one volume per annum) in January, March, May, July, September, and November. The 2010 subscription rate is USD 110.00 for organizations and USD 50.00 for individuals. Subscription orders may be placed directly with the IUPAC Secretariat. Affiliate Members receive *CI* as part of their Membership subscription, and Members of IUPAC bodies receive *CI* free of charge.

Periodicals postage paid at Durham, NC 27709-9990 and additional mailing offices. POSTMASTER: Send address changes to *Chemistry International*, IUPAC Secretariat, PO Box 13757, Research Triangle Park, NC 27709-3757, USA.

ISSN 0193-6484

From the Editor

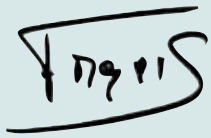
While joking over our iconic "C" logo for the 2011 International Year of Chemistry, a friend of mine suggested that the "C" should be for Communication. "Yes," I replied, and from there we went on debating the many communication challenges we all experience in our professional and personal worlds.

We agreed that most chemists are not at the forefront of exploiting communication opportunities readily available in the online world. Fortunately, we noted, there are "explorer chemists" out there who do adapt selected technologies, which then percolate into our world, bringing unforeseen benefits to how we do things. It may be true that other scientific communities embrace new tools much faster, but in the end, I am sure we will get there. A new generation of chemists will undoubtedly bring along new tools, some transferred from other social contexts.

The discussion changed course when we realized that there are many folks, including specialists in communication, who are very interested in the behavior of chemists and their challenges in communicating. One key reference I recommend reading is a recent commentary titled "Communicating Chemistry" by Theresa Velden and Carl Lagoze, published in *Nature Chemistry* on 1 December 2009 (Vol 1, p. 673–678; doi:10.1038/nchem.448), and the related white paper.

Related to this topic, I was delighted by the suggestions from Javier Garcia-Martinez, one of our youngest members and an advocate of new communication opportunities. On page 4, he offers *CI* readers his views on Chemistry 2.0 and how new social networking tools can bring folks closer to chemistry. Javier's enthusiasm is palpable. He shares with us his favorite sites and apps, and highlights the many educational opportunities.

To keep IUPAC moving forward, relevant, and sustainable in today's changing world, new voices and views are necessary. I believe it is important that we keep bringing into our community a wide range of expertise and folks with "outside the box" attitudes and ideas, and that we continue to embrace global diversity. Since IUPAC functions through the hard work of dedicated volunteers worldwide, it is up to everyone to step in, get engaged, and bring change. A perfect opportunity for involvement is upon us: IUPAC is requesting nominations for members of all divisions and commissions (see p. 19 for details). This only happens once ever two years and meanwhile, for now, in an old fashioned way, you won't find us on Facebook, nor be able to follow us on Twitter.



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The image depicted on the cover is a reproduction of the book cover from *Analogue-based Drug Discovery*—see feature on page 12; reproduced with permission from Wiley-VCH.

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The IUPAC Presidency—A Happy Recollection

by Jung-Il Jin

The importance and responsibility of the IUPAC presidency and the multiplicity of its functions are greater than one might imagine. Yet, these are rightfully reflected in the status of its position. In my term as president, I was helped and aided by a large group of capable and dedicated people: members of the Executive Committee, Bureau, and staff, as well as the IUPAC Officers.

After assuming the office of president, it immediately became evident that frequent and effective communication among and between the various branches of IUPAC and its constituent members is essential for the big machine of IUPAC to operate effectively. I quickly became aware that communications between IUPAC and the NAOs and ANAOs needed significant improvements. To this end, the Membership Relations Committee was formed earlier within the Bureau and already is functioning. Moreover, the Council Meetings, held every two years, do not provide sufficient opportunity for sharing ideas and deep discussions among IUPAC and NAO representatives. Such opportunities inevitably will help focus more of IUPAC's and the NAOs' attention to areas of mutual concern.

While the IUPAC presidency carries much prestige, it also requires considerable work and effort to respond to the opinions, and needs, of the local units. Frequently, constituents would like to see IUPAC leadership make faster decisions and take firm actions without delay. Because of this, a wide range of criticisms are steadily reaching the IUPAC Bureau. On the other hand, a continual stream of information, supporting various positions, also reach the Bureau, aiding in making better decisions.

By necessity, IUPAC is conservative: it maintains standards, making changes only when necessary. This carries through to the presidency, making it necessary to be exceedingly prudent when coming to important decisions. Inevitably, this made me consider my presidential roles:

- as an innovative leader bringing in progressive changes urged by the less patient reformist groups
- as the guardian of history and tradition, resisting the temptation for hasty change
- as a democratic negotiator restraining himself from expressing his personal philosophy and opinions

In a short time, I learned that the IUPAC president should maintain a relatively flexible stance whenever he or she has to consider any controversy. A president with a charismatic personality and viewpoint can be less desirable than one with a practical mind. My own principle on taking any leadership position, regardless of rank, is not simply to be satisfied by the honor of being in the leader's chair but, through diligent involvement and devotion, to do my best to elevate the position.

A tour of the IUPAC website <www.iupac.org> makes apparent the diversity of the Union's services and operations—and the structural complexity of the organization. Then, there are the differing circumstances and opinions of the NAOs, the diversity of opinions on various technical matters. These are made more difficult by the inevitable communication barriers that exist in any large international organization.

The president's term of office can make it stressful to make progress and reach goals in his/her limited period of service. Fortunately, in my case at least, this feeling disappeared relatively quickly because of the good advice provided by the superior analytical minds of the IUPAC officers and staff. Among them, the secretary general and the executive director occupy the most important and demanding positions. To keep the president constantly supplied with information, advice, and opinions, is only part of their jobs.

The wisdom of one's predecessors is another invaluable asset for the president. But besides these, the president should keep his or her eyes and ears wide open might they miss any suggestions or complaints coming from any corner of the organization, including the NAOs and the members.

The president also has duties and obligations outside the sphere of IUPAC. As the leader of IUPAC, the president must maintain friendly relations with other international organizations and collaborate with them on areas of mutual interest. He or she also must represent the Union in dealing with other chemical organizations outside of IUPAC and present chemistry to the people of the world, in general. As a consequence, the president must maintain a significant degree of fairness and impartiality in such extra-organizational

dealings. I felt the pull of external demands on IUPAC to expand its role as a scientific leader in dealing with questions of international concern, particularly the sustainable development of the world community. There is no doubt that IUPAC should be more proactively involved in global affairs, utilizing its capacity to mobilize the experience, knowledge, and capabilities of its constituents.

The cooperation that has just begun between IUPAC and the United Nations is an outstanding example of this and we are hopeful it will become the cornerstone for further contributions to the well-being of people and protection of the planet. The president's enthusiasm alone is inadequate to sufficiently raise IUPAC's visibility, impact, and international status. To do this, it is necessary to improve the Union's financial position. Money will be needed to become more deeply involved in a wider range of global problems. Therefore, I feel that a significant role for the president is to strengthen the financial capabilities of the constituent units. Increasing the number of member countries is another important responsibility. IUPAC undoubtedly will do its utmost during the International Year of Chemistry, 2011, to improve its worldwide recognition and image as a leading voice for the international chemistry community.

My experience has taught me that the IUPAC presidency requires keen insight, vision, and courage to cope with contemporary and future global issues. It also involves proselytizing and convincing the world that chemistry is "our life, our future." Any leader without the strong support and cooperation of his or her constituents will be doomed, like an eagle without wings. Happily for me, and for the new office holder, the IUPAC presidency is blessed with the unstinting support and cooperation of its constituents.

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Stamps International

See also www.iupac.org/publications/ci/indexes/stamps.html

The Wizard of Protein Crystallography

Dorothy Crowfoot Hodgkin, a pioneer of protein crystallography and Great Britain's first female Nobel laureate, was born in Cairo, Egypt, almost exactly a century ago, on 12 May 1910. She received her undergraduate degree from Somerville College at Oxford and, after carrying out her doctoral research with famed crystallographer J.D. Bernal at Cambridge, she returned to her alma mater and started her independent career in 1934.

The molecular structures of a string of important biomolecules of unprecedented complexity at the time, including penicillin and vitamin B_{12}, were elucidated within the next three decades, and her ingenuity and resourcefulness were recognized with the 1964 Nobel Prize in chemistry. Far from slowing down, Hodgkin solved the structure of insulin in 1969, concluding a piece of work that she had started almost 35 years before. She devoted a good part of her time in the 1970s and 1980s to a wide range of peace and humanitarian causes, primarily in developing countries, and she remained active in the field of protein crystallography until her death in 1994.

The stamp illustrated here honors Hodgkin and is part of a set of 10 stamps issued in the United Kingdom earlier this year to celebrate the 350th anniversary of the Royal Society. The stamps portray 10 distinguished Fellows of the Society, one for each 35-year period of its history, going all the way back to Robert Boyle. Although Hodgkin is the only woman in the exclusive cohort, she is certainly in good company since the eclectic group also includes the likes of Isaac Newton, Benjamin Franklin, Joseph Lister, and Ernest Rutherford. The upper half of the stamp depicts the electron density levels in the three-dimensional structure of vitamin B_{12} (cyanocobalamin), with three of the four pyrrole subunits (labeled A, B, and D) that make up the corrin ring surrounding the central cobalt ion and the 5,6-dimethylbenzimidazole and cyanide groups included in the structural diagram.

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

Chemistry 2.0
Creating Online Communities

by Javier Garcia-Martinez

How things have changed since we were kids. Nowadays, teenagers spend almost as much time watching TV as using social networking websites, technology that did not exist just a few years ago. More precisely, accordingly to a survey of over 1200 students organized by the National School Boards Association in the USA, 9- to 17-year olds in the USA spend 10 hours a week watching TV compared to 9 hours a week on web-based social networking activities. However, when our kids network online, they are much more active and innovative—creating content, sharing information, and blogging—than when they watch TV.[1]

This generation is totally into the web. In the USA, an astonishing 96 percent of students who have online access report that they have used social networking technologies. Fairly new technologies, such as chatting, text messaging, blogging, Facebook, and MySpace, are part of the daily lives of the kids who fill our classes. And it's not all about sharing music or organizing a plan for next weekend. Nearly 60 percent of our students use social networking to discuss education-related topics, and more than 50 percent specifically discuss schoolwork to support their education.[1]

Recognizing the potential risks of irresponsible use of the web, there is great potential in the new social networking technologies to reach our kids using their own language and help them find their own interests. In many cases, this simply consists of using *their* channels of communication to share information. In other cases, it means creating opportunities for them to share and create content that is useful for *them*. Doing so, will allow students to discover their own passions and share their own interests with kids from all around the world.

According to one study, students using the web 2.0 have excellent communication, creativity, collaboration, and leadership skills and technology proficiency.[1] Their natural interest in new technologies makes them ideal candidates to learn and share more about science and technology. Many educational institutions realize that using the web 2.0 they can reach this targeted audience. The Massachusetts Institute of Technology has put 1900 courses online. Hundreds of videos and additional educational material can be downloaded for free as part of the MIT OpenCourseWare initiative launched in 2002. iTunes U, part of Apple's iTunes Store, launched in 2007, already has over 75 000 files from universities from all around the world available to download for free. And of course, there is Wikipedia, 15 million articles written collaboratively by volunteers around the world, which has changed the way we share and look for information.

Additionally, professional chemical associations such as the American Chemical Society (ACS) or the Royal Society of Chemistry (RSC) have created a wonderful set of web 2.0 initiatives. On 15 March 2010, the ACS Mobile Application "ACS Mobile" became available on Apple's iTunes store. The new application provides readers with a live stream of peer-reviewed research content from across the spectrum of ACS journals right in their cell phones. More recently, Molecule of the Week, a popular feature on the ACS website since 2001, has been launched as a Mobile App. A new molecule is delivered to subscribers' iPhones each week for them to guess what each molecule is, based on an image and the clue supplied.

Both the ACS and its flagship journal, the *Journal of the American Chemical Society* (JACS) are now on Facebook, both with thousands of followers. These sites are regularly used to announce events, hold discussions, and provide breaking news, making them probably the fastest and most up-to-the-minute way to know what is going on in chemistry. But there is much more, the JACS beta site is a truly web 2.0 expe-

From Web 1.0 to Web 2.0

The term web 2.0 is typically used to define a new generation of websites characterized by community content creation, user-centered design, and interactive collaboration. Some typical web 2.0 applications include social-networking sites, wikis, and blogs. The web 2.0 is based on the goal of moving from a web-as-information-source to a web-as-participation platform in an effort to build a more participatory web. According to Wikipedia, "A web 2.0 site allows its users to interact with other users or to change website content, in contrast to noninteractive websites where users are limited to the passive viewing of information that is provided to them."

rience, with podcasts, mobile applications, and online interviews about new chemical discoveries, published weekly.

The Royal Society of Chemistry also has a wonderful set of web 2.0 initiatives, like the RSC and *Chemistry World* blogs. Personally, I am a big fan of its podcast on the chemical elements, *Chemistry in its Element*, as I am of *Distillations*, the "extracts from the past, present, and future of chemistry" from the Chemical Heritage Foundation.

Nature.com is another excellent web 2.0 site. Nature Network is probably the best example of the use of social networking technologies to connect scientists. Whereas, *Nature Chemistry's* blog, The Sceptical Chymist, is one of the best of many blogs on chemistry that are available today, including the very popular CENtral Science of *Chemical and Engineering News*. Chemistry@nature.com brings together all of the chemistry content from Nature Publishing Group in one place. A unique resource mainly for the academic chemistry community, this attractive site effectively integrates various services such as chemistry news, research highlights, blog posts, and podcasts in one single place.

But online social networking also can be used to solve problems, really big problems. InnoCentive is a global innovation marketplace, and a great example of open-innovation, where creative minds solve some of the world's most important problems for cash awards up to USD 1 million. Hundreds of "challenge problems" can be found on its website for anyone to solve. For example, if you manage to come with an environmentally friendly method for converting a di-olefin to a mono-alcohol, a cash award of USD 10 000 awaits you. For those posting the challenge, called the "seekers," there are greater benefits. For a relatively modest amount of money, they can get hundreds of minds thinking about an innovative solution. Some of their challenges have over 1000 active "solvers" thinking about how to crack the problem. Of course, the number and quality of the "solvers" are of critical importance. That is why InnoCentive has teamed up with Nature Publishing Group to offer its readers the opportunity to participate in research and development challenges through an online platform called Open Innovation Pavilion. There are many other open innovation companies, each one with its own characteristics and focus, like NineSigma, Starmind, yet2.com, MillionBrains, and Tekscout, One Billion Minds, PRESANS, and Innoget, among others.

Even well-established large chemical companies like Procter & Gamble are now fully engaged in online open innovation: 50 percent of product initiatives at the company already involve significant collaboration with outside innovators. Now, they are asking everyone to become their "partner of choice" for solving their R&D challenges, which range from polymers to cosmetics, by participating in their P&G Connect + Develop web portal. As stated in its presentation video: "click the link below and open the door."

The Periodic Table of the Web 2.0.

Sure, the academic and professional community has plenty of web-based resources, and the institutions and publishers behind them are quickly expanding their online services as they attract more well-targeted costumers. Unfortunately, there are fewer high-quality educational 2.0 websites for students, who are actually the ones who use the networking sites more frequently. A good example of the great potential of high-quality and entertaining content is the series of YouTube videos called Periodic Videos, a collection of short videos, originally on the elements of the Periodic Table but now also on useful or just curious molecules and other chemical-related topics, made by a team of chemists from Nottingham University. This effort is led by Martyn Poliakoff, who is a fairly popular figure now, since his videos have been seen over 8 million times. Periodic Videos is now a truly 2.0 platform, with its own website and YouTube channel, a great behind-the-scenes blog, a Facebook group, and, of course, a Twitter presence, with hundreds of followers. Unsurprisingly, many of them are quite young and passionate about chemistry. Just the right audience, connected with the click of a mouse, all sharing content, interests, and common projects.

As part of the 2009 U.S. National Chemistry Week, the American Chemical Society's Division of Chemical Education started a nationwide project on Facebook to build public awareness and interest in the periodic table through the "Become a fan" feature of Facebook.[2] The organizers of this initiative asked students to support their favorite element of the Periodic Table. More than 7 000 students joined the project. Regardless of which element won the competition, and yes, it was carbon, this was an extraordinary opportunity for thousands of students to revisit the Periodic Table, learn more about the properties of the chemical elements, and delve into the wonders of their favorite element. The University of Greenwich Department of Chemistry probably has the most popular Facebook group dedicated to chemistry, with more than 11 000 followers who share news, discussions, and future events about chemistry. Not bad at all.

The beauty and novelty of web 2.0 over conventional sources of information is that the content is collectively created by its users. Nowhere is this more obvious than in Wikipedia, a web-based, collaborative, multilingual encyclopedia project built by millions of volunteers. The Wikipedia Chemistry Portal, created by people who share a common passion for chemistry, contains feature articles, selected biographies, news, and plenty of information about chemical techniques, chemical databases, and online resources.

Most of us were attracted to chemistry because of the colors, explosions, and surprises of chemical demonstrations. Unfortunately, many students do not have access to such wonderful experiences. The web now has excellent online resources, with stunning videos and safe demonstrations for the classroom. Some of the experiments can even be safely performed at home. The websites Chemistry Comes Alive!, of the *Journal of Chemical Education*, and Delights of Chemistry, of the Leeds University Department of Chemistry, are just two great examples of how to attract students and create enthusiasm for chemistry among the next generation through online videos of chemical demonstrations.

Many traditional chemistry demonstrations can be found in *Classical Chemical Experiments*, a book from the RSC that can be downloaded for free from LearnNet, an RSC website for teachers and students of chemistry at all levels. This website provides access to products and resources, most of them available for free.

A number of virtual chemistry labs offer interactivity and web 2.0 content. The Virtual Lab of

2.0 opportunities for the 2011 IYC

The three goals of the 2011 IYC, namely i) increase the public appreciation of chemistry in meeting world needs, ii) encourage interest in chemistry among young people, and iii) generate enthusiasm for the creative future of chemistry have in common the need to reach a large audience, mostly young people. Coordinating and promoting this effort is really where the web 2.0 can help by providing a large and inclusive platform, efficient networking tools, and enabling technologies for everybody to contribute. It is the perfect tool to encourage people to participate; they can spontaneously self-organize in groups of interest, share ideas, and post them for everyone to know about.

This is exactly what chemistry2011.org is trying to do with the National Nodes and the Participation area, where everyone can share ideas, post activities, or announce events. There are more than 1000 members already registered, who have contributed dozens of ideas. But there is much more that can be done to make the site a truly web 2.0 experience. Perhaps a video welcoming all visitors and asking for ideas and their active participation, interviews with famous scientists supporting the IYC, news, podcasts, a blog, and links to social networking sites.

Last summer, I conducted an experiment to check the potential of social networking sites to reach young people from all around the world. I opened a Facebook group on the International Year of Chemistry, and I sent a message to my Facebook friends asking them to join. After a week, there were already more than 100 members; today the group has almost 1000. Most of them I have never met. Many are college students, some even younger. We share information, videos, ideas, and an excitement for chemistry, and the group is quickly growing as we get closer to the beginning of the year 2011.

Oxford University, launched eight years ago, contains interactive organic mechanisms, a virtual laboratory (LabChem), and many chemical demonstrations.

For those of us who love the periodic table, WebElements.com is a must-visit site. The site is not only an inexhaustible source of information about the chemical elements and their main compounds, but also an excellent source for news on everything related to chemistry through the WebElements Nexus. In addition, the site showcases books on chemistry, and much more, like T-shirts, mugs, games, and posters for periodic table maniacs.

Sure, all of this is great, but not everybody has access to a computer. What about those living in low-income countries? One solution may involve cell phones, which are widely available in many developing countries. It is estimated that in India alone, there are over 545 million cell phones and it is estimated that by 2015 there will be over a billion.[3,4] Both the cell phone and internet providers know this and are working together to change the way we use our cell phones. Content providers are working quickly to make sure they also show up on the screens of our smart phones. As mentioned before, the professional chemical associations and many universities are providing applications for smart phones (apps) that complement their online offerings. This is a new and increasingly more important platform through which to promote science among the youth and increase public appreciation of chemistry. As *Chemistry World* recently stated "Mobile chemistry has arrived." And it has done so with excellent apps for publishers, educators, and students, such as online journals, study guides, chemical calculators, databases, and much more.[5]

The web is a huge and user-friendly source of quickly updated content, but more important, it is a great platform for interacting with people sharing common interests. What better place for education to occur. The web doesn't substitute for the invaluable personal interaction between teacher and student, but it does open up new opportunities that, without being a silver bullet, should be added to our ammunition to increase public understanding and appreciation of chemistry, especially among the new generation of scientists and technologists.

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Perspectives on Chemistry and Global Climate Change

by Fulvio Zecchini and Pietro Tundo

Global warming is one of the most appropriate case-studies to introduce to students since it involves extensive problem-based learning and class discussion. In order to understand such phenomenon, students must explore several aspects of chemistry, physics, and biology in a holistic and multidisciplinary fashion.

A number of IUPAC projects are focused on educating students and the general public about the central role of chemistry in understanding and devising countermeasures to the global warming phenomenon. The Organic and Biomolecular Chemistry Division's Subcommittee on Green Chemistry has completed three projects concerning the translation, updating, adaptation, and distribution of a monograph on global climate change for secondary schools. Read more in the sidebar below.

Another IUPAC project, entitled Visualizing and Understanding the Science of Climate Change (2008-043-1-050), is currently underway. A project of the Committee on Chemistry Education, it treats the topic from a different perspective using Internet-based communication/educational tools. (See page 11.)

A Timely Topic

Based on data from the Intergovernmental Panel on Climate Change (IPCC Report 2007), there is firm evidence of global warming, and proof that human activity is the major cause. According to the panel, mean global surface temperature has increased by 0.7 °C ca. from 1906–2005. In recent decades, glaciers have begun melting faster all over the world, and the snow cover has been shrinking in the Northern Hemisphere. Model-based estimates of sea-level rise for the decade 2090–2099 range from 0.18 to 0.59 metres compared to the average for 1980–1999.

It is widely accepted by the scientific community that global warming is caused by the emission of anthropogenic greenhouse gases (GHGs) into the atmosphere. In 2007, the IPCC completed an analysis of 2004 climate data and found that CO_2 remains the most prevalent GHG, accounting for 76.7% of emissions (56.6% derived from the use of fossil fuels, 17.3% from deforestation, and 2.8% from other sources),

Teaching about the Role of Green Chemistry

by Fulvio Zecchini, Aurelia Pascariu, Patrizia Vazquez, Ligia Maria Moretto, Anthony Patti, Panayotis Siskos, Pietro Tundo

Originally published in 2004 in Italian, *Il Cambiamento Globale del Clima* (*Global Climate Change*) was written by Fulvio Zecchini and Pietro Tundo of the Consorzio Interuniversitario Nazionale "La Chimica per l'Ambiente" (INCA). Meant as an integrative educational tool, the booklet was designed to introduce green chemistry to seniors at secondary schools and to university freshmen. About 4000 copies were printed and distributed for free to schools and universities all over Italy. The monograph was so appreciated by Italian teachers, students, and academic experts, that a wider distribution is planned.

So far, the Subcommittee on Green Chemistry has completed three projects to translate the monograph into the following five languages: English, Spanish, and Portuguese (project 2005-015-1-300); Romanian (project 2007-035-1-300), and Greek (project 2008-018-2-300). All these editions are being, or already have been, distributed to target groups in several countries and have received positive feedback from end-users.

The monograph is structured into five chapters. The first two are focused on the composition and structure of the atmosphere and on air pollutants. The third chapter is dedicated to the interaction between matter and radiation, namely between greenhouse gases (GHGs) and infrared rays (IR).

The fourth chapter is focused on the depletion of the ozone layer. Since several GHGs also act as ozone depleting substances (ODSs), this topic is somewhat related to global warming and is presented in a comparative way, underlining that, even if often the involved pollutants are the same, the phenomena are different and

followed by methane, 14.3%; nitrous oxide, 7.9%; and F-gases, 1.1%. In terms of the human contribution, the major impact comes from energy usage, 25.9%; followed by industry, 19.4%; forestry, 17.4%; agriculture, 13.5%; transport, 13.1%; residential and commercial buildings, 7.9%; and waste and wastewater, 2.8%.

Within such a framework, it is obvious that the solution to global warming lies in international politics, since the two most effective counteractions would be to switch to alternative energy sources as soon as possible and to immediately discontinue deforestation. From a practical point of view, the solution must be a mix of countermeasures (political and scientific) and adaptation/mitigation (society and economics).

The most recent international event on climate change was the Copenhagen conference held in December 2009. Its most significant result was that all major industrial countries, including USA and China, agreed that action is necessary immediately. Such was the core philosophy of the Kyoto Protocol, whose provisions in terms of GHG reductions have not been met on a global level.

According to the *Stern Review on the Economics of Climate Change*, inaction will have a major negative impact on the world economy, costing 5%–20% of global annual GDP. Conversely, the cost of reducing GHGs by 75% by 2050 is estimated at 1% of global GDP. Such a cut would result in a CO_2 concentration of 550 ppm. The concept is reported in The European Commission's white paper "Adapting to Climate Change: Towards a European Framework for Action" makes the same general argument about inaction/action costs.

Progress on reducing GHGs has been limited following the Kyoto Protocol since several countries do not agree on specific countermeasures, although all nations acknowledge that the main solution remains abating emissions of CO_2. In this context, the European Commission has set two targets for the European Union in its "Communication 20 20 by 2020": a reduction of at least 20% in GHGs and the production of 20% of energy from renewables. The targets are intended to limit temperature increase to 2 °C. In parallel, the USA is adopting diverse initiatives such as the Mandatory Reporting of GHGs Rule, to report emissions and collect data for future policy decisions, and The Climate Change Technology Program, to foster novel technologies for the reduction of GHGs. Hopefully, some concrete decisions will be taken at the forthcoming international UNFCCC meeting in Bonn (June 2010) and during the COP-16 in Cancun (December 2010).

take place in different levels of the atmosphere.

The final chapter of the monograph is dedicated to the consequences of global warming and possible countermeasures. Being a global problem, the "political" solution must be global as well. New and effective international protocols must be agreed on in order to replace the ineffective Kyoto protocol. Nonetheless, the message of this chapter is that actual solutions can only come from scientists and namely from chemists, who must develop solutions to abate CO_2 emissions caused by human activity.

Besides the five versions sponsored by IUPAC projects, two further adaptations/translations were realized. The Arabic edition was produced in 2006–2007 using European Commission funds derived from the Tempus Joint European Project "Sustainable Environmental Development, A Curriculum Development Project," in which INCA participated.

The success of the different editions of the monograph has helped improve the public perception of chemistry as a fundamental scientific tool to solve global environmental problems, such as climate change. Each clear demonstration to younger generations of how much chemistry occurs in everyday life and of its usefulness for environmental protection contributes to raising awareness of, and engendering an interest in, this fascinating and useful discipline.

Cover image from the book* Il Cambiamento Globale del Clima *(by Francesco Tundo).

All of the above-mentioned versions of the monograph may be downloaded for free at <www.incaweb.org/publications/papers.php>.

www.iupac.org/web/ins/2005-015-1-300

The Role of Green Chemistry

From a scientific point of view, some countermeasures are quite simple to imagine: the use of fossil fuels is the major concern, but technically speaking their complete substitution is not achievable at present. Photovoltaic and wind power are sustainable ways to produce energy, but the energetic yield per used surface of such technologies is too low, being insufficient for most civil and industrial applications. On the other hand, Green Chemistry can provide significant contributions to the abatement of CO_2 emissions. Following are just a few of the many ways Green Chemistry can help:

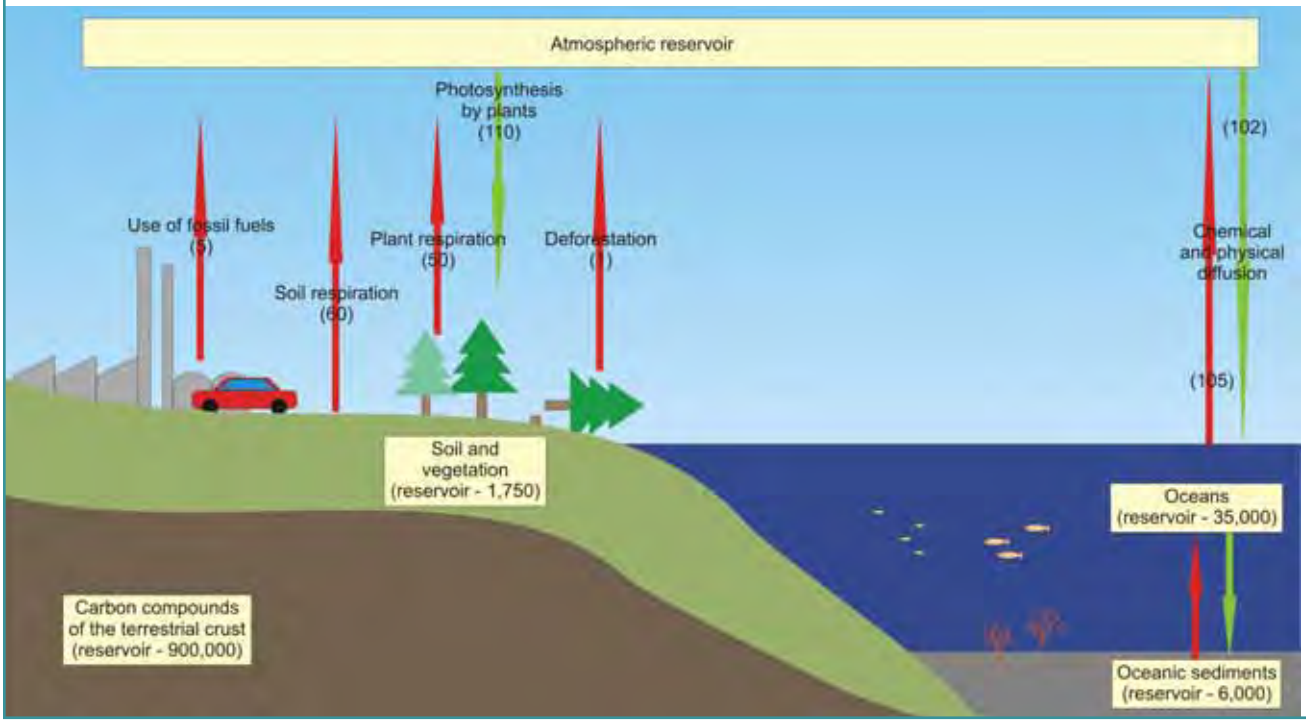
- creation of new products/processes/catalysts to reduce energy consumption and by-products/waste production
- development of products/processes/catalysts that don't use halogens or volatile organic solvents
- implementation of highly efficient processes
- use of CO_2 as a C1 building block
- generation of H_2, bio-hydrogen, from biomasses
- valorization of biomasses in bio-refineries
- syntheses of biodiesel from exhaust oils or from algae, bio-ethanol from lignin/cellulose biomasses
- creation of polymers from renewables
- use of novel materials for photovoltaic panels and fuel cells, and the improvement of battery capacity for electric vehicles
- improvement of catalytic converters for vehicles

Independence from fossil fuels still seems far off: on the one hand, we need more time, on the other hand, action is needed now. Some scientists recently proposed to adopt some extreme geo-engineering measures at a global level in order to actively capture CO_2 or to reflect part of the solar radiation. With respect to the last solution, Tom Wigley and Paul Crutzen (Nobel Prize in Chemistry in 1995) have proposed the deliberate periodic introduction of sulphate particles, aerosols, or precursors (dimethyl sulphide, sulphur dioxide, carbonyl sulphide, or hydrogen sulphide) in the atmosphere, in order to form reflecting/diffracting sulphate aerosols. If this were economically viable, Wigley thinks we could have a 20-year period during which the warming should be balanced by the reduced incoming radiation, allowing us more time to find proper long-term solutions.

Clearly, there are many aspects of chemistry that relate to climate change. For this reason, many if not most divisions of IUPAC are involved in the issue. Educational projects, such those discussed in this article, not only help make students better stewards of the planet, but they help develop the next generation of scientists and chemists who will, in all likelihood, still be developing solutions to this global problem.

Pietro R. Tundo <tundop@unive.it> and Fulvio Zecchini <zecchini_inca@unive.it> are both at the Università Ca' Foscari di Venezia, in Venezia, Italy. Tundo was president of the IUPAC Division on Organic and Biomolecular Chemistry for 2008–2009.

Simplified scheme of the carbon cycle. (Institute for the Application of Calculations, National Research Council, Napoli, Italy). Figure 3.9 reproduced from Il Cambiamento Globaled del Clima



Visualizing and Understanding the Science of Climate Change

by Peter Mahaffy

- It's -25º C today in Northern Alberta. Is climate change actually happening? How do we know?
- Our world has gone through ice ages and warm periods in the past—how is this any different?
- Why are CFCs such potent greenhouse gases? I thought they were important in stratospheric ozone depletion, not climate change.
- How does the absorption of infrared radiation by greenhouse gases in our troposphere actually lead to warming?
- Predictions of future climate are just based on models—I need to see data, not models, to believe that climate is changing.
- How do we know what the temperature was a half-million years ago?

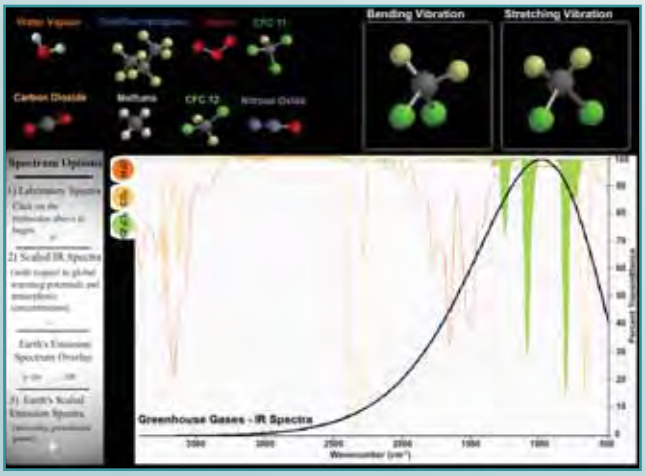
Over the past two years, students, teachers, and the general public have asked these and many other questions of the task group coordinating the project Visualizing and Understanding the Science of Climate Change. People are barraged by contradictory claims in the media about whether our climate is changing, and what is causing the changes that are seen. And at the heart of the answers to many of these questions is a basic understanding of chemistry and physics.

The IUPAC task group is working to produce 13 interactive lessons for global dissemination that will help students visualize and understand the science underlying climate change. The group started by researching common misconceptions that students have about climate change, and also fundamental principles of climate science needed to create climate-literate students and teachers.

A set of critically reviewed interactive lessons for 16–19 year old students is being created by integrating digital learning objects, developed at the King's Centre for Visualization in Science (Canada), with written materials prepared by The Royal Society of Chemistry (UK) and the American Chemical Society (USA). Task group members from IUPAC's Committee on Chemistry Education, UNESCO, and the Federation of African Societies of Chemistry will participate in the review of materials and facilitate dissemination through national and international networks.

To give readers a taste of the project, a screen capture from one of the interactive visualizations is shown to the right:

This interactive flash learning object helps to answer the third question in the list that began this report: Why are CFCs such potent greenhouse gases? Absorption of infrared radiation in the region between 700–1200 cm^{-1} causes excitation of the C-F stretching vibrational modes of CFC molecules. This happens to occur in a region of the IR spectrum where water and carbon dioxide, the two best known greenhouse gases are transparent (a spectral window). And so thinking of the earth as a giant IR source, CFCs absorb energies of IR radiation which have historically escaped into space, thus cooling our planet. This is also in a region of the spectrum close to the peak of earth's emission band (shown in the screen capture as a blue overlay).



This visualization from the King's Centre for Visualization in Science (Canada) shows how the IR signatures of a number of greenhouse gases collectively "close" the "IR window"—a phenomenon that occurs because different greenhouse gases absorb in different parts of the IR window.

When complete, the set of interactive lessons will provide tools for chemistry educators to make important connections in their classrooms to help students understand climate change, one of the defining challenges of the 21st century.

The first lessons will be completed over the next several months—meanwhile some examples of interactive digital learning objects, including the one featured above, can all ready be found at <www.kcvs.ca>.

For more information and comments, contact Task Group Chair Peter Mahaffy <peter.mahaffy@kingsu.ca>.

www.iupac.org/web/ins/2008-043-1-050

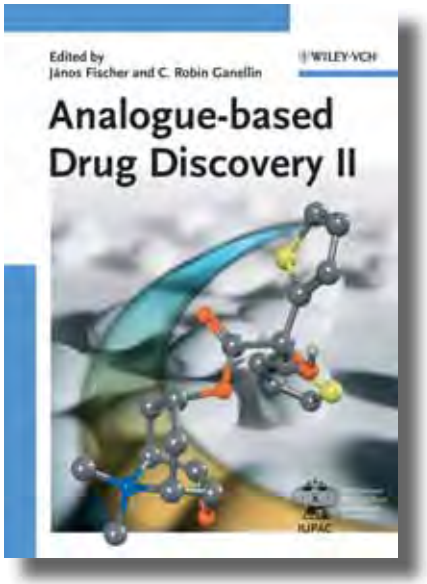
Analogue-based Drug Discovery

by János Fischer and C. Robin Ganellin

Analogy plays a very important role in scientific research, and especially in applied research. This is certainly true for the medicinal chemist searching for new drugs to treat diseases. The chemical structure and the similarities and differences in chemical and biological properties between compounds helps to guide the researcher in deciding where to position a new molecule in comparison to what is already known about other compounds.

The book *Analogue-based Drug Discovery,* published by Wiley-VCH in 2006, provided the first authoritative overview of past and current strategies for successful drug development by molecular modification of known leads was. This unique resource spanned the important drug classes in most major therapeutic fields. A second edition* was released this month that has a broader scope than the first and which not only contains descriptions of full analogues, but also includes several pharmacological analogues.

Medicinal chemistry is a relatively "young" science which has spanned the whole of the 20th century. In the first half of the century, new drug research was dominated by organic chemistry, and researchers sought improved drugs among structurally similar compounds. Full analogues dominated this kind of research. The latter half of the century saw a much greater contribution from biochemistry and pharmacology and many pioneer drugs were discovered. This opened the way for researchers to seek to improve upon these drugs by investigating analogues.



The first edition of *Analogue-based Drug Discovery* was focused on an important segment of medicinal chemistry, where an existing drug was selected as a lead compound and the research had, as a goal, to improve upon the lead by synthesizing and testing analogues. The chemical structure and main biological activity of such an analogue were often similar to the lead drug. Thus, the researchers generally sought a *structural and pharmacological analogue*, (more simply called a *full analogue*) or, if the pharmacophores were the same, a *direct analogue*. Usually the aim was to achieve an improved biological activity profile, with a greater potency.

The first edition included a description of many well-established analogue classes of drug that are indispensable nowadays for the treatment of peptic ulcer disease, gastroesophageal reflux disease, prevention of cardiovascular diseases (e.g,. antihypertensives, cholesterol-lowering agents, calcium antagonists, beta-adrenergic receptor blocking agents), pain (e.g., opioid analgesics), and many other diseases.

The last two decades, however, have witnessed great changes in the chemical and biological methods for generating a lead compound. Combinatorial chemistry affords many more compounds than traditional synthetic methods and these are tested very rapidly by high throughput screening (HTS) to deliver new hit and lead molecules. This procedure often opens the way to new types of structures for drug research, thereby decreasing the importance of having chemical similarity. At the same time, this improves the opportunity for novelty and therefore for patenting. This also gives rise to a greater need to compare the biological properties of these new lead compounds in order to arrive at the best *pharmacological analogue*.

Analogue-based Drug Discovery is not a simple research method, but it is a way of thinking that, in addition to organic synthesis, uses most of the procedures that are now available to medicinal chemists, such as the following:

- investigation of structure-activity relationships
- molecular modeling
- structure-based drug discovery

Analogue-based Drug Discovery II
Janos Fischer and C. Robin Ganellin (editors)
July 2010. 600 Pages, Hardcover, Handbook/Reference Book
ISBN-10: 3-527-32549-2 ISBN-13: 978-3-527-32549-8
Wiley-VCH, Weinheim

- fragment-based drug discovery
- early recognition of drug distribution properties and avoidance of potential toxicities

Analogue-based Drug Discovery has the merit that the therapeutic target is already validated, but it carries the hazard of potentially losing out to competitors who may start from the same approach at about the same time.

The new 2010 edition is comprised of three parts:

i. General Aspects of Analogue-based Drug Discovery
ii. Analogue Classes
iii. Case Histories

The opening chapter summarizes various ways to modify the properties of a drug to make a new drug analogue that improves patient drug therapy. There are 12 principles exemplified (see box p. 15), and within some of these principles there are several methods; hence, the chapter provides a broad overview.

A small number of the *pioneer drugs* remain without having successful analogues; we describe these by the term *standalone drug*. Among the most frequently used 100 drugs, nine such *standalone drugs* can be identified (see box to the right). Their history and present situation may be used to initiate new research activity to make analogues of them.

In addition to the traditional structure-activity relationship studies, molecular modeling is the most important method that the medicinal chemist can use to find a new drug analogue. The chapter discusses several useful examples of molecular modeling in analogue research.

Patenting activity is one of the basic tasks of drug research. Patents mostly concern a group of direct analogues; therefore, the first claim of a patent contains a general structure which describes this group of compounds. The chapter gives an overview of some of the issues that can affect the commercial protection of the discoveries made by medicinal chemists.

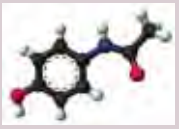
Analogue Classes

The second chapter on Analogue Classes describes the following nine categories of analogues.

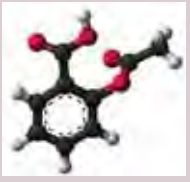
The discovery of dipeptidyl peptidase IV inhibitors opens a promising chapter for the treatment of type 2 diabetes. The *pioneer drug* sitagliptin has been followed by several analogues in order to obtain more potent and longer-acting derivatives.

Standalone Drugs Can Be Starting Points for Drug Optimizations

We analyzed the Top 100 most frequently used drugs and nine standalone drugs were identified, that is, pioneer drugs for which there are no effective analogues. These are the following drugs: acetaminophen, acetylsalicylic acid, aripiprazole, bupropion, ezetimibe, lamotrigine, metformin, topiramate, and valproate semisodium.



Acetaminophen is one of the oldest drugs, which even nowadays has a broad application as an analgesic and antipyretic agent. However, acute overdose can cause severe hepatic damage.

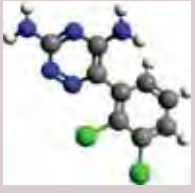


Acetylsalicylic acid (aspirin) is also one of the oldest drugs and, contrary to acetaminophen, its mechanism of action is partly known: it irreversibly inhibits the cyclooxygenase-1 enzyme. A more potent derivative with a better adverse effect profile would be advantageous.

Aripiprazole is a relatively new antipsychotic drug which acts as a dopamine partial agonist for the treatment of schizophrenia. A more effective drug is needed for the treatment of refractory patients, to improve treatment of negative symptoms and cognitive dysfunction.

Bupropion is a unique antidepressant drug. It is the first non-nicotine medication for the treatment of smoking cessation.

Ezetimibe is a relatively new cholesterol absorption inhibitor. Its mechanism of action was discovered only recently (2005). Analogue-based drug research is underway.



Lamotrigine, topiramate, and valproate are widely used anticonvulsant drugs, whose mechanism of action is not known. Several efforts have been made to find better analogues, so far without positive results.

Metformin is already an old standalone drug for the treatment of type 2 diabetes. It is used alone or in combination with new antidiabetic agents. Its mechanism of action is not known which makes it difficult to conduct an analogue-based drug research.

Serendipitious clinical observation afforded the *pioneer drug* sildenafil. Several analogues have been found that have optimized its properties (e.g., selectivity, duration of action).

Rifamycins are antibacterial antibiotics derived from fermentation. Analogue-based drug research afforded more potent derivatives. One of the derivatives, the poorly absorbed rifaximin, has a promising application for the treatment of irritable bowel syndrome.

Three analogue classes of monoterpenoid indole alkaloids are discussed: i) vincamine derivatives, ii) dimeric vinca alkaloid analogues, and iii) camptothecin analogues. The succesful natural product *direct analogues* are applied to the treatment of cerebral insufficiencies and cancer.

The natural product doxorubicin is an anthracycline antibiotic used to treat a wide range of cancers but it has a cardiotoxic adverse effect. The research into *direct analogues* had a goal to obtain drugs with a better therapeutic index.

Paclitaxel and epothilone analogues are also examples of how natural product drugs can be used to initiate analogue-based drug research to afford new drug analogues with better properties as anticancer agents.

The selective serotonin reuptake inhibitors (SSRIs) are pharmacological analogues that revolutionized antidepressant therapy. The structurally different SSRIs have different profiles for inhibiting uptake of the neurotransmitters serotonin, dopamine, and norepinephrine.

The modification of naturally occurring tropane alkaloids afforded the quaternary ammonium salts ipratropium and tiotropium, which are important drugs used for treating chronic obstructive pulmonary disease. Tiotropium—as a result of analogue-based drug discovery—has a longer duration of action that enables a once daily dosing.

The natural product adrenaline (epinephrine) was the starting point for drug research into β-adrenoreceptor agonists. From isoprenaline (isoproterenol) through the selectively acting salbutamol, and on to salmeterol, analogue research resulted in selective, more potent, and longer-acting analogues with different PK profiles, which are important drugs in asthma therapy.

Case Histories

In the final section of the book, eight case histories are described by their inventors.

Liraglutide is a new antidiabetic drug, an analogue of the natural product glucagon-like peptide 1. Among the acylated GLP-1 analogues liraglutide has been developed for a once-daily treatment.

Eplerenone is a spironolactone analogue for treating hypertension that has a greater selectivity for the mineralocorticoid receptor and reduced sexual side-effects.

Clevudine is a new drug for the treatment of the chronic hepatitis B virus (HBV) infection, which belongs to the class of nucleoside reverse transcriptase inhibitors.

Tipranavir is a new anti-HIV agent that is a protease inhibitor. The discovery of tipranavir used structure-based and fragment-based drug design and its long discovery process started from warfarin, which is a weak HIV-1 protease inhibitor.

Dasatinib can be regarded as a pharmacological analogue of imatinib. Dasatinib is more potent and it can be used in imatinib-resistant cases for the treatment of chronic myologenous leukemia (CML).

Lapatinib can be regarded as a pharmacological analogue of erlotinib. It is a tyrosine kinase inhibitor and was first approved for the treatment of solid tumors such as in breast cancer.

Venlafaxine is the first marketed serotonin/norepinephrine reuptake inhibitor and is used for the treatment of deep depression. Its active metabolite is desvenlafaxine, which has some advantageous properties (e.g., it has a more favorable metabolic profile compared to venlafaxine).

Rilpivirine is a new HIV-1 non-nucleoside reverse transcriptase inhibitor (NNRTI), an analogue of etravirine. Rilpivirine is highly potent also against strains that are resistant to the first-generation NNRTI drugs.

János Fischer <j.fischer@richter.hu> is a Ph.D. students working at Richter Plc. in Budapest, Hungary. C. Robin Ganellin <robin.ganellin@tesco.net> is a professor at University College London, in London, UK. Both have been members of the Chemistry and Human Health Division of IUPAC for several years and have collaborated on several projects involving international teams of experts.

www.iupac.org/web/ins/2008-013-1-700

Twelve Principles for Drug Optimization

1. Increasing Potency
   In the analogue class of the histamine H_2-receptor antagonists (cimetidine, nizatidine, ranitidine, roxatidine, and famotidine), an increasing potency of the drug analogues can be observed. Famotidine is the most potent member of this class.

2. Improving the Ratio of the Main Activity to Adverse Affects
   The pioneer drug of the adrenergic β-blockers is propranolol, which blocked both β_1- and β_2-receptors. However, blocking β_2-receptors in asthma is harmful. Several selective blockers were developed and used in cardiology, such as atenolol, metoprolol, etc.

3. Improving the Physicochemical Properties with the Help of Analogues
   Benzylpenicillin (penicillin G) was a pioneer antibiotic molecule, which could be administered only by intramuscular injection because of its acid-sensitivity. Through analogues, stable molecules were obtained and they could be given orally (e.g. ampicillin).

4. Decreasing Resistance to Anti-Infective Drugs
   Resistance to anti-infective drugs has become an increasing problem all over the world. The widespread use of penicillin G led to an alarming increase of penicillin-G resistant Staphylococcus aureus infections in 1960. A solution to the problem was the design of penicillinase-resistant penicillins. Several examples show that analogues can also overcome the resistance to antifungal and antiviral drugs.

5. Decreasing Resistance to Anticancer Agents
   Imatinib is the pioneer drug for the treatment of chronic myelogenous leukemia. However, a significant number of patients develop resistance to imatinib. New analogues, such as dasatinib and nilotinib, have been introduced recently and it is hoped that these analogues will be effective in imatinib-resistant cases.

6. Improving Oral Bioavailability
   A good oral bioavailability is necessary in most cases because the oral application of a drug is preferred to an injection therapy. Enalaprilat is an angiotensin-converting enzyme inhibitor which is used in intravenous administration for the treatment of hypertensive emergencies. Its ester prodrug has an excellent oral bioavailability, but it requires hydrolysis by esterases. Analogue-based drug research afforded the lysylproline analogue, lisinopril, which has an acceptable bioavailability and it does not require metabolic activation.

7. Long-Acting Drugs for Chronic Diseases
   Quaternary antimuscarinics are important drugs for the treatment of chronic obstructive pulmonary disease. Ipratropium bromide is a very active bronchodilator that is used several times daily. Its analogue is tiotropium with a longer duration of action which enables a once-daily dosing.

8. Ultrashort-Acting Drugs in Emergency Cases
   Esmolol is an adrenergic β_1-selective blocker with a very short duration of action. It is used when β-blockade of very short duration is desired in emergency situations.

9. Decreasing Interindividual Pharmacokinetic Differences
   Omeprazole is a pioneer proton pump inhibitor that shows interindividual variability. Analogue-based drug discovery afforded pantoprazole with a linear, highly predictable pharmacokinetic property.

10. Decreasing Systemic Activities
    For intranasal and inhalation applications of corticosteroids in the treatment of asthma and rhinitis, it is important to decrease the systemic availability of these drugs to avoid their adverse effects. Analogue research afforded budenoside and fluticasone with a low oral bioavailability.

11. Decreasing Drug Interactions with the Help of Analogues
    Cimetidine inhibits CYPs, an important class of drug-metabolizing enzymes. This interaction inhibits the metabolism of certain drugs, such as propranolol, warfarin, diazepam, thus producing effects equivalent to an overdose of these medicines. These effects are avoided by analogues such as ranitidine and famotidine.

12. Synergistic Interactions between Analogues
    Analogue-based drug research starting from ritonavir, which is an HIV-1 protease inhibitor, afforded the more potent lopinavir. However, it has a low plasma half- life. A combination of ritonavir and lopinavir is very successful, because ritonavir inhibits the P-450-mediated metabiolism of lopinavir.

IUPAC Announces Winners of the 2010 IUPAC Prizes for Young Chemists

The following winners of the 2010 IUPAC Prizes for Young Chemists were announced in May:

- **Guangbin Dong**, Stanford University, Palo Alto, California, USA
- **Viktoria Gessner**, Technical University Dortmund, Dortmund, Germany
- **Rafal Klajn**, Northwestern University, Evanston, Illinois, USA
- **Jason Spruell**, Northwestern University, Evanston, Illinois, USA
- **Guihua Yu**, Harvard University, Cambridge, Massachusetts, USA

The prizes are awarded for the best Ph.D. theses in the chemical sciences as described in 1000-word essays. The winners will each receive a cash prize of USD 1000 and travel expenses to the 43rd IUPAC Congress, 30 July–7 August 2011, in San Juan, Puerto Rico. Each prizewinner will also be invited to present a poster at the IUPAC Congress describing his/her award winning work and to submit a short critical review on aspects of his/her research topic to be published in *Pure and Applied Chemistry*. The awards will be presented to the winners of the 2010 and 2011 prizes during the Opening Ceremony of the Congress.

The essays describing the 2010 winners' theses can be found on the IUPAC web site and cover a wide range of subject matter:

- Guangbin Dong: Synthetic Efficiency: Using Atom-Economical and Chemoselective Approaches towards Total Syntheses of Agelas Alkaloids, Terpestacin and Bryostatins
- Viktoria Gessner: Lithiumorganic Compounds: From the Structure-Reactivity Relationship to Versatile Synthetic Building Blocks and Their Application
- Rafal Klajn: Self-Assembly of Nanostructured Materials
- Jason Spruell: Application of Copper-Catalyzed Reactions for the Efficient Synthesis of Donor-Acceptor Mechanically Interlocked Molecules as well as for Nanoscale Surface Patterning
- Guihua Yu: Assembly and Integration of Semiconductor Nanowires for Functional Nanosystems: from Nanoelectronics to Nanobiotechnology

There were 29 applications from 15 different countries. The Prize Selection Committee comprised members of the IUPAC Bureau with a wide range of expertise in chemistry.

Applications for the 2011 prizes are now being solicited. For more information, see <www.iupac.org/web/nt/2010-05-19_young_chemist>.

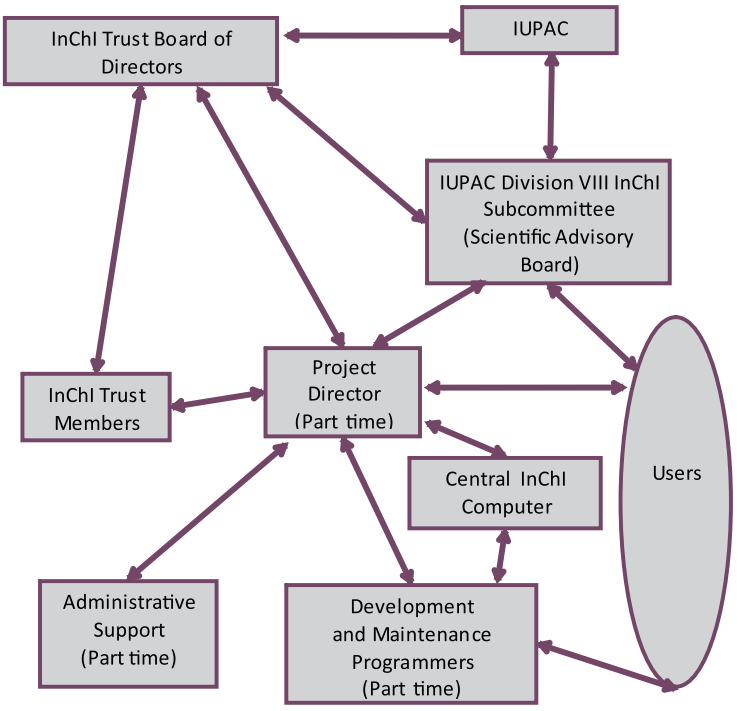
www.iupac.org/web/nt/2010-05-19_2010_winners

IUPAC and the InChI Trust Agree Upon Conditions for Collaboration

At the third meeting of the InChITrust Board of Directors, in San Francisco, USA, on 21 March 2010, an agreement (see bottom of p. 17) between IUPAC and the InChI Trust was signed by Jason Wilde (publishing director, Nature Publishing Group, and chairman of the InChI Trust Board) and Terry Renner (IUPAC executive director). This sets out the conditions under which the two organizations intend to further develop and maintain the International Chemical Identifier (InChI). The diagram on page 17 explains how the relationship will work.

The InChI Trust was constituted in May 2009 to develop and support the nonproprietary IUPAC InChI standard and promote its uses to the scientific community. Members make annual contributions to the operating costs of the Trust, and IUPAC's Division VIII InChI Subcommittee acts as a Scientific Advisory

Jason Wilde, left (publishing director, Nature Publishing Group, and chairman of the InChI Trust Board), and Terry Renner (IUPAC executive director) at the InChI Trust signing on 21 March 2010.



While InChI might be a simple concept—its maintenance and further development require intricate consideration by various groups; here is how, schematically, the organizations and individuals involved with InChI interact.

www.inchi-trust.org

Board, with responsibility for continued authentication of the InChI standard. The following organizations are now members of the Trust:

- ACD Labs
- ChemAxon
- Elsevier
- FIZ CHEMIE Berlin
- Informa/Taylor & Francis
- IUPAC
- Microsoft
- Nature Publishing Group
- OpenEye
- Royal Society of Chemistry
- Symyx Technologies
- Thomson Reuters
- Wiley-Blackwell

Questions about the Trust should be routed to the project director, Stephen Heller <Steve@InChI-Trust.org>, or to the IUPAC Division VIII InChI Subcommittee and InChI Trust Secretary, Alan McNaught <mcnaught@ntlworld.com>.

InChI Trust and IUPAC: Heads of Agreement

1. The InChI Trust, established in May 2009, provides a means of continuing the development and maintenance of the InChI standard with funds from annual membership dues.
2. The IUPAC Division VIII InChI Subcommittee (hereinafter called the "IUPAC InChI Subcommittee") represents IUPAC's authority for recognition of the InChI standard.
3. The InChI Trust Board of Directors includes a IUPAC representative with full voting rights.
4. Requests for changes, whether corrections or extensions, to the InChI algorithm and/or the related InChIKey hash algorithm can arise from InChI Trust members or other InChI users, or from within IUPAC.
5. The IUPAC InChI Subcommittee and the InChI Trust Project Director will consider any requests for change, define corresponding requirements and communicate these requirements to the InChI Trust with suggestions for prioritization if necessary.
6. The InChI Trust will make arrangements for work needed to implement accepted changes, discussing any prioritization issues with the IUPAC InChI Subcommittee. In case of disagreement over priorities, the Trust, as provider of funds for the work, will have the final say. However, it is open to IUPAC to provide alternative sources of funding for any work connected with InChI development. Conversely, the Trust may contribute funding towards projects of the IUPAC InChI Subcommittee.
7. Any new (corrected/extended) version of InChI/InChIKey will require IUPAC approval (i.e. endorsement by IUPAC Division VIII) before release. New versions of InChI/InChIKey will be released simultaneously on the IUPAC and the InChI Trust websites.
8. All releases of InChI algorithm will be on behalf of IUPAC and the InChI Trust (as joint licenser) and will continue to be made available under the GNU Lesser General Public License version 2.1, or other open-source license as mutually agreed between IUPAC and the InChI Trust.

Denis Hamilton to Receive the First International Award for Advances in Crop Protection Chemistry

The IUPAC Division on Chemistry and the Environment has established the IUPAC International Award for Advances in Harmonized Approaches to Crop Protection Chemistry, which will recognize individuals in government, intergovernmental organizations, industry, and academia who have exercised personal leadership for outstanding contributions to international harmonization for the regulation of crop protection chemistry. The award will be administered by the division's Subcommittee on Crop Protection Chemistry, and will be presented on a biennial basis in conjunction with an IUPAC-sponsored conference or special symposium organized by IUPAC.

Nominations for the award will be solicited for receipt by December 1 of odd-numbered years, with the award to be made during even-numbered years. A call for nominations will be published in *Chemistry International*. Corporate sponsorship for the award has been arranged with Dow AgroSciences of Indianapolis, USA. Awardees will receive a USD 3000 honorarium plus meeting registration, travel, and per diem reimbursement.

Rationale

Why is international harmonization for the regulation of crop protection chemistry an important goal to encourage? Historically, it has been common for regulatory authorities in each country to require unique safety and environmental studies, follow individualized testing schemes, and complete stand-alone evaluations for each new crop protection chemical or use—all of which have yielded great waste and redundancy. Today's extensive batteries of chemistry, toxicology, ecological, and environmental studies may cost upwards of USD 200 million for each new active ingredient brought to market. The lack of standardization also creates an animal welfare issue since many more animals have to be tested when studies must be repeated in different countries. In addition, the lack of common standards creates trade barriers—in the sale of crop protection chemicals and of agricultural commodities bearing trace residue of these chemicals.

Denis J. Hamilton will receive the first IUPAC International Award for Advances in Harmonized Approaches to Crop Protection Chemistry.

Although many governments and organizations are on record as promoting international regulatory harmonization and have endeavored to develop cooperation, there has been no formal mechanism in place for recognizing outstanding individual contributions toward the effort. The IUPAC award will fill this gap.

Denis Hamilton Announced as First Awardee

The first IUPAC International Award for Advances in Harmonized Approaches to Crop Protection Chemistry will be presented to **Denis J. Hamilton**, a chemist recently retired from the Queensland Department of Primary Industries (DPI), Australia, after more than 45 years of service. The award is to be presented on 7 July 2010 during a gala banquet organized as part of the 12th IUPAC International Congress of Pesticide Chemistry to be held in Melbourne, Australia <www.iupacicpc2010.org>.

Hamilton joined DPI in 1963, and after some 20 years of laboratory experience with the analysis of pesticide residues in crop protection chemicals and in foods, he began a truly extraordinary, quarter-century of work on the international harmonization of crop protection chemistry regulation. He has served on the FAO Panel of Experts on Pesticide Residues in Food and the Environment within the JMPR (Joint FAO/WHO Meeting on Pesticide Residues) since 1986. The JMPR reviews data on pesticides and recommends Codex MRLs, the maximum residue limits for pesticides in food in international trade. He has also served since 1997 on the FAO/WHO Joint Meeting on Pesticide Specifications (JMPS), which sets international quality specifications for pesticides to be used in agriculture and public health. With both JMPR and JMPS, Hamilton played leadership roles in organizing scientific panels, evaluations, and reports and in development of guidelines and novel assessment approaches.

From 1991 to 2009, Hamilton participated in IUPAC crop protection chemistry activities through the Commission on Agrochemicals and

the Environment and its successor the Subcommittee on Crop Protection Chemistry. He led several successful IUPAC projects to completion, contributed to numerous others, and was a frequently invited keynote lecturer at IUPAC-sponsored conferences and workshops spanning the globe. It may be that Hamilton's most enduring contribution will be expressed in the lives of the myriad chemists, regulatory officials, industry leaders, and researchers whom he collaborated with, lectured to, or trained.

For further information on the award, please contact Ken Racke <kracke@dow.com>.

Nominations Requested for Members of IUPAC Divisions and Commissions

Nominations are requested for candidates for all membership positions on IUPAC division committees and commissions (titular member, associate member, and national representative) for the 2012–2013 biennium. The ratification of memberships and terms of service will be finalized at the Bureau meeting in the second quarter of 2011.

A complete list of the current membership of the division committees and commissions is provided on the IUPAC website. Titular members are chosen by election. Associate members and national representatives are appointed, usually following the determination of titular membership.

IUPAC hereby requests proposals for membership on the following division committees:

- I Physical and Biophysical Chemistry
- II Inorganic Chemistry
- III Organic and Biomolecular Chemistry
- IV Polymer
- V Analytical Chemistry
- VI Chemistry and the Environment
- VII Chemistry and Human Health
- VIII Chemical Nomenclature and Structure Representation

and commissions:

- Physicochemical Symbols, Terminology, and Units
- Isotopic Abundances and Atomic Weights

Guidance for Proposing Nominees

Each member of an IUPAC body is expected to become an active participant in the work of the body in helping to decide on the program and in initiating and reviewing proposals for projects. These duties require the members to have expertise in the relevant disciplinary area and to be able to exercise sound scientific judgment. Much of each committee's work is conducted by e-mail correspondence. The Union is able to guarantee travel expenses to a meeting at the General Assembly only for Titular Members of division committees. Travel expenses for other members and for meetings outside the General Assembly are dependent on each division committee's budget and on the availability of outside funds.

IUPAC is sometimes criticized for having a membership that is predominantly male, relatively old, and drawn principally from academic institutions. In many instances, this is understandable because of the need to select senior, experienced people who are able to devote adequate time to this activity along with their full time jobs; however, the Union is making a serious effort to diversify the membership of IUPAC bodies. In making nominations, please make every effort to consider well-qualified female chemists, "younger" chemists with the required expertise and commitment, and industrial chemists.

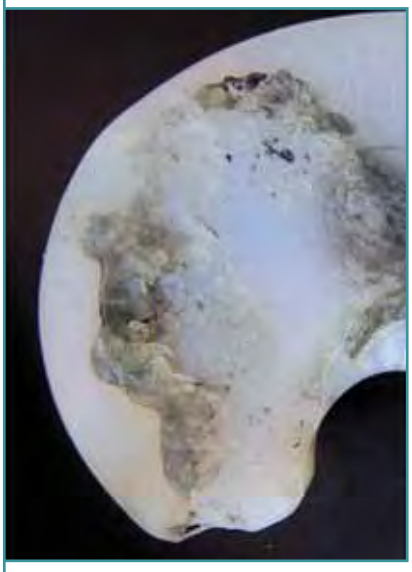
Each proposal for consideration for membership on a division or commission must identify the intended committee or commission and must be accompanied by a curriculum vitae and/or adequate information on the individual's qualifications to permit an informed evaluation and selection. Each nominee will be considered for all vacant positions on the committee unless otherwise specified.

Proposals should be submitted to the IUPAC Secretariat, preferably by e-mail attachment <secretariat@iupac.org>, by 31 July 2010. All proposed names for divisions received by this date will be forwarded to the relevant Division Nominating Committee for consideration as nominees for titular membership according to Bylaw 4.103. Those not elected as titular members subsequently will be considered for appointment as associate members or national representatives.

Nominating committees are charged with looking broadly for well-qualified candidates. Your proposals will help them ensure that we are able to establish significant pools of candidates to permit competitive selection.

Structure, Processing, and Performance of Ultra-High Molecular Weight Polyethylene

Compression moldings made from ultra-high molecular weight polyethylene (UHMWPE), are widely used in hip and knee replacements, where they generally perform well over many years. However, in a few cases, service lifetimes are drastically shortened by microcracking and wear. The aim of the present project is to develop improved quality-assurance procedures that can overcome this problem. There are major challenges in characterizing products based on PE with Mw > 1 MDa: conventional solution-based methods cannot be used to measure molecular weight distributions, and melt viscosities are so high that reactor powder is consolidated by sintering at elevated temperatures, so that tensile strength depends critically on the extent to which polymer chains have diffused across interfaces and formed entanglements. The outcome varies with processing temperature, pressure, and time.



Delaminated UHMWPE knee component after revision surgery due to pain and instability (E. Gomez-Barrena et al. Acta Orthopaedica 2008, 79(6), 832-840; doi:10.1080/17453670810016939).

Clive Bucknall will lead a task group comprising 21 academic and industrial researchers from America, China, Korea, and 5 European countries, which will study three grades of HMWPE, having Mw ≈ 0.4, 5 and 9 MDa, and develop methods for observing and quantifying the changes that occur during processing. The emphasis will be on changes that could affect fracture and wear resistance, which will also be measured.

For more information, contact Task Group Chair Clive B. Bucknall <c.b.bucknall@cranfield.ac.uk>.

www.iupac.org/web/ins/2010-019-1-400

Definitions and Notations Relating to Stereochemical Aspects in Polymer Science

Several conflicting, if not contradictory, systems for describing the absolute and relative configuration of macromolecules have been described in the literature. Some of these issues were addressed nearly 30 years ago in an IUPAC document that advanced recommendations on the stereochemical description of polymers.[1] However, some of the definitions of terms provided in that document appear inconsistent with definitions for the same terms and descriptors in organic chemistry. It is perhaps unfortunate that these terms are those which see the most widespread usage as descriptors of polymer stereochemistry. This, nonetheless, indicates the need for, and importance of, a clear unambiguous terminology that is suitable for widespread adoption. Furthermore, in the period since that publication,[1] the field of stereochemistry has undergone tremendous development, both in polymer science and in organic chemistry. It is therefore necessary to revise and update the said document in the light of current IUPAC recommendations and recent scientific developments.

This project will result in the preparation of a comprehensive document that will:

- provide the relevant terminology
- function as a basic guide to the scientific community on the stereochemical description of polymers
- highlight common misunderstandings of the different approaches used
- remove inconsistencies in recommendations that have been published at different times
- where possible, provide a concordance of formerly used terms and descriptors and classify these into preferred, acceptable, and not acceptable

The scope of the document will be limited to that of the 1981 article,[1] a version of which was recently republished, with some minor updating, in the second edition of the Purple Book.[2]

References

1. A.D. Jenkins, Stereochemical Definitions and Notations Relating to Polymers (IUPAC Recommendations 1980), *Pure Appl. Chem.* 53, 733–752 (1981) [doi:10.1351/pac198153030733]
2. *IUPAC Compendium of Polymer Terminology and*

Nomenclature (Purple Book), 2nd ed., R.G. Jones, J. Kahovec, R. Stepto, E.S. Wilks, M. Hess, T. Kitayama, W.V. Metanomski † (Eds.), RSC Publishing, Cambridge, UK 2009

For more information contact the task group chairmen Karl-Heinz Hellwich <hellwich.iupac@web.de> or Graeme Moad <graeme.moad@csiro.au>.

www.iupac.org/web/ins/2009-047-1-400

Young Ambassadors for Chemistry in Cyprus

The YAC adventure continues. This time, the Young Ambassadors for Chemistry program set up shop in Cyprus, where 45 teachers and 37 students from secondary schools participated in workshops and public events.

Held in Nicosia, Cyprus, 8–11 April 2009, the program was facilitated by the Cyprus Ministry of Education and Culture. A small group of chemistry teachers guided by Valia Angeli-Partassidou and Tasoula Karamichali, under the direction of the Inspector of Chemistry Loukia Anastasidiou, organized the YAC course at the Paedagogical Institute and the event at Eleftheria Square in Nicosia, the capital of Cyprus. A detailed report is available from the project web page listed below.

Students (roving reporters) interview Nicosia's mayor on her ideas about chemistry

The YAC team—working with the Ethiopian Chemical Society and the Federation of African Chemical Societies—hopes to visit Ethiopia during the 2011 International Year of Chemistry. See <www.chemistry2011.org/participate/ideas/show?id=6>.

For more information, contact Task Group Chair Lida Schoen <amschoen@xs4all.nl>.

www.iupac.org/web/ins/2003-055-1-050

Guidelines for Measurement of Luminescence Spectra and Quantum Yields of Inorganic Compounds, Metal Complexes, and Materials

Many fields of basic and applied chemistry, as well as material chemistry and the biosciences, employ luminescent inorganic compounds and materials. The number of researchers, who are synthetic chemists but carry out photophysical measurements, is continually increasing. While some experimental procedures have been published, there remains a need for standardized protocols, especially for quantitative measurements for such materials. Once accepted as standards, these will provide guidelines for such measurements and they can be available to all researchers, regardless of their previous experience in photophysics or theoretical chemistry, thereby allowing for objective comparisons of results generated in different laboratories.

This project aims to prepare a document describing guidelines for accurate measurements of luminescence spectra and quantum yields of metal complexes, inorganic compounds, and materials. The document will disseminate basic knowledge, rules, and protocols, not only to experts, but also to those new to this field.

In 1988, the IUPAC Organic Chemistry Division Commission on Photochemistry published "Reference Materials for Fluorescence Measurement", D. F. Eaton, *Pure Appl. Chem.*, 1988, 60, 1107-1114 (doi:10.1351/pac198860071107). This covers basic knowledge in fluorescence spectroscopy and quantum yield determination. However, there are some problems specific to inorganic compounds, which are not usually fluorescent but phosphorescent. Phosphorescence is generally air-sensitive and emits at longer wavelengths, and it may be temperature dependent. Therefore, the experiments require additional attention. For instance, the correction function for the spectrometer is generally difficult to establish in the near-infrared (NIR) range. Detectors such as CCD cameras are starting to replace the classical photomultiplier tube and reliable response curves are needed. Moreover, a major point in these experiments is the availability of highly reliable standards for relative-emission quantum-yield measurements.

Recently, some quantum yields of luminescent organic and inorganic compounds in solution have been reevaluated (Kengo Suzuki, et al., *Phys. Chem.*

Chem. Phys., 2009, 11, 9850; doi:10.1039/b912178a). The emission quantum yield of ruthenium tris(bipyridine) complex, which is internationally used as a reference, has now been reevaluated to have a significantly higher value than previously reported.

For these reasons, new guidelines should be established for the measurement of luminescence spectra and quantum yields of inorganic compounds and metal complexes. The document should describe a precise methodology for establishing the correction function, particularly in the NIR. It should also provide adequate standards for quantum yield determination of both highly and poorly luminescent inorganic compounds and complexes.

The task group is hopeful that this project will result in an inspiring and enlightening pamphlet for chemists and material scientists who join the fast developing field of photochemistry and photophysics.

For more information, contact the Task Group Chair Hitoshi Ishida <ishida@sci.kitasato-u.ac.jp>.

www.iupac.org/web/ins/2009-045-1-200

Technical Guidelines for Isotope Abundances and Atomic Weight Measurements

The Commission on Isotopic Abundances and Atomic Weights is charged with the responsibility of evaluating published data that presents new evidence on isotopic abundance measurements and consequent atomic weight values. Recommendations emerging from such evaluations, which are carried out every two years, are confirmed by IUPAC before dissemination to the scientific community. Experience at recent commission meetings has indicated that there is sometimes a lack of understanding regarding the isotopic information required. Details of the mass spectrometric protocols, including an accurate assessment of the uncertainties associated with the isotope abundance measurements, should be provided in the published work to enable the commission to evaluate the measurement results of researchers. The extent of the mass spectrometric protocols required are not always well-understood by workers in the field of isotope abundance measurements, especially with respect to uncertainty calculations. To this end, the commission will produce a readily understandable paper on the Technical Guidelines required to enable mass spectrometrists to report their data in a form suitable for evaluation.

For more information contact the task group chair John R. de Laeter <j.delaeter@curtin.edu.au>.

www.iupac.org/web/ins/2009-025-1-200

Analytical Chemistry in Action

The scientific work of the Union is undertaken by the divisions via a series of individual projects. The following division meeting report, which focuses mostly on ongoing projects, therefore seems most at home in The Project Place section.

by Brynn Hibbert, secretary of Division V

Following its well attended and successful meeting in Glasgow in 2009, the Analytical Chemistry Division was kindly hosted by the Portuguese chair of its Subcommittee on Solubility and Equilibrium Data (SSED), Maria Clara F. Magalhães. Known as the "Portuguese Venice," Aveiro is on the Atlantic coast with waterways crossing the town. The university has a vibrant chemistry department, with a strong analytical chemistry component.

Establishment of a new Subcommittee on pH

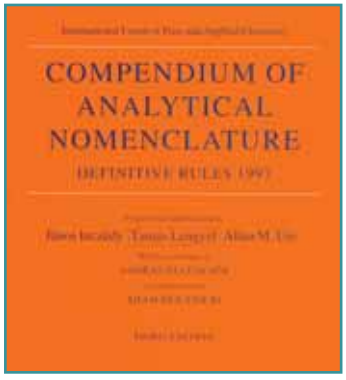
One of the strengths of the Analytical Chemistry Division is its system of subcommittees and working groups. At the meeting, the division decided to create a subcommittee on pH. Taking into account IUPAC leadership in this field, the importance of pH

The Analytical Chemistry Division in Aveiro, Portugal, in February 2010.

measurements in general, and the historical place of electrochemical methods in the past IUPAC structure, the Analytical Chemistry Division was considered the appropriate organizational entity to host this group. Maria Filomena Camões will chair the new subcommittee. She is currently vice president of the division and has been a leader of the group that in recent years brought a clear IUPAC policy to the field of pH. One immediate task for the subcommittee is to provide thoughtful input into the debate about worldwide experiments for young people in the 2011 International Year of Chemistry, which will focus on the quality of water used by communities.

The Orange Book

Like many divisions, the Analytical Chemistry Division is responsible for a color book. *The Compendium of Analytical Nomenclature: Definitive Rules* (the Orange Book) was last revised in 1997, and a web version made available in 2002 (http://media.iupac.org/publications/analytical_compendium/). The challenge for any division intending to revise a color book is how to maintain compatibility with the definitive Gold Book, while properly updating concepts and terms. After initial debates in Glasgow, the division decided that it would produce a new text version, with any new terms being abstracted into the on-line Gold Book. Bringing together definitions in a single text, and in chapters that are well understood by analytical chemists, will mean that the Orange Book will still have a future in a world dominated by the internet. The division agreed on a work flow in which any definition that eventuates in the Orange Book must come from the Gold Book or International Vocabulary of Metrology, or be included in *PAC* recommendations that will duly feed into the Gold Book. The chapters and task group chairs responsible for each chapter are shown in the next column. Brynn Hibbert is coordinating the group and will edit the final text. Please contact a task group chair if you can help with the revision of a particular chapter.



Revision of the Orange Book

Chapter	Title	Chair
Chapter 1	Fundamental concepts and terms (metrology), chemometrics (and statistics), quality assurance.	Paul De Bièvre
Chapter 2	Sampling and sample preparation	Paulo DeZorzi
Chapter 3	Methods of analysis depending on measurements of mass and volume	Maria F. Camões
Chapter 4	Separation	Tatyana Maryutina
Chapter 5	Spectroscopic methods of analysis	Zoltán Mester
Chapter 6	Mass spectrometry	David Bunk
Chapter 7	Electrochemical methods of analysis	José M. Pingarrón
Chapter 8	Radioanalytical methods	Zhifang Chai
Chapter 9	Surface analysis	Luisa Abrantes
Chapter 10	Thermal methods of analysis	Carlos Castro
Chapter 11	Immuno- and bio-analytical methods of analysis	Jan Labuda

It is interesting to compare the present 11 chapters with the 19 in the 1997 edition. There has been consolidation around fundamental methods, with the loss of explicit chapters on auto-analysis, titrimetry and gravimetry, thermal methods, magnetic methods, and a chapter on applications. It has also been decided to stick to definitions of use and importance. The new edition will not be a textbook, but a genuine compendium of terms.

Salute to Retiring Member Walter Lund

Participants at the division meeting in Aveiro also received the news that Walter Lund is retiring from the University of Oslo, and from the division after many years of service. Division president Ales Fajgelj wrote the following to the head of Lund's department:

"Following his field of speciality in chemistry, Walter became a very active member of the IUPAC Analytical Chemistry Division, and more specifically the IUPAC Commission on Microchemical Techniques and Trace Analysis in 1990. Walter served as Norwegian national representative between 1990 and 1997, was a titular member between 1998 and 2001 and became the vice president of the Analytical Chemistry Division in 2008 and with this also one of the officers of the Analytical Chemistry Division Committee. I had the

Walter Lund

opportunity to work closely with Walter in recent years. There is no need to mention his scientific contribution, as it is well reflected in numerous publications and educational work. But what I would like to point out are Walter's strong personality, openness, critical, but positive thinking, perseverance, and continuous willingness to contribute to the voluntary IUPAC work. Actually, Walter had been elected to serve as president of the IUPAC Analytical Chemistry Division for this biennium: 2010–2011. This fact alone indicates the high esteem Walter has obtained among IUPAC members. It was purely Walter's decision to reduce his work for IUPAC at this stage. We tried several times to convince him to change his mind, but unfortunately we were unsuccessful. Although we will remain in contact with Walter through IUPAC projects, members of Analytical Chemistry Division, as well as IUPAC in general, are going to miss an excellent scientist and a very good friend."

The Analytical Chemistry Division is in an exciting phase, with its members actively contributing to the work of IUPAC. There is a clear succession plan for its officers and with its subcommittees and Orange Book project, the division will have plenty to do in the coming biennium.

www.iupac.org/web/ins/500

Terminology for Chain Polymerization

During recent decades, a sometimes conflicting and contradictory terminology for describing chain polymerization processes has emerged. IUPAC has recently addressed this problem for the case of radical polymerizations which derive some of the characteristics of living polymerization from the presence of a reversible deactivation mechanism.[1] However, the issues are more pervasive and extend beyond the confines of radical polymerization, such that there is now an evident need to address the development of an even wider terminology that is being applied across all polymerization processes, often leading to conflicts of understanding at the boundaries of chain polymerization, addition polymerization, and condensation polymerization.

This project will review current terminology for chain polymerization processes in light of current IUPAC recommendations and recent developments in what continues to be a very rapidly developing field.

The project will result in the preparation of a comprehensive document that will:

- provide definitions of the relevant important terminology
- be a basic guide to terminology of mechanisms of chain polymerization processes
- highlight common misunderstandings evident in the prior literature
- remove inconsistencies in recommendations that have been published at different times
- where possible, provide a concordance of formerly used terms and descriptors and classify these either as preferred, acceptable, or not acceptable

The intention is that terminology should, where possible, be consistent with that presented in recent IUPAC documents, in particular, the "Glossary of Terms Related to Kinetics, Thermodynamics, and Mechanisms of Polymerization."[2] However, it is also recognized that some terminology may need to be modified.

References

1. A. D. Jenkins, R. I. Jones, and G. Moad, *Pure Appl. Chem.*, 2010, **82**, 483–491.
2. S. Penczek and G. Moad, *Pure Appl. Chem.*, 2008, **80**, 2163–2193.

For more information, contact Task Group Chair Graeme Moad <graeme.moad@csiro.au>.

www.iupac.org/web/ins/2010-007-1-400

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

Glossary of Terms Used in Photocatalysis and Radiocatalysis

This glossary of terms covers phenomena considered under the very wide terms "photocatalysis" and "radiocatalysis" or "radiation catalysis." A clear distinction is made between phenomena related to either photochemistry and photocatalysis or radiation chemistry and radiocatalysis. Consistent definitions are given of terms in these areas, as well as definitions of the most important parameters used for the quantitative description of these phenomena. Terms related to the up-scaling of photocatalytic processes for industrial applications have been included. This Glossary should be used together with the "Glossary of Terms used in Photochemistry," 3rd version, IUPAC Recommendations 2006: as well as with the *IUPAC Compendium of Chemical Terminology*, 2nd edition (the "Gold Book") because many terms used in photocatalysis are defined in these documents.

Comments by 31 July 2010
Prof. S.E. Braslavsky
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Mülheim/Ruhr, Germany
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www.iupac.org/web/ins/2001-036-1-300

Terminology of Polymers and Polymerization Processes in Dispersed Systems

A large group of industrially important polymerization processes is carried out in dispersed systems. These processes differ with respect to their physical nature, mechanism of particle formation, particle morphology, size, charge, types of interparticle interactions and many other aspects. Polymer dispersions, and polymers derived from polymerization in disperse media, are used in diverse areas such as paints, adhesives, microelectronics, medicine, cosmetics, biotechnology and others. Frequently, the same names are used for different processes and products or different names are used for the same processes and products. The present list of recommended terms and definitions is necessary for the unambiguous description of processes, products, parameters and characteristic features relevant to polymers in dispersed systems.

Comments by 30 November 2010
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www.iupac.org/web/ins/2002-017-1-400

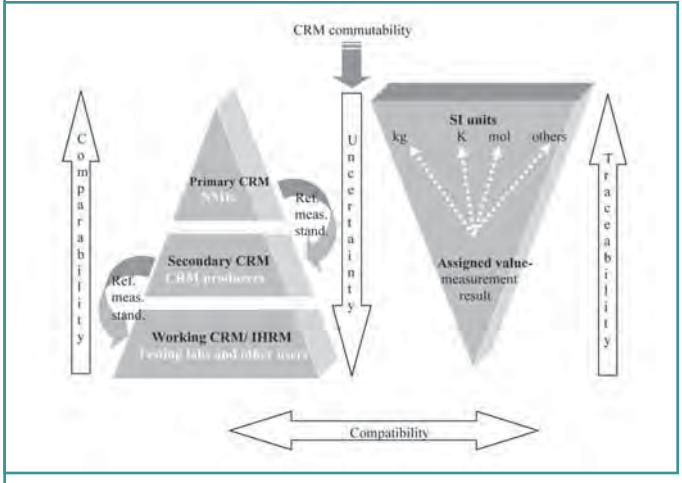
IUPAC/CITAC Guide: Selection and Use of Proficiency Testing Schemes for a Limited Number of Participants—Chemical Analytical Laboratories (IUPAC Technical Report)

Ilya Kuselman and Aleš Fajgelj

Pure and Applied Chemistry 2010
Vol. 82, No. 5, pp. 1099–1135

A metrological background for implementation of proficiency testing (PT) schemes for a limited number of participating laboratories (fewer than 30) is discussed in this paper. Such schemes should be based on the use of certified reference materials with traceable property values to serve as PT items whose composition is unknown to the participants. It is shown that achieving quality of PT results in the framework of the concept "tested once, accepted everywhere" requires both metrological comparability and compatibility of these results. The possibility of assessing collective/group performance of PT participants by comparison of the PT consensus value (mean or median of the PT results) with the certified value of the test items is analyzed. Tabulated criteria for this assessment are proposed. Practical examples are described for illustration of the issues discussed.

http://dx.doi.org/10.1351/PAC-REP-09-08-15



A scheme of calibration hierarchy, traceability and commutability (adequacy or match) of RMs used for PT, comparability and compatibility of PT results; reproduced from ref. 16 by permission of Springer.

Empirical and Theoretical Models of Equilibrium and Non-Equilibrium Transition Temperatures of Supplemented Phase Diagrams in Aqueous Systems (IUPAC Technical Report)

Horacio R. Corti, C. Austen Angell, Tony Auffret, Harry Levine, M. Pilar Buera, David S. Reid, Yrjö H. Roos, and Louise Slade

Pure and Applied Chemistry, 2010
Vol. 82, No. 5, pp. 1065–1097

This paper describes the main thermodynamic concepts related to the construction of supplemented phase (or state) diagrams for aqueous solutions containing vitrifying agents used in the cryo- and dehydro-preservation of natural (foods, seeds, etc.) and synthetic (pharmaceuticals) products. It also reviews the empirical and theoretical equations employed to predict equilibrium transitions (ice freezing, solute solubility) and non-equilibrium transitions (glass transition and the extrapolated freezing curve). The comparison with experimental results is restricted to carbohydrate aqueous solutions because these are the most widely used cryoprotectant agents. The paper identifies the best standard procedure to determine the glass transition curve over the entire water-content scale, and how to determine the temperature and concentration of the maximally freeze-concentrated solution.

http://dx.doi.org/10.1351/PAC-REP-09-10-24

The IUPAC-NIST Solubility Data Series: A Guide to Preparation and Use of Compilations and Evaluations (IUPAC Technical Report)

Heinz Gamsjäger, John W. Lorimer, Mark Salomon, David G. Shaw, and Reginald P.T. Tomkins

Pure and Applied Chemistry, 2010
Vol. 82, No. 5, pp. 1137–1159

The IUPAC-NIST Solubility Data Series (SDS) is an ongoing project that provides comprehensive reviews of published data for solubilities of gases, liquids,

and solids in liquids or solids. Data are compiled in a uniform format, evaluated, and, where data from independent sources agree sufficiently, recommended values are proposed. This paper is a guide to the SDS and is intended for the benefit of both those who use the SDS as a source of critically evaluated solubility data and who prepare compilations and evaluations for future volumes. A major portion of this paper presents terminology and nomenclature currently recommended by IUPAC and other international bodies and relates these to obsolete forms that appear in the older solubility literature. In addition, this paper presents a detailed guide to the criteria and procedures used in data compilation, evaluation, and presentation and considers special features of solubility in gas + liquid, liquid + liquid, and solid + liquid systems. In the past, much of this information was included in introductory sections of individual volumes of the SDS. However, to eliminate repetitive publication, this information has been collected, updated, and expanded for separate publication in this report.

http://dx.doi.org/10.1351/PAC-REP-09-10-33

Electrochemical Nucleic Acid–Based Biosensors: Concepts, Terms, and Methodology (IUPAC Technical Report)

Jan Labuda, Ana Maria Oliveira Brett, Gennady Evtugyn, Miroslav Fojta, Marco Mascini, Mehmet Ozsoz, Ilaria Palchetti, Emil Paleček, and Joseph Wang

Pure and Applied Chemistry, 2010
Vol. 82, No. 5, pp. 1161–1187

An electrochemical nucleic acid–based biosensor is a biosensor that integrates a nucleic acid as the biological recognition element and an electrode as the electrochemical signal transducer. This report provides concepts, terms, and methodology related to biorecognition elements, detection principles, type of interactions to be addressed, and construction and performance of electrochemical nucleic acid–based biosensors, including their critical evaluation, which should be valuable for a wide audience, including academic, biomedical, environmental, food-testing, and drug-developing laboratories and sensor producers.

http://dx.doi.org/10.1351/PAC-REP-09-08-16

Japanese Versions of the IUPAC Red Book and Green Book Available

A Concise Summary of Quantities, Units, and Symbols in Physical Chemistry

A Japanese translation of a concise summary of the Green Book has been completed by Kozo Kuchitsu, Tadamasa Shida, and Yutaka Kuroda. It was produced under the auspices of the Chemical Society of Japan.

For information on how to purchase the book, see <www.chemistry.or.jp>.

Nomenclature of Inorganic Chemistry, IUPAC Recommendations 2005

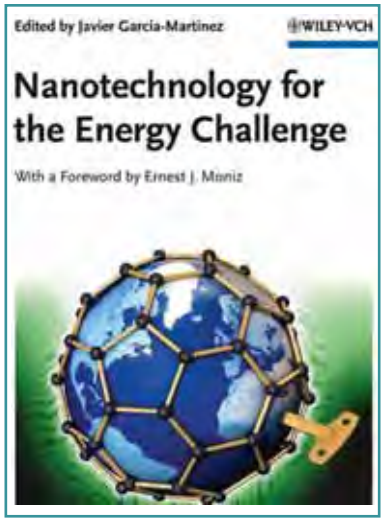
The IUPAC Red Book also has been translated into Japanese. The translation was made by members of the Committee for Nomenclature of the Chemical Society of Japan: Hiroshi Ogino, Toschitake Iwamoto, Masaaki Okazaki, Taro Saito, and Masayoshi Nakahara. It is hoped that the book, published in March 2010 by Tokyo Kagaku Dozin Co., Ltd., will facilitate the exchange of ideas and interests between Japanese chemists and chemists in other countries.

Nanotechnology for the Energy Challenge

Javier Garcia-Martinez (editor), Ernest J. Moniz (foreword)
ISBN: 978-3-527-32401-9
Wiley, April 2010

reviewed by Alan Smith

The editor, Javier Garcia-Martinez, has done a great job in this 477-page "epic," pulling together a host of experts from different parts of the energy sector.



Hardly anyone questions the predictions that nanotechnology will have a major impact on the energy sector, and *Nanotechnology for the Energy Challenge* should leave no doubt among readers that nanotechnology will dramatically change all aspects of energy generation, storage, and transmission over the next few years. The book covers recent progress as well as exciting activities at the development stage.

This major contribution to the energy debate does not aim to cover all the additional energy savings that nanotechnology will bring through more durable coatings and new composite materials, but focuses on three main themes: sustainable energy production, efficient energy storage, and energy sustainability. The chapters are written by world leaders in the specific fields, and the information contained in those chapters is extremely comprehensive and up to date, and is well illustrated where necessary.

There are five chapters in the section on sustainable energy production that describe the impact of nanotechnology on photovoltaics, thermal-electrical energy conversion, fuel cells, and hydrogen production. The section on efficient energy storage has four chapters covering hydrogen and electrochemical energy storage, as well as developments in nanomaterials for supercapacitors. The final section on energy sustainability has six chapters on topics such as green nanofabrication, nanocatalysts, carbon dioxide capture, organic light emitting devices, and progress in energy efficient buildings.

Nanotechnology for the Energy Challenge is a "must" read for those with a science education and an interest in the future of our energy supply, storage, and use.

www.wiley.com/WileyCDA/WileyTitle/productCd-3527324011.html

The Future of the Chemical Industry

Roger F. Jones, editor
ACS Symposium Series 1026,
2009, ISBN 978-0-8412-0002-9
doi:10.1021/bk-2009-1026

reviewed by Michael J. Droescher

Books describing future developments are always a challenge. The day they appear, the future has already become the present. When the book is the proceedings from a conference, the challenge is even greater. Roger F. Jones—a veteran of the chemical industry with a 50-year-long career at more than five global companies—undertook such an adventure in producing *The Future of the Chemical Industry* as part of the ACS Symposium Series.

The symposium was held at the ACS National Meeting in Philadelphia on 18 August 2008. At that time, the financial crisis was brewing but it was not yet an industrial crisis. So, the five papers in the book were presented in view of a bullish market and strong industrial growth.

When Jones edited the book in early 2009, he wrote in the preface, "The speed of change in our industry seems only to continue accelerating". However, he also knew that "portions of the book will be dated by the time of publication."

If I stopped my review here, I would not give full respect to the value of the book. The authors have assembled a strong database of industrial data up to 2007, which will be of value by itself. Let us have a closer look at the contributions.

The first chapter, written by Jones, focuses on the U.S. chemical industry. Even in a time of industrial prosperity he offers a pessimistic outlook. He discusses the negative impact of governmental policies, the low number of chemistry graduates, and a slowing of innovation activities outside the strong pharmaceutical branch.

This leads directly to the second chapter, written by Faiz Kermani and Susan Wollowitz, dealing with R&D in the global pharmaceutical markets, where the U.S. sector is running ahead of Europe and Japan. Here, as in the other chapters, the data basis is very strong. The chapter also provides deep insight into how the different pharmaceutical markets work economically and how governmental policies will influence future developments.

Chapters 3 and 4 examine the Chinese chemical markets. Klaus Griesar reports the results from a European research project comparing European Union and Chinese chemical industries. This paper, which is a well-documented source of economic data for 2003 to 2007 with forecasts for 2015, also provides a profound discussion of weaknesses and strengths in the Chinese market. Similarly, Timothy C. Weckesser describes the movement of the Chinese chemical industry up the value chain, from low-cost producer to specialty chemicals producer, thereby challenging the rest of the world and gaining market position.

The fifth chapter is somewhat unrelated to the former part of the book. It is a short article on Hydrogen PEM Fuel Cells.

From a readability standpoint, it is unfortunate that each article has its own design and that some of the pictures are barely readable. Overall, however, the book has value to readers who are interested in data on the economic development of the chemical industry and are looking for a sound discussion of its future development.

http://dx.doi.org/10.1021/bk-2009-1026

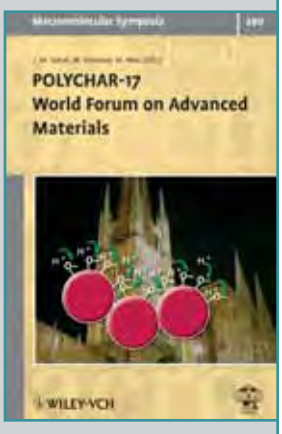
Macro- and Supramolecular Architectures and Materials

Macromolecular Symposia
Volume 287, pages 1–176 (January 2010)
Helmut Ritter, Ella Bezdushna, Carsten Koopmans, Maricica Munteanu, Monir Tabatabai, Kurt E. Geckeler (editors)

POLYCHAR-17 World Forum on Advanced Materials

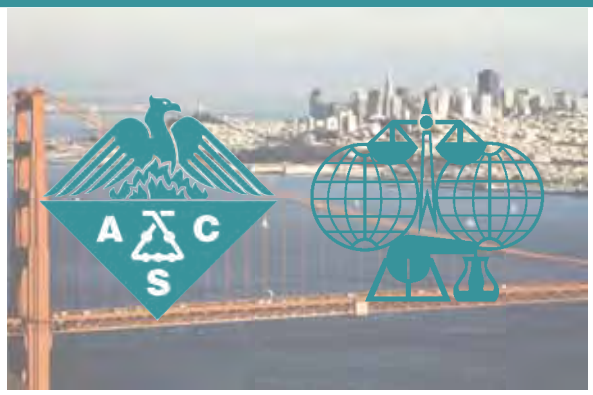
Macromolecular Symposia
Volume 290, pages 1–184 (April 2010)
Jean-Marc Saiter, Witold Brostow, Michael Hess
(editors)

www.iupac.org/publications/macro/2010



IUPAC–ACS Collaboration Summit

by Katherine Bowman and Francisco Gomez



The **Second IUPAC–ACS Collaboration Summit** was convened on 21 March 2010 during the American Chemical Society (ACS) meeting in San Francisco, California, USA, under the auspices of IUPAC, ACS, and the U.S. National Academies (through its role as the U.S. adhering member to IUPAC). The meeting—attended by approximately 40 representatives of IUPAC and ACS technical divisions and committees—built on the success of an inaugural collaboration event held on 15 August 2009 in Washington, D.C. While the previous summit focused on developing broad awareness of the activities and interests of participating IUPAC and ACS groups, the second summit focused on generating concrete collaborative ideas to be taken forward by these groups. The International Year of Chemistry (IYC) 2011 provided a framework for these plans, particularly potential outreach events and symposia to be held at the December 2010 Pacfichem meeting in Hawaii and the August 2011 IUPAC Congress in Puerto Rico.

Overview of the Meeting

The summit was moderated by Bryan Henry, past president of IUPAC and a member of the ACS International Activities Committee. Welcome remarks were given by David Black, IUPAC secretary general, and Joseph Francisco, ACS president and vice chair of the U.S. National Committee for IUPAC, who challenged participants to explore opportunities that reached across disciplinary and divisional boundaries. A brief review of the celebration and goals of IYC 2011 followed these welcomes. Participants also discussed background information on Pacifichem 2010 and the 2011 IUPAC Congress, with the focus on these upcoming events as targets for potential collaborative division activities. Participants discussed potential funding opportunities for IUPAC–ACS divisions wanting to initiate collaborative projects. These included providing seed money through IUPAC–ACS Mini Planning Awards and the IUPAC project system. In addition, it was announced that ACS has made three Challenge Grants available for symposia that will be held during the Puerto Rico Congress.

An example of the type of collaborative symposium that could be organized was presented to the group by Hessy Taft, who is currently preparing a session on "Advances in Alternative Energy" with likely co-sponsorship from ACS divisions such as Industrial and Engineering Chemistry and Environmental Chemistry. The symposium will feature talks on key forms of energy including wind, solar, hydrogen, and biofuels, as well as how information on alternative energy can be incorporated into the K–12 curriculum.

The second half of the meeting allowed participants to brainstorm ideas for events and symposia; these ideas were further discussed and refined in smaller breakout groups. For each idea, groups were asked to consider a plan of action including next steps, timelines, metrics, and who would carry out the needed tasks. The small groups reported their progress back to the full meeting and submitted an informal written report. The meeting concluded with remarks by Judith Benham, chair of the ACS International Activities Committee, who expressed her thanks for the productive discussions and her hope that IUPAC and ACS would continue to foster these valuable collaborative relationships.

Proposed Collaborative Events and Symposia

An important component of the summit was the generation of potential collaborative activities. Initial ideas were generated in a group brainstorming session, followed by six breakout discussion groups to create initial plans of action for who will be involved and how these proposals will be carried forward. The topics selected for discussion included potential outreach events to students as well as IUPAC Congress symposia.

Outreach Events

1. Pre-IYC launch events at Pacifichem on the theme of water
2. Student/teacher outreach event at the 2011 IUPAC Congress

IUPAC Congress Symposia

3. Contributions of Crystallography to Structure-Based Drug Discovery
4. Worldwide Research and Development in Materials Chemistry
5. Global Water Quality Issues
6. Women in Science Symposium + Marie Curie Reenactment
7. Organic Chemical Terminology
8. Chemical Safety and Security

Brief Overviews of Proposed Events and Plans

Outreach: Pre-IYC Launch at Pacifichem

Group leader: Peter Mahaffy, IUPAC Committee on Chemistry Education

- Several activities will focus on advertising IYC and the planned program of IYC Global Water Experiments
- Inclusion in the Pacifichem opening ceremonies of a well-known water quality scientist to provide an introduction to global water issues, their connection to chemistry, and the program of global experiments on "Water: A Chemical Solution"
- A display and demonstration on the global water experiments program at the IUPAC exhibition booth
- Organization of a public event in Hawaii, perhaps at the beach, to announce IYC and demonstrate the Global Water Experiments
- A link with the YouTube video project of ACS' Younger Chemists Committee (YCC) and Women Chemists Committee (WCC), which will be ready to show at Pacifichem

Potential partners: ACS and IUPAC divisions/committees in environmental chemistry, agricultural and food chemistry, CHED, Chemrawn, IUPAC IYC Management Committee, ACS International Activities Committee, YCC, WCC, and others

Outreach: Student/Teacher Event at IUPAC Congress

Group leader: Ram Lamba, IUPAC Bureau and IUPAC Committee on Chemistry Education

The event "Chemistry in Our Lives: A Chat with Nobel Laureates" will be organized for middle school and high school teachers and students. The activity will also include the development of interactive materials in English and Spanish for the teachers and students, such as a lesson plan discussing the roles of chemistry, Marie Curie, and IYC.

Potential partners: ACS divisions/committees on chemistry education, local sections, IYC management committee, Congress organizing committee, teachers associations, and others

Symposium: Contributions of Crystallography to Structure-Based Drug Discovery

Group leaders: Katherine Kantardjieff, U.S. National Committee for Crystallography, and Mukund Chorghade, IUPAC Division on Chemistry and Human Health

This one-day symposium will focus on neglected and orphan diseases. It will feature a series of coordinated talks addressing both structure solution/description and the application of structure in organic/medicinal/clinical aspects.

Potential partners: ACS Division of Medicinal Chemistry, Small Chemical Business Division, and partner societies like ACA, AsCA, ECA, and AAAS

Symposium: Worldwide Research and Development in Materials Chemistry

Group leader: Len Interrante, IUPAC Interdivisional Subcommittee on Materials Chemistry

This symposium will be led by the IUPAC Interdivisional Subcommittee on Materials Chemistry, with assistance from relevant ACS divisions and other chemical society partners. It will include a session of talks followed by a panel discussion/workshop on the needs and opportunities for materials chemistry in science and technology.

Potential partners: ACS divisions such as PHYS, PMSE, INORG, CATAL, COLL, ENVR, I&EC, and others and societies such as the U.K. Royal Society of Chemistry and the European Association for Chemical and Molecular Sciences (EuCheMS)

Symposium: Global Water Quality Issues

Group leader: Sut Ahuja, ACS Divisions of Analytical and Environmental Chemistry

This symposium series will include four topical sessions on aspects of water quality including environ-

mental, analytical measurement, impact on development and agriculture, and industrial issues. The sessions will feature both invited overview talks as well as contributed papers.

Potential partners: IUPAC groups in analytical and environmental chemistry, IUPAC Committee on Chemistry and Industry (COCI), ACS Division of Agricultural and Food Chemistry, industrial and engineering chemistry, corporation associates, and Global Innovation Imperatives

Symposium: Women in Science Symposium + Marie Curie Reenactment

Group leader: Ingrid Montes, Gabriel Infante, and Janet Bryant

This proposed project would include the following activities:

- series of 12 online profiles over the course of a year (2011): one woman per month to be highlighted
- Eminent Scientists Symposium (Puerto Rico)
- Marie Curie Reenactment (Puerto Rico)

Potential partners: ACS Women Chemists Committee, Puerto Rico Section, Younger Chemists Committee, Committee on Minority Affairs, International Activities Committee

Two additional symposia were proposed for the 2011 IUPAC Congress program: Organic Chemical Terminology (leaders: Victor Snieckus, ACS Division of Organic Chemistry and Leiv Sydnes, IUPAC Committee on Chemistry Research Applied to World Needs [Chemrawn]) and Chemical Safety and Security (Leader: Mark Cesa, COCI). Although these two symposia were not discussed in detail during the second summit, the group welcomed further development of these ideas.

The ACS's YCC is also planning a YouTube collaboration with the European Youn Chemists Network of EuCheMS called the "World of Chemistry": three-minute shorts featuring young chemists from different countries who discuss, in their native language, what chemistry means to them. The YCC also is working on expanding the international exchange program that exists between the Gesellschaft Deutscher Chemiker (i.e. the german chemical society) and Northeastern Section of the American Chemical Society to other European Union chemical societies and the ACS (this initiative is for more than 2011, but likely will start then).

Conclusion

Work on these proposals will begin immediately in order to meet the deadlines for the ACS Challenge Grants, to allow enough time to seek alternative sources of funding, and to allow enough time to ensure the success of the projects. An IUPAC/ACS Summit Discussion Forum will be created on the ACS Network. All participants will be invited to join and will be encouraged to share their progress, exchange ideas, and collaborate with each other. A follow-up-meeting take place in August 2010 at the ACS National Meeting in Boston, Massachusetts, USA, that will focus on progress made on the specific proposals.

Katherine Bowman was, at the time of the meeting, the U.S. representative to IUPAC for the National Academy of Sciences (that position is currently held by Lois Peterson <LPeterson@nas.edu>. Francisco Gomez <F_Gomez@acs.org> is Global Alliances & Partnerships Manager for the ACS Office of International Activities.

Environmental Best Practices

by Maciej Góra

The **2nd International Environmental Best Practices (EBP-II) Conference** was held in Krakow, Poland, 14–18 September 2009. This symposium was chaired by Maciej Góra and Miroslaw Luczynski and was hosted by the Faculty of Chemistry of the Jagiellonian University, one of the oldest universities in Europe. The EBP-II Conference attracted over 100 participants from scientific and industrial institutions from 24 countries. Symposium topics covered a broad spectrum of environmental issues and solutions to the challenges facing the world today. One plenary lecture, 7 keynote

addresses, 20 oral papers, and 87 posters were presented over five days during the following sessions:

- Environmental Remediation
- Wastewater Treatment
- Solid Waste Management
- Alternative Energy Sources
- Environmental Toxicology
- Interfacial Phenomena in Environmental Sciences
- Resources and Ecosystems Management

The EBP II conference was organized in collaboration with the Ohio State University, Columbus, Ohio, USA; the University of Warmia and Mazury in Olsztyn, Poland; Institute of Catalysis and Surface Chemistry, PAS, Poland; and the University of Applied Sciences in Offenburg, Germany. The conference successfully brought together researchers from academic, governmental, and industrial institutions to discuss new developments and results in the field of environmental science.

The AGFES Workshop moderated by Delia Gallinaro, MPA (Sam Houston State University), was an integral part of the meeting and provided participants with brief but valuable information on funding opportunities for research and scholarly activities, grant proposal development and submission, and the dissemination of results.

One of the highlights of the meeting was a discussion about the problems of simultaneous toxicological impact of xenobiotics on water organisms and methods used in their determination.

The contributions to EBP II will be published in *Environmental Biotechnology* journal <www.environmentalbiotechnology.pl>. In addition, all conference participants have been invited by the editor of *EB* to submit manuscripts based on lectures or posters.

This symposium was sponsored and supported by IUPAC, the Polish Ministry of Science and Higher Education, City of Krakow, and the Pro Chemia Foundation.

Full details of the conference program, including a list of speakers and lecture titles are available on the conference website at <www.chemia.uj.edu.pl/ebp.html>.

The EBP III will be held in 2011 at the University of Applied Sciences, Offenburg, Germany.

Maciej Gora <mgora@chemia.uj.edu.pl> is a scientist in the Department of Organic Chemistry, Jagiellonian University, Krakow, Poland. He was the co-chair of the EBP-II conference.

Advanced Polymeric Materials

by Werner Mormann and Michael Hess

The **18th Word Forum on Advanced Polymeric Materials**—POLYCHAR 18—was held in Siegen, Germany, 7–10 April 2010. It was proceeded by the Short Course on Polymer Characterization, a regular tutorial with a long tradition, held on 6 April by designated experts in their field. The name POLYCHAR is derived from polymer characterization and addresses the whole field of polymeric materials.

The conference was hosted by the Department of Macromolecular Chemistry of the University of Siegen in the southern tip of the State of North-Rhine-Westfalia, County of Siegen-Wittgenstein. Although located in a water-rich hill country with vast forests, it has been a center of iron ore mining and the manufacturing of high-tech materials and products for a long time. Hence, it proved to be a good place for non-metal materials scientists to meet.

About 250 registered participants (23 from industry) from 5 continents and 41 countries attended this intensive three-day meeting that offered 129 oral contributions, arranged in three parallel sessions, and one poster session with 112 contributions. Six keynote speakers and 38 invited speakers formed the framework of the sessions which covered Synthesis, Physico-Chemical Properties, Surfaces & Interfaces, Characterization, Application, and Processing.

Delegates were welcomed by the Conference Chair Werner Mormann. He was followed by Jung-Il Jin, IUPAC past president, in his function as official IUPAC representative.

Goerg Michler (left), chair of the POLYCHAR Prize Committee; Andrezej Galeski, recipient of the Paul J. Flory Medal 2010; and Werner Mormann, chair of POLYCHAR 18.

The titles of the following keynote lectures demonstrate the borad range of subjects covered by the conference:

- Gero Decher, Strasbourg (France), "Toward Soft Matter Thin Film Devices"
- David Grainger, Salt Lake City (USA), "Molecular Sorting at Surfaces: Protein-Protein Capture to Pattern and their Analysis"
- Tony Ryan, Sheffield (UK), "The Quest for Motility: Making Polymers Swim"
- Jiasong He, Beijing (China), "Microfoaming of Polymers by Supercritical CO2-Technique"
- Michael Buchmeiser, Stuttgart (Germany), "Ring-Opening Metathesis Polymerization Derived Materials for Heterogeneous Catalysis, Separation Science and Tissue Engineering"
- Kwang-Sup Lee, Daejeon (Republic of Korea), "Recent Advances in Two-Photon Stereolithography"

As an IUPAC-sponsored international conference, POLYCHAR attracts internationally renowned scientists from all over the world. The philosophy of POLYCHAR from the very beginning was to give young scientists and advanced students a forum in which to present their results themselves as oral presentations or posters, and to allow them to meet and establish contacts with the established scientists from academia and industry.

IUPAC sponsorship and a German Academic Exchange Service grant were used to support the attendance of 24 students from developing and underprivileged countries and a researcher from the University of Nigeria. The German Research Council and Funds of Chemical Industry enabled conference organizers to attract high-level scientists from all over the world.

The conference concluded with two P.J. Flory Award Speeches and a prize ceremony honoring the recipients of the award:

- Hans Wolfgang Spiess, Max-Planck-Institute for Polymer Research, Mainz, for his pioneering work in the field of Solid-State-NMR for the analysis of structure and dynamics of polymer systems
- Andrzej Galeski, Centre of Molecular and Macromolecular Studies, Polish Academy of Sciences, Lodz, for his pioneering work on strength and toughness of semicrystalline polymers, blends, and filled polymer systems

Jung-Il Jin (right), past president of IUPAC, presents an IUPAC-poster prize to Lei Nie, University of Sheffield, England.

The International Materials Science Prize was given to Peter Mallon, Stellenbosch (South Africa), who gave a talk on "Synthesis, Morphology, and Electrospinning of Polydimethylsiloxane-based Copolymers."

The Jürgen Springer Award for a Young Scientist was given to Davide Tranchida, Humboldt fellow at the University of Siegen, for his presentation on "Mechanical Properties of Morphologies Studied by Atomic Force Microscopy Nanoindentation: Polymer Brushes and Polymeric Nanophases"

Because of strong competition, the Carl Klason Prize for the Best Student Paper was awarded to three *ex aequo* winners:

- Victor Baukh, Eindhoven University of Technology, the Netherlands (advisor Henk Huinink) for his paper on "NMR-Imaging of Water Absorption by Multilayer Coatings"
- Gareth Bayley, University of Stellenbosch, South Africa (advisor Peter Mallon) for his presentation on "Carbon Nanotube-Filled Electrospun Polyacrylonitrile-Graft-Poly(dimethylsiloxane) Fibers for Silicone Elastomer Composites"
- Anais Vuillequez, University of Rouen, France (advisor Jean-Marc Saiter) for her paper on "Glass Transition and Enthalpy Relaxation in Glassy Materials: from Polymers to Food Industry"

IUPAC Poster Prizes were awarded as follows:

- Nattaya Muksing, Chulangkorn University Bangkok, Thailand (advisor Rathanawan Magaraphan), for her poster "Peroxide Cured Natural Rubber/Fluorelastomer/High-Density Polyethylene via Dynamic Vulcanization"
- Lei Nie, University of Sheffield, England (advisor Tony J. Ryan), for his poster "Water Vaper Transport in Liquid Crystalline Thermosets"
- Nataliia Puzko, Lviv Polytechnic National University, Lviv Ukraine (advisor Michail Bratychak), for her poster "Regulation of Carbon-Chain Polymer Surface Properties"

Winners of the Wiley Poster Prize:

- Anton Ginzburg, Deutsches Kunststoffinstitut Darmstadt Germany (advisor Tibor Macko), for his poster "Characterization of Polyolefines with High-Temperature Two-Dimensional Liquid Chromatography"
- Fritjof Nilsson, Royal Institute of Technology Stockholm, Sweden (advisor Ulf W. Gedde), for his poster "Modelling the Permittivity of Anisotropic Composites"

The POLYCHAR-18 Poster Prize was given to Anna Trinker, University of Cologne (advisor Bernd Tieke), for her poster "Functionalization of Hydrogels Based on N-Isopropylacrylamide and Cationic Surfactant Monomers via Counterion Exchange."

IUPAC sponsorship was vital in supplying international recognition, credibility, and attracting many high-quality speakers from all over the world and all fields of polymer science and technology.

With more than 80 registered participants from academia and industry, this IUPAC-sponsored Short Course on Polymer Characterization was very popular and provided newcomers with a better understanding of the field. Following are some highlights:

- "Atomic Force Spectroscopy: Morphology and Surface Analysis Beyond Topography," H. Schönherr, Siegen (Germany)
- "Dynamic Mechanical Thermal Analysis," M. Hess, Siegen (Germany)
- "Comprehensive Characterization of Macromolecules by Liquid Chromatography," P. Kilz, PSS Darmstadt (Germany) and C. Johann, Wyatt Technology Europe, Dernbach (Germany)
- "Characterization of Thin Polymer Films by Quartz Crystal Microbalance with Dissipation Monitoring (QCM-D)," S. Svedhem, Lund (Sweden)
- "Assessing Transport Properties of Polymers by Experimental Techniques and Simulation Techniques," U.W. Gedde, Stockholm (Sweden)

Manuscripts will be published in *Macromolecular Symposia*, as well as in *Polymer Engineering & Science* after the usual process of peer review.

Future POLYCHAR conferences are scheduled as follows:

- POLYCHAR-19, Katmandu, Nepal, March 2011
- POLYCHAR-20, Zagreb, Croatia, 2012
- POLYCHAR-21, Gwangju, South Korea, 2013

For more information, see <www.unt.edu/POLYCHAR>.

Heterocyclic Chemistry

by Lisa McElwee-White

The **11th Annual Florida Heterocyclic and Synthetic Conference** was held 7–10 March 2010 in Gainesville at the University of Florida. Attendees had the opportunity to participate in an excellent program that included 11 plenary lectures, 39 invited lectures, 5 short courses, and a poster session. Short courses were taught by John Joule (University of Manchester) on azines, Ronald Castellano (University of Florida) on non-covalent interactions of aromatics and heterocycles in molecular recognition, Gordon Gribble (Dartmouth College) on the applications of metals in heterocyclic chemistry, Girolamo Cirrincione (University of Palermo) on eight-membered heterocyclic rings, and Victor Zhdankin (University of Minnesota) on hypervalent iodine reagents.

The following scientists delivered plenary lectures:

- Michael Collins, CEM Corporation, USA
- Amos Smith, University of Pennsylvania, USA
- Ciarán McArdle, Henkel AG, Germany
- Oleg G. Kulinkovich, Belarusian State University, Belarus
- Ronald Breslow, Columbia University, USA
- Bernd Giese, University of Basel, Switzerland
- Henri Kagan, Université Paris-Sud, France
- Bill Murray, Johnson & Johnson Pharmaceutical R&D, USA
- William Roush, Scripps Florida, USA
- Richard Houghten, Torrey Pines Institute for Molecular Studies, USA
- Malcolm Stevens, University of Nottingham, USA

Over 200 attendees included approximately 55 graduate students and postdocs, along with academic and industrial research chemists from more than 25 countries. Heterocyclic compounds are of particular importance to the pharmaceutical industry and many of the industrial delegates came from this area. The conference attracted a number of commercial exhibitors, including publishers, chemical suppliers, and instrument makers.

Proceeds from the conference are used to support *ARKIVOC* (Archive for Organic Chemistry), a free peer-reviewed online journal covering all aspects of organic chemistry <www.arkat-usa.org>.

Lisa McElwee-White is a professor of chemistry at the University of Florida and a former titular member of the Organic and Biomolecular Chemistry Division Committee.

Where 2B & Y

Vanadium

6–9 October 2010, Toyama, Japan

Vanadium chemistry and biochemistry have become more attractive in part because of the synthetic utility of several vanadium complexes and in part because of new findings that vanadium compounds have insulin-mimic and anti-tumor properties. In addition, the discovery of several vanadium enzymes and proteins from marine organisms are the subject of intensive research. The **Seventh International Symposium on the Chemistry and Biological Chemistry of Vanadium** (V7 Symposium), 6–9 October 2010, Toyama, Japan, will encourage international and interdisciplinary exchange of the most up-to-date information among the chemistry and biochemistry fields, thereby promoting the advancement of vanadium chemistry.

The scientific topics for the V7 Symposium are as follows:

- Vanadium Inorganic Chemistry—Coordination, Speciation, and Structure
- Vanadium Bioinorganic and Biological Chemistry
- Vanadium Transport, Toxicology, and Enzymology
- Therapeutic Applications of Vanadium Compounds
- Vanadium-Induced or -Catalyzed Reactions

- New Materials Containing Vanadium and their Processes

The deadline for abstract submissions for poster presentations is 31 July 2010. Several posters will be selected as oral presentations on the basis of the quality and creativity of the research presented in the provided abstract.

See Mark Your Calendar on page 37 for contact information.

www.vanadiumseven.com

Liquid Chromatography–Mass Spectrometry

10–12 November 2010
Montreux, Switzerland

Since its inception in the early '80s, the Montreux **Liquid Chromatography–Mass Spectrometry Conference** has been the world's premier conference on LC/MS and all related hyphenated technologies, including important application challenges such as sample pretreatment, separation technologies, and novel software/bioinformatics. This year, LC/MS will take place 10–12 November 2010.

Novel instrumentation and analytical strategies are keys to the success of the meeting. It is anticipated that new developments will be introduced as during previous meetings. An attractive oral and poster session will take place in a relaxed format to allow maximum interaction among participants. Introductory courses will stimulate newcomers to enter the exciting world of LC/MS.

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

The exhibition is key to the conference and all major companies involved in LC/MS will be present, while ample time is available in the program for discussions and introduction into novel concepts and instruments.

The charm of Montreux will provide an excellent atmosphere for combining intense science and business with ample opportunities for making new friends and meeting old friends!

www.lcms-montreux.com

Organometallic Chemistry Directed Towards Organic Synthesis

24–28 July 2011, Shanghai, China

The **16th IUPAC International Symposium on Organometallic Chemistry Directed Towards Organic Synthesis** (OMCOS 16) will be held in Shanghai, China, from 24–28 July 2011. It will be organized by the Shanghai Institute of Organic Chemistry, Chinese Academy of Sciences, and the East China Normal University.

Shanghai will host the OMCOS meeting for the first time following the successful series of symposia held at Fort Collins (1981), Dijon (1983), Kyoto (1985), Vancouver (1987), Florence (1989), Utrecht (1991), Kobe (1993), Santa Barbara (1995), Gottingen (1997), Versailles (1999), Taipei (2001), Toronto (2003), Geneva (2005), Nara (2007), and Glasgow (2009). The venue for the symposium will be the Shanghai International Convention Center, located in the heart of Lujiazui—Shanghai's financial and trade zone, southwest of the Oriental Pearl TV Tower.

OMCOS brings together chemists from industry and academia from all over the world to present and discuss the latest advances in organic synthesis with organometallic reagents, metal-mediated or -catalyzed reactions, asymmetric synthesis and catalysis, structural and mechanistic aspects of organometallics, and environmentally benign processes using metals.

The conference chairs are Shengming Ma and Kuiling Ding.

See Mark Your Calendar on page 40 for contact information.

www.omcos16.org

Visas

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

How to Apply for IUPAC Sponsorship

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

www.iupac.org

Mark Your Calendar

Upcoming IUPAC-sponsored events
See also http://www.iupac.org/indexes/Conferences for links to specific event websites

2010 (later than 1 August)

IUPAC poster prizes to be awarded

1–6 August 2010 • Chemical Thermodynamics • Tsukuba, Japan
21st International Conference on Chemical Thermodynamics
Prof. Kazuya Saito, Department of Chemistry, Graduate School of Pure and Applied Sciences, University of Tsukuba, Tsukuba, Ibaraki 305-8571, Japan
Tel.: +81 29 853 4239, Fax: +81 29 853 6503, E-mail: kazuya@chem.tsubuka.ac.jp

1–6 August 2010 • Organic Synthesis • Bergen, Norway
18th International Conference on Organic Synthesis
Prof. Leiv K. Sydnes, Department of Chemistry, University of Bergen, Allégaten 41, N-5007 Bergen, Norway
Tel.: +47 55 58 34 50, Fax: +47 55 58 94 90, E-mail: leiv.sydnes@kj.uib.no

1–6 August 2010 • Carbohydrate • Chiba, Japan
25th International Carbohydrate Symposium
Prof. Yukishige Ito, RIKEN Advanced Science Institute, 2-1 Hirosawa, Wako, Saitama 351-0198, Japan
Tel.: + 81 48-467-9430, Fax: + 81 48-462-4680, E-mail: yukito@riken.jp

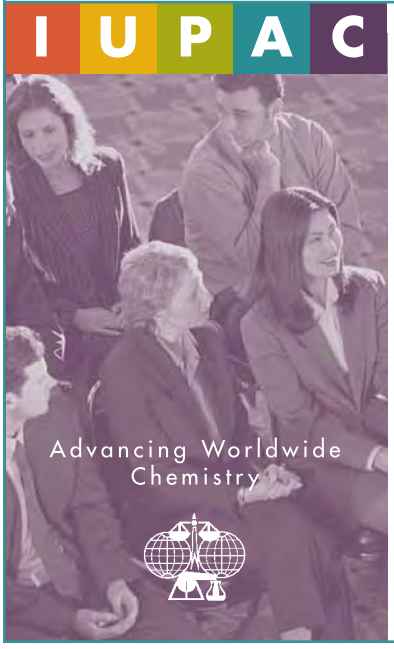
8–13 August 2010 • Chemical Education • Taipei, Taiwan
21st International Conference on Chemical Education—Chemistry Education and Sustainability in the Global Age
Prof. Mei-Hung Chiu, National Taiwan Normal University, No. 88, Ding-Zhou Road, Section 4, Taipei, 116, Taiwan
Tel.: + 886 2-2932-2756, Fax: + 886 2-2935-6134, E-mail: mhc@ntnu.edu.tw

15–19 August 2010 • Green Chemistry • Ottawa, Canada
3rd IUPAC Conference on Green Chemistry (ICGC-3)
Prof. Philip Jessop, Department of Chemistry, Queen's University, 90 Bader Lane, Kingston, ON, K7L 3N6, Canada
Tel.: +1 613-533-3212, Fax: +1 613-533-6669, E-mail: info@icgc2010.ca

15–20 August 2010 • Supramolecular Architectures and Materials • Montego Bay, Jamaica
5th International Symposium on Macro- and Supra-molecular Architectures and Materials
Professor Ishenkumba A. Kahwa, Faculty of Pure and Applied Sciences, University of the West Indies, Mona Campus, Kingston 7, Jamaica, Tel.: +1 876 927 1910, Fax: +1 876 805 5580, E-mail: MAM-10@uwimona.edu.jm

22–27 August 2010 • Physical Organic Chemistry • Busan, Korea
20th International Conference on Physical Organic Chemistry
Prof. Dae-Dong Sung, Department of Chemistry, Dong-A University, Saha-Gu, Busan 604-714, Korea
Tel.: +82 51 200 7243, Fax: +82 51 200 7259, E-mail: ddsung@dau.ac.kr

13–17 September 2010 • Hyperfine Interactions and Nuclear Quadrupole Interactions • CERN, Switzerland
Joint International Conference on Hyperfine Interactions and Symposium on Nuclear Quadrupole Interactions
Professor Reiner Vianden, Universität Bonn, Helmholtz Institute für Stahlen und Kerphysik (HISKP), Nussallee 14-16, D-53115 Bonn, Germany, Tel.: +49 228 733 355, Fax: +49 228 732 505, E-mail: vianden@hiskp.uni-bonn.de



IUPAC Prize for Young Chemists

Supporting the future of chemistry

The encouragement of young research scientists is critical to the future of chemistry. With a prize of USD 1000 and paid travel to the next IUPAC Congress, the **IUPAC Prize for Young Chemists** encourages young chemical scientists at the beginning of their careers. The prize is based on graduate work and is given for the most outstanding Ph.D. thesis in the general area of the chemical sciences, as described in a 1000-word essay.

Call for Nominations: **Deadline is 1 February 2011.**

For more information, visit www.IUPAC.org/news/prize.html or contact the Secretariat by e-mail at secretariat@iupac.org or by fax at +1 919 485 8706.

14–18 September 2010 • Biotechnology • Rimini, Italy
14th International Biotechnology Symposium and Exhibition
Prof. Fabio Fava, Università di Bologna, Via Terracini, 28, I-40131 Bologna, Italy
Tel.: +39 051 209 0330, Fax: +39 051 209 0348, E-mail: fabio.fava@unibo.it

19–23 September 2010 • Heavy Metals in the Environment • Gdansk, Poland
15th International Conference on Heavy Metals in the Environment
Prof. Jacek Namiesnik, Department of Analytical Chemistry, Gdansk University of Technology, G. Narutowicza 11/12, PL-80 233 Gdansk, Poland, Tel.: +48 58 347 1345, Fax: +48 58 347 2340, E-mail: chemanal@pg.gda.pl

20–23 September 2010 • Polymer Behavior • Lodz, Poland
4th International Conference on Polymer Behavior
Professor Andrzej Galeski, Centre of Molecular & Macromolecular Studies, Polish Academy of Sciences, PL-90 363 Lódz, Poland, Tel.: + 48 426 803 250, Fax: +48 426 803 261, E-mail: andgal@cbmm.lodz.pl

6–9 October 2010 • Vanadium • Toyama, Japan
7th International Symposium on the Chemistry and Biological Chemistry of Vanadium
Tatsuya Ueki, Department of Biological Science, Hiroshima University, Higashi-Hiroshima, Hiroshima 739-8526, Japan
Tel.: +81 82 424 7437, Fax: +81 82 424 7437, E-mail: secretariat@vanadiumseven.com

6–10 October 2010 • Eurasia Chemistry • Amman, Jordan
11th Eurasia Conference on Chemical Sciences
Dr. Amal Al-Aboudi, Chemistry Department, University of Jordan, Amman 11942, Jordan
Tel.: +962 6 535 5000, Fax: +962 6 535 5522, E-mail: alaboudi@ju.edu.jo

11–14 October 2010 • Novel Materials • Wuhan, China
6th International Symposium on Novel Materials and their Synthesis
Prof. Yu-Ping Wu, Department of Chemistry, Fudan University, No. 220 Handan Road, Shanghai 200433, China
Tel.: +86-21-6564-2141 +86-21-5566-4223, Fax: +86-21-5566-4223, E-mail: nms@fudan.edu.cn

24–29 October 2010 • Polymer Science • Hersonissos, Greece
8th Hellenic Society Symposium on Polymer Science and Technology
Professor Marinos Pitsikalis, Department of Chemistry, University of Athens, Panepistimiopolis, Zografou, GR-15771, Greece, Tel.: +30 210 727 4440, Fax: +30 210 722 1800, E-mail: pitsikalis@chem.uoa.gr

20–23 November 2010 • Chemistry in Africa • Luxor, Egypt
11th International Chemistry Conference in Africa
Professor Ahmed El-Saghier, University of Sohag, Department of Chemistry, Sohag, 82542 Egypt
Tel.: +20 128 307 176, Fax: +20 934 601 159, E-mail: africaconf2010@yahoo.com

13–16 December 2010 • Nanomaterials and Nanotechnology • Tiruchengode, India
International Conference on Nanomaterials and Nanotechnology 2010
V. Rajendran, K.S.R. College of Technology, Centre of NanoScience and Technology, K.S.R. Kalvi Nagar, Tiruchengode 637 215, India, Tel.: +91 428 827 4880, Fax: +91 428 827 4880, E-mail: veerajendran@gmail.com

2011

IUPAC poster prizes to be awarded

16–21 January 2011 • African Chemical Societies • Johannesburg, South Africa
40th South African Chemical Society Convention & 3rd Federation of African Chemical Societies Meeting
Prof. James Darkwa, University of Johannesburg, Department of Chemistry, Auckland Park 2006, South Africa
Tel.: +27 11 559 2838, Fax: +27 11 489 2819, E-mail: jdarkwa@uj.ac.za

26–29 April 2011 • Functional Polymeric Materials and Composites • Stellenbosch, South Africa
11th UNESCO/IUPAC Workshop and Conference on Functional Polymeric Materials and Composites
Prof. Harald Pasch, University of Stellenbosch, Department of Chemical and Physical Science, Private Bag X1, Matieland 7602, South Africa
Tel.: +27 21 12 808 3173, Fax: +27 21 12 808 4967, E-mail: hpasch@sun.ac.za

22–26 May 2011 • Analytical Sciences • Kyoto, Japan
IUPAC International Congress on Analytical Sciences 2011 (ICAS-2011)
Prof. Koji Otsuka, Department of Material Chemistry, Graduate School of Engineering, Kyoto University
Katsura, Nishikyo-ku, Kyoto 615-8510, Japan
Tel.: +81 75-383-2447, Fax: +81 75-383-2450, E-mail: otsuka@anchem.mc.kyoto-u.ac.jp

Conference Call

23–27 May 2011 • Advanced Materials • Pretoria, South Africa
11th International Conference on Frontiers of Polymers and Advanced Materials
Prof. Walter W. Focke, University of Pretoria, Department of Chemical Engineering, Menlo Park, Pretoria 0102, South Africa, Tel.: +27 21 12 420 3728, Fax: +27 21 12 420 2516, E-mail: walter.focke@up.ac.za

10–14 July 2011 • Biodiversity and Natural Products • Brisbane, Australia
7th International Conference on Biodiversity & 27th International Symposium on the Chemistry of Natural Products
Prof. Mary J. Garson, School of Chemistry & Molecular Biosciences, University of Queensland, Chemistry Building, Room 307, Brisbane, QLD 4072, Australia,
Tel.: +61 7 3365 3605, Fax: +61 7 3365 4273, E-mail: m.garson@uq.edu.au

24–29 July 2011 • Novel Aromatic Compounds • Eugene, Oregon, USA
14th International Symposium on Novel Aromatic Compounds
Prof. Michael M. Haley, Department of Chemistry, University of Oregon, Eugene, OR 97403-1253, USA
Tel.: +1 541 346 0456, Fax: +1 541 346 0487, E-mail: haley@uoregon.edu

24–28 July 2011 • Organic Synthesis • Shanghai, China
16th International Conference on Organometallic Chemistry Directed Toward Organic Synthesis
Dr. Shuli You, Chinese Academy of Sciences, Shanghai Institute of Organic Chemistry, State Key Laboratory of Organometallic Chemistry, 345 Fenglin Lu, Shanghai 2000032, China
Tel.: +86 21 6223 7360, Fax: +86 21 6260 9305, E-mail: slyou@mail.sioc.ac.cn

30 July–7 August 2011 • 43rd IUPAC Congress • San Juan, Puerto Rico
Chemistry Bridging Innovation Among the Americas and the World
Gabriel A. Infante, Pontifical Catholic University of Puerto Rico
E-mail: ginfante@iupac2011.org, www.iupac2011.org

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International Union of Pure and Applied Chemistry

Advancing the worldwide role of chemistry for the benefit of Mankind

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

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Brazilian Chemistry Committee for IUPAC *(Brazil)*
Bulgarian Academy of Sciences *(Bulgaria)*
National Research Council of Canada *(Canada)*
Sociedad Chilena de Química *(Chile)*
Chinese Chemical Society *(China)*
Chemical Society located in Taipei *(China)*
Croatian Chemical Society *(Croatia)*
Sociedad Cubana de Química *(Cuba)*
Pancyprian Union of Chemists (*Cyprus*)
Czech National Committee for Chemistry *(Czech Republic)*
Det Kongelige Danske Videnskabernes Selskab *(Denmark)*
National Committee for IUPAC *(Egypt)*
Chemical Society of Ethiopia *(Ethiopia)*
Suomen Kemian Seura—Kemiska Sällskapet i Finland *(Finland)*
Comité National Français de la Chimie *(France)*
Deutscher Zentralausschuss für Chemie *(Germany)*
Association of Greek Chemists *(Greece)*
Hungarian Academy of Sciences *(Hungary)*
Indian National Science Academy *(India)*
Royal Irish Academy *(Ireland)*
Israel Academy of Sciences and Humanities *(Israel)*
Consiglio Nazionale delle Ricerche *(Italy)*
Caribbean Academy of Sciences—Jamaica Chapter *(Jamaica)*
Science Council of Japan *(Japan)*
Jordanian Chemical Society *(Jordan)*
Korean Federation of Science and Technology Societies *(Korea)*
Kuwait Chemical Society *(Kuwait)*
Fonds National de la Recherche *(Luxembourg)*
Institut Kimia Malaysia *(Malaysia)*
Koninklijke Nederlandse Chemische Vereniging *(Netherlands)*
Royal Society of New Zealand *(New Zealand)*
Norsk Kjemisk Selskap *(Norway)*
Chemical Society of Pakistan *(Pakistan)*
Polska Akademia Nauk *(Poland)*
Sociedade Portuguesa de Química *(Portugal)*
Colegio de Químicos de Puerto Rico *(Puerto Rico)*
Russian Academy of Sciences *(Russia)*
Serbian Chemical Society *(Serbia)*
Slovak Chemical Society *(Slovakia)*
Slovenian Chemical Society *(Slovenia)*
National Research Foundation *(South Africa)*
Ministerio de Educación y Ciencia *(Spain)*
Institute of Chemistry, Ceylon *(Sri Lanka)*
Svenska Nationalkommittén för Kemi *(Sweden)*
Swiss Chemical Society *(Switzerland)*
Tanzania Chemical Society *(Tanzania)*
Chemical Society of Thailand *(Thailand)*
Société Chimique de Tunisie *(Tunisia)*
Türkiye Kimya Dernegi *(Turkey)*
National Academy of Sciences of Ukraine *(Ukraine)*
Royal Society of Chemistry *(United Kingdom)*
National Academy of Sciences *(USA)*
Programa de Desarrollo de Ciencias Básicas *(Uruguay)*

43 rd IUPAC World Chemistry Congress
46 th IUPAC General Assembly
70 th CQPR Annual Conference and Exhibition
July 30 to August 7, 2011

"Chemistry Bridging Innovation Among the Americas and the World"

Organized by the Colegio de Químicos de Puerto Rico (CQPR) on behalf of IUPAC, the Congress will provide the appropriate forum to foster the bridging of innovation in Chemistry and related fields among the Americas and the World and establish a gateway for the new interdisciplinary fields of science developed in the last decade.

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The IUPAC Congress call for abstracts opens in summer 2010. For your opportunity to present your work at this prestigious international congress submit an abstract by March 31, 2011 through *www.iupac2011.org*.

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- Chemical Education and Heritage
- Chemical Synthesis
- Chemistry and the Environment
- Chemistry of Life
- Industrial and Applied Chemistry
- Macromolecular, Supramolecular and Nanotechnology
- Materials Science
- Theoretical, Physical and Computational Chemistry

A more detailed list of topics and invited speakers are published on our regularly updated website.

Confirmed Plenary Speakers

- **Professor Aaron Ciechanover**
  Israel Institute of Technology, Israel
- **Professor Richard R. Ernst**
  ETH Zürich, Switzerland
- **Professor Robert H. Grubbs**
  Caltech, USA
- **Professor Roald Hoffmann**
  Cornell University, USA
- **Professor Mario Molina**
  UC-San Diego, USA and Mexico
- **Professor Richard R. Schrock**
  MIT, USA
- **Professor Ada E. Yonath**
  Weismann Institute of Science, Israel

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