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

# CHEMISTRY International





# From the Editor

#### **CHEMISTRY** International

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

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ach time I write this column, I look back through the proof of the issue at hand or I simply think about what has come across my desk recently. This time, most immediate in my mind was IUPAC's 2009 General Assembly in Glasgow. And, as expected, the buzzword at the GA was "the International Year of Chemistry."

"I Y C two eleven" is now "something" tangible to which we are all committed, and throughout the GA one could sense the enthusiasm and eagerness to participate. Every scheduled meeting had an agenda item devoted to the IYC, including the Council Round Table Discussions and the World Chemistry Leadership Meeting.



For those of you eager to get started on IYC 2011, there is one thing you can do right away, and that is to visit <www.chemistry2011. org> (or iyc2011.org) and join the IYC network. In its current phase, the website offers background information and ideas, and is essentially a virtual meeting place.

We will be building on the site and soon it will provide more functionality. In the end, it will be the central repository of resources and references and of activities being planned for the IYC.

Reflecting now on the GA and reviewing this issue, there is something I read in the treasurer's column which makes me appreciate why IUPAC is special. Aside from the numbers and the flux in the financial markets, the treasurer points out the extraordinary good value that the enormous range of activities carried out within IUPAC represent. This, he added, we owe to the willingness of our numerous volunteers. It is exactly this willingness that makes the GA a pretty unique event. Individuals come to meet, but not in a selfish pursuit; it is not about singular accomplishments, but clearly about a better good. Accordingly, each committee sets its goals to match up with the Union's mission of promoting the norms, values, standards, and ethics of science.

Glasgow was my sixth GA; Berlin in 1999, Brisbane in 2001, Ottawa 2003, Beijing 2005, Torino 2007, they were all different. The pace is set by the officers, and more so by the problems at hand. In Berlin, and for several GAs after that, the project system was the buzzword, which was followed by improving communication and efficiency, and streamlining operations. These were, and still are, internal challenges. However, to embrace now the IYC 2011, which we do with so much enthusiasm, seems to me a reflection of how confident we are that we can do better, not only for IUPAC, not only for chemistry, but for the world. Start planning, and keep in touch with us, with your national chemical society, academy, colleagues, and friends.

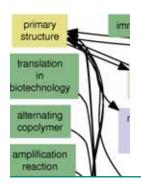


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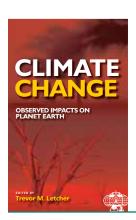
\*Because of the timing, there is nothing about the GA in this issue; do check again in the next issue for the first reports from Glasgow.

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### Treasurer's Column

# When You Walk through a Storm . . .



by John Corish

uring the past 12 months the global financial situation and the states of health, or otherwise, of individual national economies have been analyzed more frequently and with more concern than ever before. And not without good reason, because the rapidity with which the current global

depression descended upon us and its severity are without precedent. We have become almost immune to hearing about new records being set for losses by heretofore profitable and trusted banks, to the size of company bankruptcies, and to the disappearances of what were household names in the commercial world. Thankfully, we have also seen concerted action by the major financial countries and we can at least hope that the worst has now passed.

Before writing this column I read through the Treasurer's Columns published in *Chemistry* International for the past five years. Two of these reported significant increases in our reserves culminating some two years ago in an overall value of our portfolio of in excess of USD 5.5 million. So how have we fared during the current financial difficulties? Well, the blunt answer is not too badly and we are certainly still afloat and with the ability to continue to run the full range of our important programs and to plan with confidence for the upcoming major opportunity that will be provided us in 2011 by the International Year of Chemistry. Given the spread of our financial activities, it would have been quite impossible for us to escape unscathed from the current storm. However, the prudent investment policy adopted and adhered to by our Finance Committee as well as the decision taken some years ago to bill national subscriptions in national currencies rather than only in U.S. dollars and to carry part of our capital in a Euro account has protected us from the worst of the recent downturn.

The values of the three elements of our income stream, national subscriptions, profits from our publishing activities, and investments, have all been maintained. Our investment income is from long-term bonds and has not been adversely affected, and the

billing in national currencies has, taken on average, been of benefit to us. The value of some of our other investments, which are in equities, has fallen and resulted, at the worst point, in a loss of just less than 30 percent of the value of our portfolio. The Finance Committee at its meeting this year considered all our holdings and these have all now been carefully reviewed. The most recent figures to hand show a steady increase in the value of our portfolio since the beginning of this year. In overall terms, there has been a significant recovery and the portfolio has now regained in excess of 40 percent of its losses. This is due in part to the improvement in the markets and also in part to the increased valuation of our Euro holdings. Even in these uncertain times it is reasonable to suppose that this recovery will be at least partially maintained as the world recession is expected to recede and markets to continue to regain value. More detailed figures can be found online in the Financial Report presented to Council in Glasgow on 5 August 2009 <www.iupac.org/symposia/conferences/ga09/ council agenda.html>.

There are two further points that have been made before in Treasurer's Columns, but which bear repeating, particularly during this financially difficult period. The first is to remind ourselves that IUPAC will need to actively pursue alternative sources of income, including sponsorship, if we are to maintain and increase our current range of activities. In particular, extensive fundraising will be required for our effective participation in the IYC in 2011 and I am glad to be able to report that this has been included in the planning process. The second is to stress again that the enormous range of activities that is carried on across the full spectrum of our subject and its applications represents extraordinary good value for money. Critically, it is made possible through the project system only by the dedicated efforts of so many members of IUPAC divisions, standing committees, and their task forces and other groups which do the work voluntarily. To them we continue to owe an incalculable debt of gratitude.

If by some chance you do not know the words of the next line of the anthem used in the title of this column, they are "Hold your head up high," and we can certainly do that.

John Corish <jcorish@tcd.ie> has been treasurer of IUPAC since January 2008. He has served IUPAC at many levels since 1979, including chair of the Subcommittee on Materials Chemistry, president of the Inorganic Chemistry Division, and member of the Finance Committee.

# Institut Kimia Malaysia

# In Pursuit of Excellence in Chemistry

by Ting-Kueh Soon

fter several years as an Associate National Adhering Organization of IUPAC, the Institut Kimia Malaysia, or the Malaysian Institute of Chemistry, has become a full member of the Union—a National Adhering Organization. The Institute's NAO status was ratified unanimously by IUPAC Council at its meeting on 5 August 2009 in Glasgow, Scotland.



The Institut Kimia Malaysia's 41st annual meeting, 29 March 2008.

The Institut Kimia Malaysia (IKM) is a professional organization established to regulate and represent the profession of chemistry in Malaysia. IKM, which has its headquarters in Kuala Lumpur and six branches in other regions of the country, has grown in tandem with the rapid development of the country. With a membership of 2 562 as of 1 January 2009, IKM enjoys a prominent place among the professional scientific organizations in Malaysia. The Institute is also playing a leading role in the development of chemistry in Asia.

The Institute regulates the practice of chemistry in Malaysia, represents the profession of chemistry,

and promotes chemistry education and the public understanding and appreciation of chemistry. IKM also plays a key role in socioeconomic development, including encouraging sustainable development of natural resources and preserving and conserving the natural environment.

### Chemists Act 1975

The IKM was registered under the Societies Act 1966 on 8 April 1967 with 27 founding members. It was subsequently incorporated as a professional body under the Chemists Act 1975 on 1 November 1977. The act gave IKM the authority to regulate and promote the practice of the profession of chemistry in Malaysia.

The act states that only registered chemists of IKM can do the following:

- a. practice as a registered chemist
- b. advertise as a registered chemist
- adopt, use, or exhibit the term "registered chemist"
- sign or certify any report or certificate of analysis intended for the public

Among the key functions of the Institute are determining the qualifications of persons for admission as members and providing training, education, and examinations for those intending to practice chemistry. IKM also regulates the practice of chemistry and promotes the interests of the profession.

Membership of the Institute is open to all persons over 21 years old with a recognized pass or honors degree in chemistry or equivalent academic qualifications and the requisite practical experience. Membership is of three grades: fellowship, associateship and licentiateship. Fellows, associates, and licentiates are entitled to use the initials FMIC, AMIC, or LMIC, respectively, after their names.



IKM meeting with the Ministry of Science, Technology, and Innovation.



Malaysian Chemistry Festival in 2008.



New fellows of IKM in 2008.

### <u>Institut Kimia Malaysia</u>

### **Activities of the Institute**

The Institute carries out a wide range of professional, educational, social, and promotional activities, including membership examinations, chemistry conferences, professional courses and continuing education programs, chemistry publications, and technical and professional visits and study tours. A number of IKM's activities are focused on promoting public understanding and appreciation of chemistry, including the Chemistry and Technology Information Series, the Malaysian Chemistry Festival, and the Malaysian National Chemistry Quiz ( $K_3M$ ).

The Institute also regularly holds regional and international meetings. Among the major regional and international chemical conferences organized by the Institute in recent years are the following:

- Asia Pacific Symposium on Information and Communication Technology in Chemical Education, Research and Development (2002)
- Malaysian Chemical Conference and Exhibition on "Macromolecular Science and Its Impact on Industries" (2004)
- 4th International Conference on Essential Oils, Fragrance, and Flavor Materials (2005)
- MCC International Conference and Exhibition on Green Chemistry (2006)
- 12th Asian Chemical Congress (2007)
- 5th International Conference on Essential Oils, Fragrance and Flavour Materials (2008)

The Institute organized the 10th Asian Conference on Analytical Sciences (ASIANALYSIS X) in Kuala Lumpur, Malaysia, from 11-13 August 2009. LabAsia 2009, an exposition on instrumentation, laboratory equipment, and services, was held in conjunction with ASIANALYSIS X. Another upcoming conference organized by IKM is the Malaysian International Chemical Congress 2010.



Question and answer session at the IKM annual meeting.

### **IKM Moving Forward**

The Institute plans to continue playing a leading role in advancing chemistry in Malaysia and Asia. It intends to focus on chemistry education, research, and development. Strong emphasis will be placed on promoting chemistry education in schools, elevating the level of undergraduate chemistry programs in universities, and promoting cutting-edge research and development in chemistry.

The Institute's strategic goals call for it to emphasize membership development and continuing professional education and training. IKM plans to conduct training courses and workshops on instrumentation and method development in analytical chemistry, chemical safety and security, occupational safety and health, standards, national and international laws and regulations, and other related areas.

The Institute will also play an active role in promoting public awareness and understanding of chemistry, and the roles played by chemistry in socioeconomic development and improving quality of life.

### Council of IKM and Its Committees

The Institute is managed by a 13-member Council elected from its membership, with the director general of chemistry as the registrar. The principal office bearers are elected annually from among the Council members.

The principal office holders of the IKM Council for 2009/10 are as follows:

President:	Datuk Dr. Ting-Kueh Soon
Vice President:	Dato' Chang Eng Thuan
Registrar:	Mr. N. Hithaya Jeevan
Honorary Secretary:	Prof. Datin Dr. Zuriati Zakaria
Honorary Treasurer:	Mr. Steven Tea Hing San
Honorary Asst Secretary:	Assoc. Prof. Dr. Teh Geok Bee
Honorary Asst Treasurer:	Mr. Chee Ong Koh

The Council also establishes a number of committees to ensure the smooth operation and management of the Secretariat and various activities. Members of the Council are appointed as chairpersons of these committees.

### Institut Kimia Malaysia

# National, Regional, and International Cooperation

Under the Chemists Act 1975, the Institute is under the provisions of the Ministry of Science, Technology, and Innovation. The director general of the Chemistry Department Malaysia is the registrar of the Institute.

The Institute is a founding member of the Confederation of Scientific and Technological Associations in Malaysia and the Malaysian Professional Centre. The Institute plays a major role in the governance, operation, and activities of both organizations.

The Institute also works closely with a number of government ministries and agencies including the Ministry of Education, Ministry of Higher Education, Ministry of Health, Ministry of International Trade and Industry, Chemistry Department Malaysia, and the Department of Standards Malaysia.

IKM is represented in the following national councils and committees:

- Malaysian Council of Standards and Accreditation
- National Measurement Council
- Malaysian Council of Food Safety and Nutrition
- Technical Committees and Working Groups of SIRIM Berhad

In addition, the Institute cooperates with Malaysian universities and other institutions of higher learning to promote chemistry education, research, and development. IKM and these institutions are jointly developing undergraduate chemistry programs to suit national development goals and the latest developments in chemical sciences.

IKM is a founding member of the Federation of Asian Chemical Societies (FACS) and takes an active part in FACS activities. The Institute hosted the 12th Asian Chemical Congress in Kuala Lumpur in 2007.

### **IKM Publications**

The Institute publishes the following journals and publications:

- Malaysian Journal of Chemistry (an electronic refereed journal of IKM)
- Berita IKM—Chemistry in Malaysia (a quarterly publication for members)
- Kimia Kini (a semi-annual publication of the Chemistry Education Section)
- Directory of Laboratory Services and Consultancy (an annual publication)



Preparing questions for the 2009 Malaysian National Chemistry Quiz.

### **IKM Awards**

The Institute presents a number of annual awards to recognize professional contributions, academic excellence, and outstanding meritorious service within its membership and profession. Among these awards are the following:

- IKM Gold Medal for Distinctive Contribution to the Profession of Chemistry in Malaysia
- IKM Gold Medal for Excellence in Chemical Research and Development
- Tan Sri Datuk Amar Stephen K.T. Yong Award for significant contribution to development in the industrial sector in Malaysia
- Tan Sri Dato' Sri Law Hieng Ding Award for significant contribution to chemistry education and/or public understanding of chemistry
- Tan Sri Ong Kee Hui Postgraduate Chemistry Medal
- Graduate Chemistry Medals
- IKM Citation Awards for Meritorious Service

In conclusion, the Institute will continue to play a key role in the socioeconomic development of Malaysia. IKM will also play a major role in safeguarding the quality of our environment and ensuring the sustainable management of our natural resources. We will also work closely with other chemical societies from Asia and the rest of the world to ensure that chemical knowledge and innovations are put to good use to serve humankind.

Ting-Kueh Soon <soontk@ikm.org.my> is president of the Institut Kimia Malaysia.



# Consistency and Clarity in Chemical Concepts

# How to Achieve a Codified Chemical Terminology—A Pilot Study

by Ture Damhus, Peder Olesen Larsen, Bodil Nistrup Madsen, and Sine Zambach

onsistency and clarity are essential when defining chemical concepts. However, currently available glossaries in chemistry are lacking in these respects to a certain extent. General terminology methods involving the construction of concept systems and the specification of relations between concepts can be of use here. A pilot study indicates that improvements of the term definitions in enzyme and protein chemistry are possible. Our aim is to raise a discussion about these issues, hopefully resulting in further projects.

IUPAC has made enormous progress through the years in providing systematic chemical nomenclature and terminology. The efforts in terminology are collected in the Gold Book: The IUPAC Compendium of Chemical Terminology. However, the development of new terms via IUPAC projects concerned with delimited areas of chemistry has resulted in glossaries typically with a narrow focus, which means that the Gold Book has become, in principle, an uncritical compilation of glossaries established by various specialist groups for their specific needs. This entails a risk of creating inconsistencies in the overall terminology. We address this problem using fundamental principles of terminology<sup>2</sup> to create concept systems, also referred to as terminological ontologies, as well as to attain clearer and mutually consistent definitions.

# Two Types of Debatable Entries in the Gold Book

Users may find definitions in the Gold Book unsatisfactory for at least two reasons. A definition may be unambiguous and consistent with related definitions in the Gold Book, but may differ from what the user expects or wants as the definition. This type of entry is illustrated in Table 1, comparing definitions from the Gold Book and the Oxford Dictionary of Biochemistry and Molecular Biology,<sup>3</sup> or ODBMB, for short. Perhaps a bit discomforting, text books and dictionaries do not agree on the definitions of a number of fundamental chemistry concepts. Gold Book definitions in those cases, however phrased, will disagree with the opinion of large numbers of practitioners. For cases like this, systematic terminology work will not solve the problem. Somebody has to make a decision, which is often more or less arbitrary, such as whether a molecule may be monoatomic or not, as illustrated in Table 1. Although important enough, this type of situation will not be dealt with in this article.

The second type of unsatisfactory definitions is those that contain inconsistencies that may be widely accepted in the scientific community. This makes it difficult to enlarge such sets by adding new terms and definitions. Also, it may confuse nonexperts like students who are trying to learn what the concepts are about. Examples of this second category will be given below.

<b>Definition from Gold Book</b>	Defir
An electrically neutral entity consisting of more than one atom $(n > 1)$ . Rigorously, a molecule, in which $n > 1$ must correspond to a depression on the potential energy surface that is deep enough to confine at least one vibrational state.	A str cons atom part or or co chem all its
Smallest particle still characterizing a chemical element. It consists of a nucleus of a positive charge ( <i>Z</i> is the proton number and e the elementary charge) carrying almost all its mass (more than 99.9%) and <i>Z</i> electrons determining the size.	A unit single one of The innormal the a addirective of the conventive of the convention of the convent
	An electrically neutral entity consisting of more than one atom $(n > 1)$ . Rigorously, a molecule, in which $n > 1$ must correspond to a depression on the potential energy surface that is deep enough to confine at least one vibrational state. Smallest particle still characterizing a chemical element. It consists of a nucleus of a positive charge ( $Z$ is the proton number and e the elementary charge) carrying almost all its mass (more than 99.9%) and $Z$ electrons determining

Definition from ODBMB
A structural unit of matter

consisting of one or more atoms; the smallest discrete part of a specified element or compound that retains its chemical identity and exhibits all its chemical properties.

A unit of matter consisting of a single nucleus surrounded by one or more orbital electrons. The number of electrons is normally sufficient to make the atom electrically neutral; adding or removing electrons converts the atom into a negative or positive ion, but this is regarded as a state of the same atom since the atom is characterized by its nucleus.

Table 1. Comparison of two basic definitions presented in the Gold Book and the ODBMB.

### The Pilot Study

Our purpose in the pilot study is to create an ontology or ontologies and a term database for enzyme chemistry, based on available recommendations, in particular from the Gold Book and ODBMB.<sup>1,3</sup> For a start, we have chosen to work in two narrow subfields: enzyme inhibition and protein structure. By using principles of terminology we intend to avoid creating inconsistencies when expanding the ontologies. We are using the concept modelling tool i-Model from i-Term;<sup>4</sup> the system i-Term is a terminology and knowledge management system that combines facilities of a traditional term base with a concept modelling tool.

### **How to Define Terms**

Instead of focusing on each definition, we work according to the terminological method with the concepts in a concept system (an ontology). Therefore, we need to formalize the relations between the concepts and to introduce characteristics delimiting related concepts (feature specifications, consisting of attribute-value pairs). On the basis of these feature specifications, subdivision criteria are introduced, which group concepts and thereby give a good overview. These methods are described in conference proceedings referenced below.<sup>5,6</sup>

In our work, we use an iterative process: analyzing the concepts as well as placing them in draft concept systems in the form of hierarchies or networks on the basis of their characteristics, then drafting definitions, and, finally, refining concept systems as well as definitions. In this way, we arrive at consistent definitions referring to the superordinate concept (i.e., *genus proximum* or nearest kind) and followed by the delimiting characteristic.

In the example shown to the right in Figure 1, the *genus proximum* is inhibition, one subdivision criterion or attribute is MECHANISM, and one of the attribute values is "a product of the reaction is the inhibitor."

The superordinate concept and the attribute of the feature specification must be the same in definitions of *subordinate* concepts falling under one subdivision criterion.

# Inhibition as Kinetics and Mechanism

Figure 1 clarifies the differences between various subtypes of *inhibition*. Seven of these concepts fall within two groups according to the two subdivision criteria: KINETICS and MECHANISM.

The three concepts allosteric inhibition, substrate inhibition, and product inhibition differ with respect to

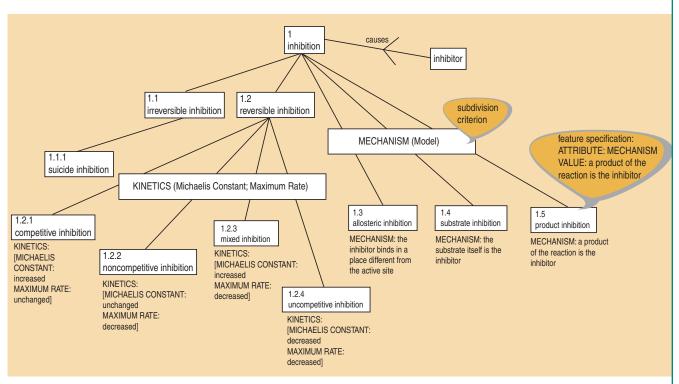


Figure 1. Extract of the inhibition diagram.

### Consistency and Clarity in Chemical Concepts

MECHANISM, and, therefore, the definitions of these concepts should focus on *mechanism*. However, as may be seen from Table 2, the definitions from ODBMB do not clearly reflect this.

Concept	Definitions from ODBMB	Characteristic features
allosteric inhibition	Any inhibition of an enzyme by a negative allosteric effector.	MECHANISM: the inhibitor binds at a place different from the active site
substrate inhibition	The inhibition of an enzyme's activity by its substrate by an allosteric mechanism.	MECHANISM: the substrate itself is the inhibitor
product inhibition	The inhibition of an enzymatic reaction caused by increased concentration of one or more products of that reaction	MECHANISM: a product of the reaction is the inhibitor

Table 2. Comparison of the definitions from ODBMB and characteristic features (as shown in figure 1), for three inhibition concepts falling under the attribute 'mechanism'.

According to the terminological principles described in the conference proceedings referenced below, <sup>5,6</sup> two concepts with the same superordinate concept must not differ with respect to more than one characteristic, except if they belong to a "polyhierarchy," where the concepts in question have two or more superordinate concepts belonging to different subdivision criteria. In our area of study, however, concepts are often delimited by a combination of characteristics. In Figure 1, the four subordinate concepts to the concept *reversible inhibition* differ with respect to KINETICS, which is a composite characteristic having two feature specifications with the attributes MICHAELIS CONSTANT and MAXIMUM RATE.

The diagram in Figure 1 also illustrates that a concept system may comprise *hierarchical* relations (*type* relations) as well as *associative* relations. Associative relations have a relation name and an arrow indicating the direction of the relation (e.g., the relation *causes* between *inhibitor* and *inhibition*).

#### What Is Protein Structure?

Everybody dealing with protein chemistry uses the terms *primary, secondary, tertiary,* and *quaternary structure*. Nevertheless, writing an agreeable set of definitions for them is not easy. Table 3 shows the ODBMB and Gold Book definitions for the three first concepts. We also add the definitions of the structural elements  $\alpha$ -helix and  $\beta$ -pleated sheet, mentioned in

both sources in their definitions of secondary structure, but only defined in ODBMB.

There are several observations to be made. First of all, the two definitions of primary structure clearly do not agree on whether one is allowed to regard cross-linking as part of primary structure. This difference is of the same kind as we noted above with the definitions of atom and molecule (see Table 1). Another observation is that in each of the two sources, the style of wording varies considerably from primary over secondary to tertiary structure. ODBMB speaks of "first order of complexity in structural organization," then of "arrangement of . . . structure" and then "level of structure." Gold Book has "constitutional formula . . . abbreviated to sequence," then "conformational arrangement," and, for tertiary structure, "spatial organization." A third comment is that the ODBMB explanations in particular contain more than is needed for defining the term; there is commentary and additional information. However, ODBMB is a dictionary and readers will expect this kind of material to be included.

The terms  $\alpha$ -helix and  $\beta$ -pleated sheet appear in both sources as examples of secondary structure elements. The definitions in ODBMB look very different in that some geometrical facts about  $\alpha$ -helices are included that are actually a consequence of the definition of the concept and the way amino acids bind to each other. The definition of  $\beta$ -pleated sheet looks much briefer, but it turns out that if one looks up the term  $\beta$ -strand appearing in the definition, this is defined again via  $\beta$ -conformation, the explanation for which is just as lengthy as the one for  $\alpha$ -helix. We note in particular that a definition may rely on a term that itself needs to be defined before the first definition is understandable. Another example of this in Table 3 is conformation and conformational, which appear in several places.

We have attempted to put the definitions on a more equal footing and to explore whether they can be satisfactorily arranged in a hierarchy. The column to the far right in Table 3 shows the definitions we suggest at the moment and the diagram proposed in Figure 2 shows the hierarchy. The concepts secondary and tertiary structure (and quaternary structure, which we have tentatively included in the diagram) have the superordinate concept conformation, while primary structure is seen as a subordinate concept to constitution; conformation and constitution are subordinate concepts to molecular structure. The characteristic feature LEVEL (inspired by one of the wordings in the sources) distinguishes the three structure terms. The job is not finished, however; we still need to resolve

### How to Achieve a Codified Chemical Terminology—A Pilot Study

the issue about the disulfide bonds, and we have to deal with the definitions of *conformation* and of  $\beta$ -strand, both of which may turn out to necessitate even further definitions until we end at basic terms that may be assumed to have unique interpretations by all practitioners.

All in all, the establishment of usefully worded and consistent definitions of concepts in a hierarchy is an iterative process, in which all steps are subjected to the principles explained above.

# Future Steps towards a Consistent Terminology

Among the advantages of working with concept systems is that they can clarify concepts by pruning the descriptions. This is achieved by identifying the characteristics delimiting terms derived from the same superior concepts, which makes the differences between the concepts clear (e.g, competitive inhibition versus noncompetitive inhibition and secondary

structure versus tertiary structure). Using this methodology, the definitions of the concepts themselves can be clarified as well as the relations between concepts (such as causes, inhibits, or activates), which provides a better understanding of the concepts and their use.

The online edition of the Gold Book provides the possibility of seeing the relations between concepts. Figure 3 shows an example of the relations existing in Gold Book for a number of the concepts included in our work. This facility is useful for finding additional related concepts. However, it is not possible to figure out the types of relations.

Presenting concept systems with specified concept relations and concept characteristics can be useful not only for the general chemist to understand the enzyme chemist, but also for students at all levels to obtain a more conceptual understanding of the words used in chemical textbooks and articles. Just as the periodic table can help students get an overview of electro-negativity, number of electrons in each orbital shell, and atomic radii, a systematic display of the

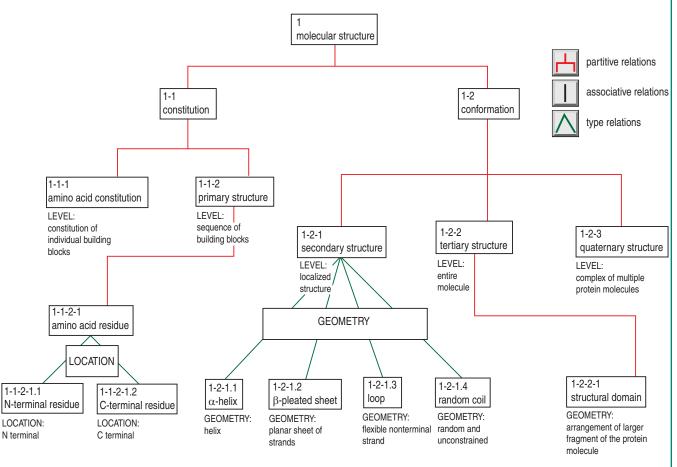


Figure 2. Extract of the protein structure diagram.

### Consistency and Clarity in Chemical Concepts

Concept	Definitions from ODBMB	Definitions from Gold Book	Characteristic feature	Proposed definitions based on concept diagram
primary structure	The first order of complexity of structural organization exhibited by polypeptide and protein molecules, and by polynucleotide and nucleicacid molecules. When applied to a segment of a polypeptide chain, or to a polypeptide or protein molecule, it refers to the linear sequence of the amino-acid residues of the polypeptide chain(s), without regard to spatial arrangement, apart from configuration at the $\alpha$ -carbon atoms (and excluding positions of any disulfide bonds).	In the context of mac- romolecules such as proteins, constitutional formula, usually abbrevi- ated to a statement of the sequence and if appropriate cross-linking of chains.	LEVEL: sequence of building blocks	Sequence of building blocks in a linear macromolecule, such as the sequence of amino acid residues in a polypeptide chain.
secondary structure	Arrangement of the polypeptide structure into locally-organized, hydrogen-bonded structures, in particular $\alpha\text{-helices}$ and $\beta$ sheets	The conformational arrangement ( $\alpha$ -helix, $\beta$ -pleated sheet, etc.) of the backbone segments of a macromolecule such as a polypeptide chain of a protein without regard to the conformation of the side chains or the relationship to other segments.	LEVEL: local- ized segments	Part of the conformation of a polypeptide (or other macromolecule) specifying the internal spatial arrangement of individual backbone segments without regard to the conformation of side chains or the relationship to other segments.
tertiary structure	The level of protein structure at which an entire polypeptide chain has folded into a 3-D structure. The tertiary structure results from interactions between amino-acid residues that may be widely separated in the primary structure, but may be brought into proximity by the folding of the polypeptide chain.	The spatial organization (including conformation) of an entire protein molecule or other molecule consisting of a single chain.	LEVEL: entire molecule	Part of the conformation of an entire polypeptide (or other macromolecule consisting of a single chain) specifying the spatial arrangements of all backbone segments relative to each other.  Comment: The tertiary structure results from interactions between amino-acid residues that may be widely separated in the primary structure, but may be brought into proximity by the folding of the polypeptide chain.
α-helix	A helical, or spiral conformation of a polypeptide chain in which successive turns of the helix are held together by hydrogen bonds between the amide peptide links, the carbonyl group of any given residue being hydrogen-bonded to the imino group of the third residue behind it in the chain. An $\alpha$ -helix has 3.6 residues per turn, and the pitch is 5.4 Å per turn. The helix may be left- or right handed, the latter being much more common.	Not defined.	GEOMETRY: helix	Secondary structure element consisting of a helical conformation in which turns of the helix are held together by hydrogen bonds between the amide links in such a way that the carbonyl group in every amide link is bonded by a hydrogen bond to the imino group in the amide link three residues behind the first amide link. $ \textit{Comment:} \   \text{An } \alpha \text{-helix has } 3.6 \ \text{residues per turn, and the pitch of the helix is } 5.4 \ \mathring{\text{A}}. \   \text{The helix may be left- or right-handed, the latter being much more common.} $
β-pleated sheet	An approximately planar array of two or more adjacent $\beta$ -strands such that hydrogen bonds may be formed between C=O groups of one $\beta$ -strand and NH groups of another.	Not defined.	GEOMETRY: planar sheet of strands	Secondary structure element consisting of a planar array formed by two or more adjacent $\beta\text{-strands}$ via hydrogen bonds between carbonyl groups of one $\beta\text{-strand}$ and imino groups of another.

Table 3. Definitions from ODBMB and Gold Book of selected molecular structure concepts illustrated in figure 2.

### How to Achieve a Codified Chemical Terminology—A Pilot Study

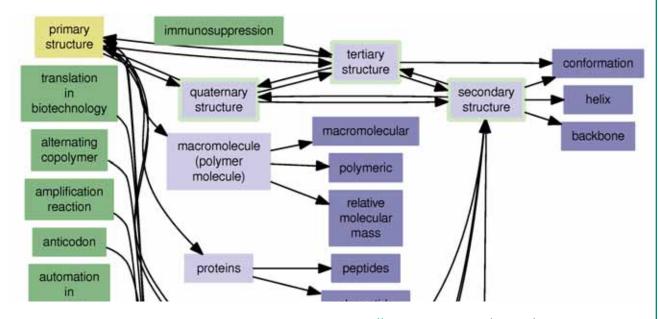


Figure 3. Example of interactive link map from the Gold Book <a href="http://goldbook.iupac.org/Graphs/P04843.2.map.html">http://goldbook.iupac.org/Graphs/P04843.2.map.html</a>.

concepts used in chemistry and biochemistry may help the student toward a better understanding of the meaning of the terms involved.

Our work aims to identify and rectify inconsistencies in the two selected subject areas. We feel it is important to extend this work to larger fields. This will require cooperation among chemists and terminologists. As a first step, we are proposing a joint IUPAC-IUBMB project to extend our first results and set up guidelines for future work.

This study is still at an early stage. Therefore, we encourage readers to contact us if they want to comment or contribute and/or eventually to participate in forthcoming projects.

### Acknowledgements

Annemette Wenzel and Lone Bo Sisseck, both then at the DANTERM terminology centre, contributed in the early phases of this study.

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's a professor at Copenhagen Business School, Denmark, Dept. of International Language Studies and Computational Linguistics, and head of the terminology centre, DANTERMcentret; she is also chair of ISO TC 37, SC 3 (systems to manage terminology, knowledge, and content). Sine Zambach <sz@ruc.dk> is a Ph.D. fellow in Computer Science at Roskilde University. She holds a master's degree in biochemistry and bioinformatics.

# Increasing the Global Impact of the Polymer Division

### by Christopher K. Ober

he IUPAC Polymer Division recently created several new prestigious research awards. These awards, presented at the biennial IUPAC World Polymer Congress (WPC), have the effect of recognizing the talents of remarkable polymer chemists from around the world while and at the same time attract-

ing researchers to the WPC and raising the visibility and prestige of the Polymer Division.

The division now administers the IUPAC-Samsung Young Polymer Scientist Award, the DSM Performance Materials Award (with the cooperation of IUPAC), and the IUPAC-Polymer International Award. Both the "DSM-IUPAC" and the "IUPAC-PI" Awards were presented for the first time at the 2008 IUPAC World Polymer Congress. The Polymer Division was directly involved in the selection of the following award winners: Craig Hawker (USA), DSM-IUPAC

Award; Zhenan Bao (USA), IUPAC-PI Award: and Eric Cloutet (France), Samsung Award. Nominations for the DSM-IUPAC and the IUPAC-PI awards are underway for MACRO2010.

The first award offered by the Polymer Division was the IUPAC-Samsung Young Polymer Scientist Award. Candidates for this award are identified by the organizers of the World Polymer Congress from among the presenters who will attend the meeting. A short list is provided to selected members

of the Polymer Division who select the winner of the award. There is an award ceremony held during the plenary session of the conference and a cash prize is provided to the winner. The prize has the advantage that it recognizes younger scientists and draws them to the conference, but it also provides the winner with early career recognition in the international community. The award is new enough that previous winners are still midcareer, but to date all indications are that these individuals will have very successful careers. The

fund that is used to support the award also provides funding to help run the WPC. The division is very grateful to Samsung-Total for its sponsorship of this

The most lucrative award is the DSM Performance Materials Award. The award winner receives a 50 000 Euro prize, a symposium is held on a topic related to

> his or her research, and the winner gives one of the plenary talks at the conference. There is a public ceremony following the plenary talk during which the award winner receives his or her award. At MACRO2008 in Taipei, the talk and symposium were very well attended and among the most popular events held at the conference. The very generous sponsorship by DSM also provides for support for the special symposium and is very much appreciated by the organizers of the WPC.

> The most recent award is the IUPAC-Polymer International Award. This award, supported by the journal Polymer

> > International and its publisher Wiley Interscience, provides a cash prize to a young midcareer polymer chemist and gives an opportunity for the award winner to provide a keynote lecture during the World Polymer Congress.

> > Each award is different. but together they cover the career arc of polymer chemists from young to established. The awards also provide financial aid to the organizers of the Congress and a focal point to the program. Finally, they provide IUPAC with an opportu-

nity to reach out to the polymer chemistry community and enhance its visibility as an organization that is providing a service to chemistry in the service of society. 🛣



Award.



Craig Hawker (right) receives the first DSM Performance Materials Award from Professor Joseph Put, chief technology officer of DSM.

Christopher K. Ober <cko3@cornell.edu> is Francis Bard Professor of Materials Engineering at Cornell University. He is president of the IUPAC Polymer Division.



# **MACRO2010**

# 43rd IUPAC World Polymer Congress

**Polymer Science in the Service of Society** 

**11 - 16 July 2010** SECC, Glasgow, UK



'Macro2010' is the latest in the series of the biennial meetings of the IUPAC Polymer Division. With a history spanning several decades, this is the largest international multi-symposium conference dedicated to all aspects of polymer science and engineering.

### **Themes**

- Delivering New Polymers for Service in Society: Advances in Polymer Chemistry
- Molecular to Macroscopic Behaviour of Polymers
- Sustainability: Renewable Resources and Environmentally-Friendly Polymers
- Polymers in Support of Life
- Functional Polymers for Electronics, Energy and Analysis
- Polymer Science in Everyday Life
- Advances in Colloidal and Nanosize Polymer Materials
- Young Polymer Scientists: Contributions, Nurturing and Networking

A more detailed list of topics and invited speakers are published on our regularly updated website **www.MACRO2010.org**.

### **Confirmed Plenary Speakers**

Professor Jean M J Fréchet University of California, Berkeley, USA

Professor Sir Richard Friend, FRS University of Cambridge, UK

Professor Ming Jiang Fudan University, China

Professor Laura Kiessling University of Wisconsin-Madison, USA

Professor Kiyohito Koyama Yamagata University, Japan

Professor Ludwik Leibler ESPCI CNRS, Paris, France



### Call for Abstracts

The Macro2010 call for abstracts opens in late summer 2009. For your chance to present your work submit an abstract by 29 January 2010.

### **Sponsorship and Exhibition**

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# **IUPAC** Wire

# IUPAC Funding Opportunities in International Polymer Chemistry

UPAC announces a transnational/transcontinental call for proposals in polymer chemistry supported by a consortium of funding agencies. The goal of this first pilot call is to establish an efficient transnational funding program in chemistry, transcending national boundaries, with minimal bureaucracy.



This call is intended to foster trinational cooperation in polymer chemistry and encourages involvement of researchers from developing countries. All researchers working in this field and eligible to apply for financial support from their participating national research councils are cordially invited to apply. This program is designed for interested research teams involving three principal investigators, each working in a different country. Each team will submit one joint proposal.

Many more details can be found on the website listed below. Those interested in this opportunity should be aware of the following dates:

- 1. Letters of intent are due 15 November 2009.
- 2. For the eligible projects, the full proposals are due 15 February 2010.
- 3. The final results of this call will be conveyed to applicants by 15 September 2010.
- 4. The funding of all successful proposals will start no later than January 2011.

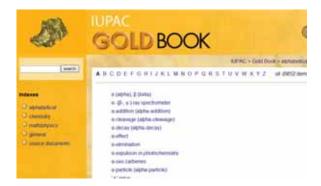


### **Gold Book Update**

t's not quite a precious resource, but the Gold Book online just became a lot more valuable. Significant enhancements have been made to the electronic version of the IUPAC Compendium of Chemical Terminology over the past few months. In June 2009, release 2.1.0 was made public-a major, new update with almost 300 entries either added or updated. This version also includes other improvements, such as better positioning of mathematical formulas on a line, acronyms as part of the title in the alphabetical index, improved support for names of characters (such as alpha, lambda) in full-text search, improved alternative text for images of mathematical formulas, and other smaller changes. The release also provides a brand new structure search that complements the standard text-based search.

In July 2009, software tools were introduced that enable the automatic addition of links to Gold Book terms contained in PDFs and HTML documents. The software tools are placed separately on SourceForge, which allows for easier collaboration on the software. The "Goldify" project consists of several parts:

- Java—This is the main tool, the goldify program itself, written in Java and containing both a standalone and a client-server version.
- Javascript—This directory contains a JavaScript version of goldify which allows client-side addition of links to Gold Book terms. It is completely separate from the Java version.
- Resources—These are XML files which describe the terms defined in the XML Gold Book. They are used by the java tool and are also a good resource for third-party tools.



One readily available resource that has been "goldified" is IUPAC's own scientific journal *Pure and Applied Chemistry (PAC)*. Each *PAC* abstract now has seamless links back to Gold Book entries. More than 1800 abstracts have terms that link back to the Gold Book, generating a total of 17 758 links! Links are made "on-the-fly"—this way the original abstracts are not modified, making future changes more manageable and keeping the load on the server pretty small.

Browse the Gold Book at <a href="http://goldbook.iupac.">http://goldbook.iupac.</a> org> and see from PAC, how it works at <www.iupac. org/publications/pac>.

For feedback/comments/ideas, please contact project leader Bedrich Kosata <kosatab@vscht.cz>.

### **IUPAC Members Recognized at Pittcon**

ittcon is the world's premier conference and exposition on laboratory science and the major meeting place for the inventors, users, manufacturers, and vendors of laboratory instruments, equipment, and supplies. At Pittcon 2009, which was held March 8-13, 2009, McCormick Place, Chicago, Illinois, 11 major awards were presented, including two to IUPAC members.

The 2009 Analytical Chemistry Award for Young Investigators in Separation Science was presented to Nelson Torto of Rhodes University. In particular, the award recognizes and encourages outstanding contributions to the field of separation science by a chemist or chemical engineer within 10 years of their degree.

Martin Quack, a member of the IUPAC Commission on Physicochemical Symbols, Terminology, and Units, was presented with the 2009 Bomem-Michelson Awardee, Quack is a full professor at the Swiss Federal Institute of Technology in Zürich. He is involved in the revision of the IUPAC Green Book and preparing it for translation. The Bomen-Michelson Award honors scientists who have advanced techniques of vibrational, molecular, Raman, or electronic spectroscopy.

www.pittcon.org/technical/awards.html

### Thieme-IUPAC Prize—Call for **Nominations**

he Thieme-IUPAC Prize is presented every two years on the occasion of the IUPAC International Conference on Organic Synthesis (ICOS). The next conference, ICOS-18, will be held in Bergen, Norway, between 1-6 August 2010.

Sponsored jointly by Georg Thieme Verlag, IUPAC, and the editors of SYNLETT, SYNTHESIS, Science of Synthesis, and Houben-Weyl, the prize is awarded to a scientist under 40 years of age whose research has had a major impact in synthetic organic chemistry.

The prize is given on the basis of scientific merit for independent research dealing with synthesis in the broadest context of organic chemistry, including organometallic chemistry, medicinal and biological chemistry, designed molecules, and materials. Candidates must be under 40 years of age as of January 1 of the year in which the prize is awarded.



www.iupac.org/news/Thieme\_prize.html www.thieme-chemistry.com/en/our-service/thieme-iupac-prize.html

### **CHEMRAWN VII Prize for** Atmospheric and Green Chemistry— Call for Nominations

he CHEMRAWN VII Future Actions Committee and the IUPAC Organic and Biomolecular Chemistry Division have established the Prize for Atmospheric and Green Chemistry, to be awarded biennially at the IUPAC Conference on Green Chemistry. Pietro Tundo, president of the Organic and Biomolecular Chemistry Division, announced the new prize at the IUPAC Council Meeting, 6 August 2009, in Glasgow, Scotland.

Beginning in 2010, the prize of USD 5 000 will be granted to a young investigator (less than 45) from a developing country. The first award will be given at the third IUPAC International Conference on Green Chemistry, 15-19 August 2010 in Ottawa, Ontario, Canada.

Nominations for the first prize are due 31 December 2009. Each nomination should include a CV and two letters of support, plus a brief summary of research, illustrating the contribution of the applicant to the field of green chemistry, and emphasizing atmospheric chemistry. Applications should be sent to the IUPAC Secretariat at <secretariat@jupac.org> or to P.O. Box 13757, Research Triangle Park, NC 27709-3757 USA.

The Selection Committee is composed of the president of the Organic and Biomolecular Chemistry Division, who serves as chair; the chair of the Subcommittee on Green Chemistry; and the chair of CHEMRAWN.

www.iupac.org/web/nt/2008-08-28\_CHEMRAWN\_VII\_Prize

### InChl Trust

he InChl Trust, a not-for-profit organization formed to expand and develop the InChl Open Source chemical structure representation algorithm, was formally launched in July 2009. Originally developed by IUPAC, the International Chemical Identifier (InChl) is an alpha-numeric character string generated by an algorithm. The InChl was developed as a new, nonproprietary, international standard to represent chemical structures. The Trust aims to develop and improve on the current InChl standard, further enabling the interlinking of chemistry and chemical structures on the web. The connection with IUPAC is maintained through IUPAC's InChl Subcommittee.

The InChI algorithm turns chemical structures into machine-readable strings of information. InChIs are unique to the compound they describe and can encode absolute stereochemistry. Machine-readable, the InChI allows chemistry and chemical structures to be navigable and discoverable. A simple analogy is that InChI is the bar-code for chemistry and chemical structures. The InChI format and algorithm are nonproprietary and the software is open source, with ongoing development performed by the community.

"The goal of the InChI Trust," says project director Stephen Heller, "is to continue to develop the InChI and InChIKey, the condensed machine-searchable version, as a tool to enable widescale linking of chemical information."

The InChI Trust was formally incorporated in the UK in May 2009, and now has six charter members: The Royal Society of Chemistry, Nature Publishing Group, FIZ-Chemie Berlin, Symyx Technologies, Taylor & Francis, and OpenEye. More organizations and publishers are in the process of joining the InChI Trust.

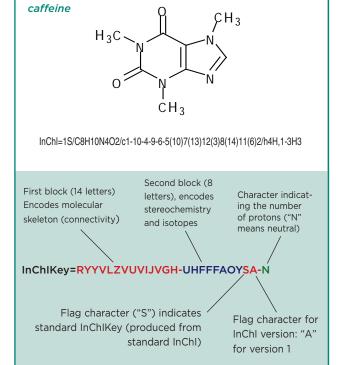
"Nature Publishing Group is delighted to be a charter member of the InChI Trust," says Jason Wilde, publisher for the physical sciences, Nature Publishing Group. "We view the ongoing maintenance of the InChI algorithm, and the resulting adoption of InChI, as important for the development of chemistry communication. The interlinking that the InChI offers between journal content and databases ensures that chemistry is the first truly web-enabled scientific discipline."

"The InChI has already gained a wide user base," says Richard Kidd, informatics manager at the Royal Society of Chemistry, "and the Trust will ensure continuing development and support for this key standard, helping to link together chemical resources

across the internet. The RSC is proud to support the InChI Trust."

Since the introduction of the InChI in 2005, there has been widespread adoption of InChI standards by public databases and journals. Today, there are more than 100 million InChIs in scientific literature and products.

To date, numerous databases, journals, and chemical structure drawing programs have incorporated the InChI algorithm. These include the NIST WebBook and mass spectral databases, the NIH/NCBI PubChem database, the NIH/NCI database, the EBI chemistry database, ChemSpider, Symyx Draw, and many others.



The initiative serves chemists, publishers, chemical software companies, chemical structure drawing vendors, librarians, and intermediaries by creating an international standard to represent defined chemical structures. This provides a consistent, credible, and compatible way for databases of chemical structures to be linked together for the benefit of users of chemical information around the world.

For further information, contact Stephen Heller at <steve@inchi-trust.org>.

www.inchi-trust.org and www.iupac.org/inchi/

### The Project Place

### Visualizing and Understanding the Science of Climate Change

Barraged by contradictory messages from media, many don't have the right tools to know what to think about the connection between human activity and our changing climate. This project brings together chemists and educators from the IUPAC Committee on Chemistry Education, The King's Centre for Visualization in Science (Canada), The Royal Society of Chemistry (UK), American Chemical Society (USA), UNESCO, and the Federation of African Societies of Chemistry to develop a set of critically reviewed, interactive, web-based materials for global dissemination to help students visualize and understand the underlying science of climate change. Target audiences are (a) teachers at the secondary and first-year tertiary levels, (b) students at those same levels, and (c) chemistry professionals. Visualizations will emphasize the fundamental chemistry of climate processes, but will also present research climate models, and place anthropogenic inputs to our atmosphere in a geo-political context.

The outcomes will contribute to the International Year of Chemistry's goal of promoting the critical role of "education in and about chemistry" in "addressing challenges such as global climate change, in providing sustainable sources of clean water, food and energy, and in maintaining a wholesome environment for the well being of all people . . . . "

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



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

### A Critical Evaluation of the Viscosity and Density of Molten Copper and Tin

There is an increasing use of mathematical models to simulate a variety of processes involving liquid metals such as "cast to shape," primary and secondary metal production, powder production by spray forming, and welding. Depending on what aspect of the process is modeled, there is a need for viscosity data for the relevant metals or their alloys.

Historically, there are wide discrepancies in the viscosity data reported for the metallic elements and for alloys (1) and in general reported values for viscosity can be up to an order of magnitude apart. Hence, only an internationally accepted committee can collect and critically evaluate such data.

In a previous IUPAC project standard reference correlations for the viscosity and density of aluminium and iron were proposed (2). The proposed standard reference correlations for the density of aluminium and iron are characterized by 0.65% and 0.77% percentage standard deviation, while the standard reference correlations for the viscosity are characterized by 13.7% and 5.7% percentage standard deviation, at the 95% confidence level, respectively.

The viscosity and density of aluminium covered a temperature range 930-1270 K and iron 1800-2100 K. The proposed study of copper and tin will cover the temperature ranges 1350-1700 K and 500-1050 K, respectively, and thus will provide a complete temperature range for the viscosity and density from 500-2100 K for industrial application.

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For more information and comments, contact Task Group Chair Marc J. Assael <assael@auth.gr> or William A. Wakeham <vice-chancellor@soton.ac.uk>.



www.iupac.org/web/ins/2008-045-2-100

### A Database of Water Transitions from Experiment and Theory

The water molecule is arguably the single most important species from a spectroscopic point of view. It is certainly molecule number 1 in the standard atmospheric database HITRAN since it is both the largest absorber of sunlight in the earth's atmosphere and the major greenhouse gas. This means, for example, that its isotopologue H<sub>2</sub><sup>18</sup>O is the fifth biggest absorber in the earth's atmosphere. Water spectra are equally important astronomically: absorption by hot water dominates the atmospheres of M-dwarfs, the most common stars in our galaxy, and has recently been identified in the extra-solar planet HD189733b.

There have been many years of work and hundreds of papers on the laboratory spectroscopy of water but

### The Project Place

obtaining reliable spectroscopic parameters for water remains an unresolved problem. The Task Group was created to synthesize the known data on water spectra, whether experimental or theoretical, and carefully validate them.

As a first major task, the project has established a protocol for inverting transition frequencies taken from high-resolution laboratory spectra to give energy levels. The procedure, called MARVEL (Measured Active Rotational-Vibrational Energy Levels) is based on the use of the so-called X-matrix method, which has been in use for some time, for producing energy levels from a single spectrum. Adapting the X-matrix to large datasets of heterogeneous data raises a number of issues to do with both consistency of the underlying data and that of the published uncertainties. These are addressed in MARVEL itself before and during the inversion process, and post hoc by comparing the labelled MARVEL energy levels with those obtained from high-accuracy variational nuclear motion calculations and with combination differences.

The Task Group recently published the first part of a series of articles reporting critically evaluated rotational-vibrational line positions, transition intensities, pressure dependence, and energy levels, with associated critically reviewed assignments and uncertainties, for all the main isotopologues of water. The article,<sup>2</sup> which also sets out the strategy the Task Group wishes to follow, contains energy levels and data for line positions of the singly substituted isotopologues  $H_2^{17}O$ and H<sub>2</sub><sup>18</sup>O. The procedure and code MARVEL is used extensively in all stages of determining the validated levels and lines and their self-consistent uncertainties. The spectral regions covered for both H<sub>2</sub><sup>17</sup>O and H<sub>2</sub><sup>18</sup>O are 0-17125 cm<sup>-1</sup>. The energy levels are checked against ones determined from accurate variational calculations. The number of critically evaluated and recommended levels and lines are, respectively, 2687 and 8614 for  $H_2^{17}O$  and 4839 and 29364 for  $H_2^{18}O$ . Among other things, the list of validated energy levels can be used to give very precise predictions of yetto-be measured line frequencies. The active nature of this activity is illustrated by the publication of new spectra subsequent to the completion of this paper by some task group members. Similar studies are now underway for HD<sup>16</sup>O, HD<sup>17</sup>O, and HD<sup>18</sup>O, which will be reported shortly, and for the main isotopologue, H<sub>2</sub><sup>16</sup>O, for which the dataset collected contains more than 100 000 transitions.

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For more information and comments, contact Task Group Chair Jonathan Tennyson <j.tennyson@ucl.ac.uk>.



www.iupac.org/web/ins/2004-035-1-100

### Host Companies Needed

The IUPAC Committee on Chemistry and Industry (COCI) is seeking host companies for the IUPAC Safety Safety Training Program, which **Training** enables experts from developing countries to learn **Program** about safety and environmental protective measures by visiting and working with IUPAC Company Associates in industrialized countries.

Several trainees are currently awaiting placement at Host Companies. All are professional scientists and engineers who are supervisors or managers in chemical companies, government institutions, or academic laboratories. IUPAC provides funding for trainee travel to the Host Company, and the Host Company provides for local expenses during training.





Contact Mark Cesa <mark.cesa@ineos.com>, COCI chair and STP coordinator, for more information and to volunteer!



www.iupac.org/standing/coci/safety-program.html

### Provisional Recommendations

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

www.iupac.org/reports/provisional

### Glossary of Terms Used in Biomolecular Screening

Biomolecular screening is now a crucial component of the drug discovery process and this glossary of terms will be of use to practitioners in the field of screening and to those who interact with the screening community. The glossary contains definitions related to various aspects of the screening process such as assay types, data handling, and relevant technologies. Many of the terms used in this discipline are not covered by existing glossaries, and in the cases where they are, the definitions are often not appropriate. This document provides new or modified definitions to better reflect the new context. The field of biomolecular screening is multidisciplinary in nature and this glossary of authoritative definitions will be useful not only for regular practitioners, but also for those who make use of the data generated during the screening process.

### Comments by 30 September 2009

John Proudfoot <john.proudfoot@boehringer-ingelheim.com> Boehringer Ingelheim Pharmaceuticals Inc 900 Ridgebury Road Ridgefield, CT 06877, USA



www.iupac.org/reports/provisional/abstract09/proudfoot\_300909.html

### Metrological Traceability of Measurement Results in Chemistry: **Concepts and Implementation**

This IUPAC study aims at formulating recommendations concerning the metrological traceability of a measurement result in chemistry. It is intended to provide the chemical measurement community with a consistent view of the creation, meaning, and role of metrological traceability and its underpinning concepts. No distinction is made between measurement results obtained in "high metrology" and in the "field". A description is given of the calibration hierarchies needed in different circumstances to arrive at metrological traceability along a metrological traceability chain. Flow charts of generic calibration hierarchies are presented as well as a variety of examples. The establishment, assessment, and reporting of metrological traceability are discussed, including the needed metrological institutional framework and the role of interlaboratory comparisons. Recommendations are made about the essential steps in planning and performing a measurement, and reporting a measurement result.

### Comments by 31 October 2009

Prof. Paul De Bièvre Tel.: +[32] 14 851 338 Fax: +[32] 14 853 908

E-mail: paul.de.bievre@skynet.be



www. iupac.org/reports/provisional/abstract09/debievre\_311009.html

### Name and Symbol of the Element with Atomic Number 112

A joint IUPAC/IUPAP Working Party (JWP) has confirmed the discovery of the element with atomic number 112 by the collaboration of Hofmann et al. from the Gesellschaft für Schwerionenforschung mbH in Darmstadt, Germany. In accordance with IUPAC procedures, the discoverers proposed a name, copernicium, and symbol, Cn, for the element. The Inorganic Chemistry Division now recommends these proposals for acceptance.

This proposal lies within the long tradition of naming elements to honor famous scientists. Nicolaus Copernicus was born on 19 February 1473 in Torún, Poland, and died on 24 May 1543 in Frombork/ Frauenburg. His work has been of exceptional influence on the philosophical and political thinking of humanmankind and on the rise of modern science based on experimental results.

### Comments by 31 January 2010

Prof. John Corish <jcorish@tcd.ie> University of Dublin Chemistry Department, Trinity College Dublin 2. Ireland



www.iupac.org/reports/provisional/abstract09/corish\_310110.html

Recent IUPAC technical reports and recommendations that affect the many fields of pure and applied chemistry.

### Making an imPACt

### **Glossary of Class Names** of Polymers Based on **Chemical Structure and** Molecular Architecture (IUPAC **Recommendations 2009)**

Máximo Barón, Karl-Heinz Hellwich, Michael Hess, Kazuyuki Horie, Aubrey D. Jenkins, Richard G. Jones, Jaroslav Kahovec, Pavel Kratochvíl, W. Val Metanomski, Werner Mormann, Robert F. T. Stepto, Jiří Vohlídal, and Edward S. Wilks

### Pure and Applied Chemistry, 2009 Vol. 81, No. 6, pp. 1131-1186

This document defines class names of polymers based on the class names of starting monomers and characteristic features of the chemical constitution of polymer molecules (macromolecules), (i.e., class names that have gained general acceptance in polymer and material literature or beyond). The glossary is divided into three parts:

- Source-based class names, which identify common classes of starting monomers such as "acrylic", "diene", "phenolic", "vinylic".
- Class names based on chemical structure, which identify characteristic groups in the main chains (backbones) of the polymer molecules such as (i) inter-unit groups derived from functional groups (e.g., "amide", "ester", "ether"); (ii) a specific group of atoms (e.g., "alkenylene", "siloxane", "sulfone"); (iii) ring structures (e.g., "benzimidazole", "benzoxazole", "quinoxaline").
- Class names based on molecular architecture, which identify mainly the overall shapes of polymer molecules through the type of their graphical representation such as "linear", "branched", "dendritic", "comb". Each part of the glossary is arranged in a non-hierarchical alphabetical order. Each entry provides: (a) the polymer class name; (b) its definition; (c) specific or generic examples including IUPAC names and a structure or graphical representation; (d) relations to other polymer classes and subclasses; (e) notes on the inclusion or exclusion of borderline cases. An alphabetical index of all class names is included.

http://dx.doi.org/10.1351/PAC-REC-08-01-30

### Discovery of the Element with **Atomic Number 112 (IUPAC** Technical Report)

Robert C. Barber, Heinz W. Gäggeler, Paul J. Karol, Hiromichi Nakahara, Emanuele Vardaci, and Erich Vogt

Pure and Applied Chemistry, 2009 Vol. 81, No. 7, pp. 1331-1343

The IUPAC/IUPAP Joint Working Party (JWP) on the priority of claims to the discovery of new elements has reviewed the relevant literature pertaining to several claims. In accordance with the criteria for the discovery of elements previously established by the 1992 IUPAC/IUPAP Transfermium Working Group, and reiterated by the 1999 and 2003 IUPAC/IUPAP JWPs, it was determined that the 1996 and 2002 claims by the Hofmann et al. research collaborations for the discovery of the element with atomic number 112 at Gesellschaft für Schwerionenforschung (GSI) share in the fulfillment of those criteria. A synopsis of Z = 112experiments and related efforts is presented. A subsequent report will address identification of higher-Z elements including those of odd atomic number.

http://dx.doi.org/10.1351/PAC-REP-08-03-05

The process of approving a name for the element of atomic number 112 has begun with the submission of a proposed name and symbol by the Gesselschaft für Schwerionenforschung (GSI) whose team was recently acknowledged as the discover of the new element. Following discussion with the discoverers, IUPAC issued (see p. 19) a Provisional Recommendation suggesting the name copernicium, with the symbol Cn, for the element with atomic number 112. This Provisional Recommendation is available for Public Comment for five months. At the end of the Public Comment period, the Inorganic Chemistry Division will review the comments made and either again revise the Recommendation or recommend approval by the IUPAC Council. After approval by the IUPAC Council, or its designate, the Recommendation of the name and symbol will be published in the IUPAC journal, Pure and Applied Chemistry.

For more details see IUPAC recommendations 2002 entitled "Naming of New Elements," Pure and Applied Chemistry, 2002, Vol. 74, No. 5, pp. 787-791; doi:10.1351/ pac200274050787.

CLIMATE

CHANGE

OBSERVED IMPACTS ON PLANET EARTH

### Bookworm

### Climate Change: Observed Impacts on Planet Earth

Edited by Trevor M. Letcher Elsevier, 2009

FISBN: 044453301X: ISBN 13: 97804445330121

Climate Change can be considered as a sequel to Trevor Letcher's recent book Future Energy (published in 2008, also by Elsevier). The two are inexorably

The book is divided into 25 chapters, each one written by an expert in the field. The first five chapters focus on the possible causes of climate change, while in particular the first chapter deals with the possible effects of anthropogenic greenhouse gases. Chapter six discusses the geological history of climate change, and puts the whole idea of climate change into perspective. The remaining 19 chapters focus on a variety of global changes brought about by climate change. These include detailed scientific observations on weather patterns; plants and plant pathogens; lichens; bird, insect, and animal ecology; sea

rising sea levels; and coastal erosion and ice sheets. If there ever was doubt about whether global and climate changes are taking place, these chapters may help put such thinking to rest.

This book supports the work done by the Intergovernmental Panel on Climate Change through experimental evidence. There has been no speculation, through computer modeling, at predicting possible future scenarios. The book is a scientific presentation of the facts surrounding climate change and no attempt has been made to offer solutions, although the basic nature of the problem is obvious; the burning of oil, coal, and gas is causing a significant rise in atmospheric carbon dioxide, water vapor, nitrogen

> oxides, and particulate matter-all of which influence our climate. This book should have a strong influence on deciding our future energy options.

> IUPAC supports the book, through its Chemistry and the Environment Division. IUPAC's adherence to the International System of Quantities is reflected in the book, with the use of SI units wherever possible.

> Climate Change is a source book and guide and is written, not only for students and researchers and their professors, but for decision makers in government and in industry, journalists and editors, corporate leaders, and all interested people who wish for a balanced, scientific, and honest look at this

major problem facing us.



www.iupac.org/web/ins/2007-050-2-600



### **Ecosystem Change and Human Well-**Being—Research and Monitoring Priorities Based on the Findings of the Millennium Ecosystem Assessment

### ICSU-UNESCO-UNU (2008), Paris, International **Council for Science**

The Millennium Ecosystem Assessment (MA) was called for by the United Nations Secretary-General Kofi Annan in 2000. Initiated in 2001, the objective of the MA was to assess the consequences of ecosystem change for human well-being and the scientific basis for action needed to enhance the conservation and sustainable use of those systems and their contribution to human well-being. The MA has involved the work of more than 1360 experts worldwide. Their findings, contained in five technical volumes and six synthesis reports, provide a state-of-the-art scientific appraisal of the condition and trends in the world's ecosystems and the services they provide (such as clean water, food, forest products, flood control, and natural resources) and the options to restore, conserve, or enhance the sustainable use of ecosystems.

The bottom line of the MA findings was that human actions are depleting Earth's natural capital, putting such strain on the environment that the ability of the planet's ecosystems to sustain future generations can

### Bookworm

no longer be taken for granted. At the same time, the assessment shows that with appropriate actions it is possible to reverse the degradation of many ecosystem services over the next 50 years, but the changes in policy and practice required are substantial and not currently underway.

The United Nations Environment Programme, as part of the Global Environment Facility procedures, initiated an independent valuation of the MA, which was completed in September 2006. In addition, the United Kingdom's Environmental Audit Committee of the House of Commons undertook an evaluation of the MA and published its results in 2007. Both evaluations reported that the MA's technical objective of assessing

the capacity of ecosystems to support human wellbeing proved both innovative and far-reaching. Thus, the MA emphasis on ecosystem services and their significance for human well-being is widely recognized as having made a major contribution to linking biodiversity conservation with poverty alleviation.

However, the evaluations also concluded that there was little evidence so far that the MA has had a significant direct impact on policy formulation and decision-making, especially in developing countries. In addition, in certain areas, the MA failed to provide the hoped for synthesis, since the scientific knowledge was lacking.

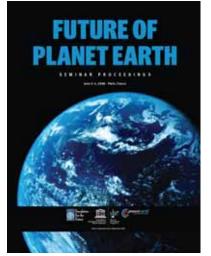


### **Future of Planet Earth**

Foundation For the Future and UNESCO Division of Ecological and Earth Sciences, 2009 (ISBN 978-0-9794081-5-1)

On 3-5 June 2008, 19 eminent scholars representing 5 continents met in Paris, France, at the UNESCO Headquarters to consider the critical factors that might have the most impact on the long-term future of Planet Earth. The seminar, called "Future of Planet Earth," was jointly sponsored and conducted by Foundation For the Future and UNESCO's Division of Ecological and Earth Sciences. The seminar was among the activities organized

in the framework of the United Nations "International



Year of Planet Earth," which focused on the impor-

tance of Earth sciences for society and human well-being. The intention behind the seminar was to provide a forum for dialogue amongst academics, scientists, conservationists, resource managers, and others dedicated to the wellbeing of the planet to explore the human-environment relationship with significant implications for the future of Planet Earth.

The seminar proceedings are now available on the FFF website under Recent Publications. The 358-page book contains transcripts of the seminar presentations and all dialogic sessions that followed.



# POLYCHAR-16 World Forum on Advanced Materials

Michael Hess (ed.)

Macromolecular Symposia, Vol. 277, March 2009
doi:10.1002/masy.200990004

The POLYCHAR 16: World Forum on Advanced Materials, organized by the University of Lucknow, was held from 17 to 21 February 2008 in the capital of the state of Uttar Pradesh. India. The annual POLYCHAR

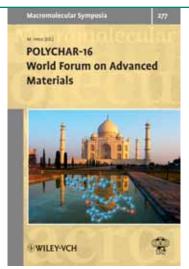
conferences have been sponsored by IUPAC for several years and are known for combining the broad field of materials sciences with a clear focus on polymeric materials (the name "POLYCHAR" is derived from the term "polymer characterization").

As in past years, POLYCHAR puts emphasis on the quality of research presented - in contrast to maximizing the number of participants. The areas covered include nanomaterials and smart materials; natural and biodegradable materials and recycling; materials syn-

### Bookworm

thesis; polymers for energy; rheology, solutions, and processing; mechanical properties and performance; characterization and structure-property relationships; biomaterials and tissue engineering; dielectric and electrical properties; surfaces, interfaces, and tribology; and predictive methods. Symptomatically, the number of papers on "green" science was higher than at POLYCHAR 15 in Búzios, Rio de Janeiro, in 2007.

This conference volume represents only a small fraction of the multitude of contributions from different parts



of materials science—48 oral contributions and 170 posters. Many of the contributions have review character, some represent excellent original contributions. Only a small number could be selected for this volume because of the limited space that is available.

In addition to this *Macromolecular Symposia* volume, an issue of *Pure and Applied Chemistry* (2009, Vol. 81, Issue 3) includes reports from this event <www.iupac.org/publications/pac/81/3/>.

# Molecular Order and Mobility in Polymer Systems

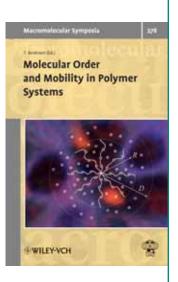
Tatiana Birshtein (ed.)

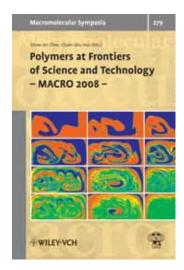
Macromolecular Symposia, Vol. 278, April 2009
doi:10.1002/masy.200990006

The main aim of this symposium was to discuss complex stimuli-responsive polymer systems that have nano-structure organization and a "soft" order that preserves a pronounced molecular mobility. Leading scientists in polymer physics from all over the world presented experimental data and the results of theory and simulation. The area receiving the most attention was equilibrium properties of polymer systems.

This issue contains the work from invited speakers.

The majority of the contributions are devoted to the systems which contain topologically complicated macromolecules with different functional groups, this resulting in a variety of interactions and possibilities of nanostructure formation. With exception of two last papers, publications are devoted to the investigation of equilibrium characteristics of the systems under consideration.





# Polymers at the Frontiers of Science and Technology—MACRO 2008

Show-An Chen and Chain-Shu Hsu (editors) Macromolecular Symposia, Vol. 279, May 2009 doi:10.1002/masy.200990011

The aim of the biannually held World Polymer Congress series is to bring together polymer scientists and engineers from around the globe to address recent developments and urgent issues in polymer science. The IUPAC-sponsored 42nd World Polymer Congress—MACRO 2008, held 29 June to 4 July 2008 in Taipei, China, had as its theme "Polymers at the Frontiers of Science and Technology."

MACRO 2008 involved 11 plenary, 157 invited, 245 contributed oral, and 595 poster papers. Two-thirds of the papers were contributed by scientists oversea. This issue contains selected papers from the conference.

# CHEMRAWN VII Prize for Atmospheric and Green Chemistry

USD 5000 will be awarded to a young scientist (under age 45) from a developing country who is contributing to the field of green chemistry through atmospheric chemistry research.

The first award will be given at the IUPAC International Conference on Green Chemistry in Ottawa, Canada, 15–19 August 2010.

# Nominations due by 31 December 2009

Each nomination should include a CV and two letters of support, plus a brief summary of research, illustrating the contribution of the applicant in the field of green chemistry and emphasizing atmospheric chemistry.

Send nominations to:

IUPAC Secretariat

PO Box 13757

Research Triangle Park, NC 27709-3757, USA

or by e-mail to secretariat@iupac.org

### Internet Connection

### Periodic Table PDF Generator

In the May-June 2008 issue of Chemistry International <a href="https://www.iupac.org/publications/ci/2008/3003/ic.html">www.iupac.org/publications/ci/2008/3003/ic.html</a>, Daniel Tofan reported on the Periodic Table Database/XML project, an effort to provide an online, open source of data about the elements in various formats. This article reports on a new online periodic table program Tofan developed that should be helpful to chemistry teachers.

### by Daniel C. Tofan

rintable periodic tables come in handy for distributing to students taking chemistry exams, particularly in lower-level courses. The ability to control what information to give students about the elements is important in such courses. For some classroom activities, it is also useful to provide "blank" periodic tables that students can be instructed to fill in with the properties they learn.

Scott Van Bramer has provided a few periodic table templates that can be used for this purpose. I created a brand new program, the Periodic Table PDF

en 4	2							
	4					Atomic	number	
	Be	Symbol						
1	Beryllium	Name						
	9.012182	Atomic mass			]			
	12							
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n 928	Magnesium 24.3050	3	4	5	6	7	8	ģ
	20	21	22	23	24	25	26	2
	Ca	Sc	Ti	V	Cr	Mn	Fe	С
ım	Calcium	Scandium	Titanium	Vanadium	Chromium	Manganese	Iron	Col
3	40.078	44.955912	47.867	50.9415	51.9961	54.938045	55.845	58.93
	38	39	40	41	42	43	44	4
	Sr	Υ	Zr	Nb	Мо	Tc	Ru	R
m 8	Strontium 87.62	Yttrium 88.90585	Zirconium 91.224	Niobium 92.90638	Molybdenum 95.94	Technetium	Ruthenium 101.07	Rho 102.9
8						[98]		102.9
	56	57	72	73 -	74	75	76	(
	Ba Barium	La Lanthanum	Hf Hafnium	Ta Tantalum	W	Re Rhenium	Os Osmium	Irid
m 519	137.327	138.90547	178.49	180.94788	Tungsten 183.84	186.207	190.23	192
	88	89	104	105	106	107	108	10
	Ra	Ac	Rf	Db	Sg	Bh	Hs	N
m	Radium	Actinium	Rutherfordium	Dubnium	Seaborgium	Bohrium	Hassium	Meitn
	[226]	[227]	[261]	[262]	[266]	[264]	[277]	[26

Part of a periodic table generated with Periodic Table PDF Generator.

Generator, which allows users to generate customized versions of the periodic table as PDF files. The software is written in Java and displays a GUI that allows the user to select what information to display for each element box (for now only the basic data is available: atomic number, symbol, name, and atomic mass) and to color the background of the element boxes based on several categories of properties. Atomic masses can be customized to display the chosen number of decimals, four significant figures, or all known digits. Two page sizes (letter and legal) are available, as well as landscape and portrait orientations.

The program is completely free and can be found at <www.intelot.com>, under Products.² In order to run the program, you need Java Runtime Environment installed on your computer. The program is launched from any browser via Java Web Start. You will need to "trust" the publisher in order to launch the program (an option that appears right after downloading the program). Selecting options is self-explanatory, and upon submission of the chosen options, a PDF file will be created and returned to you from the server, containing a printable periodic table exactly as you designed it.

I developed and tested the program on Windows machines, but it will run on any platform that supports Java (Mac, Linux, Solaris etc). I recommend installing the most recent version of the JRE<sup>3</sup> for full compatibility.

There is a "Contact us" page on the website that will send feedback directly to me. I encourage anyone who has suggestions for further improvements to let me know what you would like to see in a future version. Also, please report any bugs or unexpected behavior that you discover while using the software.

### References

- http://science.widener.edu/~svanbram/ptable. html, accessed June 2009
- 2. www.intelot.com, accessed June 2009
- http://java.sun.com/javase/downloads/ ?intcmp=1281, accessed June 2009

Contact Daniel Tofan at <intelot@gmail.com> for further information.

Daniel Tofan is an assistant professor in the Department of Chemistry at Eastern Kentucky University in Richmond, Kentucky, USA.

### **Radical Polymerization**

### by Graeme Moad

The symposium Materials of The Future, Science of Today: Radical Polymerization—The Next Stage took place in Melbourne, Australia, from 15-17 February 2009 at the University of Melbourne's Bio21 Institute.



The conference attracted approximately 116 participants from Australia, China, France, Germany, Iran, Japan, New Zealand, South Africa, and the USA. IUPAC sponsorship was vital in providing international recognition and credibility and in helping to attract high-quality speakers, many of whom came without funding from the conference.

The conference explored recent developments in radical polymerization and its application. A particular focus of the meeting was

radical polymerization with RAFT (Reversible Addition Fragmentation chain Transfer). The meeting also celebrated the 65th birthday and record of scientific achievement of Ezio Rizzardo (CSIRO Molecular and Health Technologies), a pioneer of reversible deactivation radical polymerization and one of the inventors of the RAFT process.

Following welcoming remarks by Greg Simpson (deputy chief, CSIRO Molecular and Health Technologies), the conference commenced with a plenary lecture by Rizzardo on "Perspectives of RAFT Polymerization-Something Old and Something New," in which he announced a new class of "switchable" RAFT agents. Four speakers then provided an industrial perspective on the applications of RAFT polymerization: Mike Fryd (DuPont) talked about "RAFT Technology for Microlithographic Applications," Mathias Destarac (Rhodia) discussed "Some Industrial Aspects of the MADIX Technology," Chris Such (Orica/Dulux) presented "RAFT Polymerization—A Coating Technologists View," and Kate Dawson (CSIRO), "RAFT-The New Horizon," mentioned the commercial availability of research quantities of RAFT agents through Strem and announced the formation of the "RAFT Alliance." The RAFT Alliance is a CSIRO-facilitated, global knowledge-exchange community, enabling members to network and share recent developments in both RAFT-related research findings and industrial applications. It is intended that membership will be free to academia.

Other plenary speakers included Andrew Holmes (CSIRO Molecular and Health Technologies and Bio21 Institute), "Seeing the Light with Polymers"; Thomas Davis (University of New South Wales), "The Stabilization and Biofunctionalization of Iron Oxide Nanoparticles"; Bert Klumperman (Stellenbosch University), "RAFT-Mediated Polymerization towards Advanced Macromolecular Architectures"; Krzysztof Matyjaszewski (Carnegie Mellon University), "ATRP and RAFT: Taking the Best of Each World"; Heather Maynard (University of California, Los Angeles) "RAFT Polymerization to Synthesize Polymer Bioconjugates for Therapeutic Applications"; and Charles McCormick (University of Southern Mississippi) "Aqueous RAFT Polymerization—A Technology Relevant to Biomedicine."

In all, there were 23 presentations and 23 posters presented over the two and a half days of the conference. All delegates benefited from extensive networking opportunities during both informal/social events and structured panel and poster sessions.



Bert Klumperman, San Thang, Heather Maynard, and Michael Monteiro at a poster session.

The International Advisory Board was composed of IUPAC President Jung-II Jin (Korea), Michael Buback (Germany), Takeshi Fukuda (Japan), Greg Russell (New Zealand), and Michael Fryd (USA). The meeting was sponsored by IUPAC, the Royal Australian Chemical Institute Polymer Division, CSIRO, DuPont, and Davies Collison Cave.

The conference program remains available online at <www.csiro.au/resources/RAFT-Conference-Program. html>.

Graeme Moad <graeme.moad@csiro.au> is research group leader at CSIRO Molecular and Health Technologies, in Clayton South, Australia. He was the Conference Program Committee chair.

# Clinical Laboratory and in vitro Diagnostics

### by Xavier Filella

The fifth European Symposium on Clinical Laboratory and in vitro Diagnostics, held 16-17 April 2009 at the Institut d'Estudis Catalans in Barcelona (Catalonia, Spain), focused on "Standardization and Tumor Markers." This IUPAC-sponsored conference was organized by the Catalan Association for Clinical Laboratory Sciences. Xavier Fuentes (Hospital de Bellvitge, L'Hospitalet de Llobregat) represented IUPAC at the meeting.

The main objective of the symposium was discussing the present and future of standardization in the measurement of tumor markers and, particularly, the clinical usefulness of these biomarkers. More than 100 participants from 6 countries took part in the meeting, which was based on the real experiences of laboratory and industry professionals, including members of Abbott, Beckman Coulter, Olympus, Roche Diagnostics, and Siemens.

One of the highlights of the meeting was a discussion about the problems of interchangeability in the concentrations of tumor markers in relationship to the method used in their measurement. Particularly, the speakers focused their attention on differences between methods for measuring prostate-specific antigen, or PSA, with the adoption of the International Reference Preparation WHO 96/670. The adoption of this standard in the measurement of PSA supposes the usefulness of a new cut-off of 3,1 ng/ml in substitution of the older cut-off of 4 ng/ml. On the other hand, the experts indicated that, in addition to the standard, there are other factors, such as incubation time, matrix effect, or the platform used that influence the results.

The symposium featured four roundtable discussions in which participants exchanged views and discussed opportunities for future activities regarding the following topics:

- It is necessary to obtain the standardization of tumor markers, but what are the problems?
- The industry and the standardization of tumor markers: why our results are so different?
- The clinical usefulness of tumor markers
- The interpretation of results: standardization and cut-off values

Another conclusion of the symposium was that the complexity of the substances used as tumor markers

makes it difficult to compare results obtained from different methods, although advances were made in cases such as CEA, AFP, and PSA. In this regard, speakers pointed to the International Federation of Clinical Biochemistry and Laboratory Medicine's project to clarify the nomenclature and characterization of various forms of this biomarker.

Xavier Filella <xfilella@clinic.ub.es> was the chair of the organizing committee; he is a member of the Department of Biochemistry and Molecular Genetics at the Hospital Clínic in Barcelona, Catalonia, Spain.

# Macro- and Supramolecular Architectures

by Kurt E. Geckeler

It is well known and accepted that polymer materials and architectures will play a key role in science and technology in the 21st century. In view of the general importance and dramatic recent progress made on a global basis in the area of "Synthesis, Properties, and Applications of Macro- and Supramolecular Architectures and Materials," the 4th International Symposium on Macro- and Supramolecular Architectures and Materials (MAM-08), was held from 7 to 11 September 2008 in Düsseldorf, Germany. The venue was the Conference Center on the campus of the University of Düsseldorf, which is located



The "Nobel Table" at the symposium banquet, which took place on a ship on the Rhine River. From left to right: F. Schue, K.E. Geckeler, A.H. Mueller, Y. Lee and D. Depnath (both GIST students), R. Huber (1988 Nobel Laureate in chemistry), and H. Ritter (symposium chair).



A view of Düsseldorf.

downtown in the vicinity of the Institute for Organic Chemistry and Macromolecular Chemistry. Düsseldorf is the capital of the Federal State of North-Rhine-Westphalia and is an important economic and cultural center of Germany.

Over 350 scientists, originating from about 40 countries, attended the symposium, which was the fourth in a series of MAM meetings. The conference featured 3 plenary lectures, 48 invited lectures, 65 contributed lectures, and 161 poster presentations.

The objective of the MAM series is to provide an interdisciplinary forum for scientists engaged in the full spectrum of research, development, and application, in which they can discuss the current status and recent developments of these materials. The meetings provide an opportunity to overview the field by covering a wide range of topics. Themes are selected to accommodate a wide range of interests to facilitate interdisciplinary interactions in both academic fields and industrial science and technology.

During the opening session, Michael J. Dröscher, the official IUPAC representative, gave an introduction to IUPAC. Lectures were organized in three parallel sessions due to the high number of contributions. The first plenary lecture was given by Nobel Laureate Jean-Marie Lehn on "Dynamats: Dynamic Molecular and Supramolecular Materials." The second one covered the topic of "Macromolecules, Assemblies, Particles, A Discovery Journey in Materials Synthesis," and was presented by Klaus Mullen. Nobel Laureate Robert Huber gave the third plenary lecture on "Architecture, Structure, and Function of Molecular Machines for Protein Degradation."

The high scientific level of the conference was based on the outstanding plenary and invited lectures as well as the many interesting contributed lectures and impressive posters, which were organized in two sessions in the spacious central hall that gave access to the different lecture halls. Several attractive poster awards sponsored by IUPAC, Wiley-VCH, and Springer Verlag, Germany, encouraged the presenta-

tion of excellent poster contributions. There was a tight schedule for the attendees, with the three parallel sessions only interrupted by short lunch and coffee breaks, which were the main times for scientific and other discussions.

The social program included a welcome reception and a banquet that was combined with a "cruise" on the Rhine river and a follow-up stroll through the old city of Düsseldorf. In addition, after the very well-attended final session, participants were invited to enjoy a half-day excursion to a typical German "Schloss" (castle).

Overall, the symposium was very stimulating and successful. It also provided an interdisciplinary forum for scientists and engineers to meet and discuss progress in the broad area of macromolecular and supramolecular science and technology. The next symposium in the series, MAM-10, will be held in 2010 in Montego Bay, Jamaica. The conference chair is Ishen Kahwa

Further information on the next meeting can be obtained at <www.mona.uwi. edu/mam-10>.

Kurt E. Geckeler < keg@gist.ac.kr> is chair and professor at the Gwangju Institute of Science and Technology in Gwangju, South Korea.

### Trace Elements in Food

### by Francesco Cubadda

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

The different facets of trace elements, from essentiality to toxicity, were addressed at the **3rd International Symposium on Trace Elements in Food** (TEF-3). The meeting was held 1-3 April 2009 in Rome, Italy, organized by the Istituto Superiore di Sanità (ISS), and consisted of two and one-half days of oral and poster presentations. Like the two previous meetings in this series, organized in Warsaw, Poland (2000), and in

Brussels, Belgium (2004), TEF-3 was held under the auspices of IUPAC.

The objective of this interdisciplinary symposium was to gather experts with different backgrounds to discuss all aspects of trace elements in food in rela-

tion to human health, with special emphasis on the biological effects of elements. The topics covered included essentiality, toxicity, bioaccessibility, bioavailability, speciation, sources and transfer in the food chain, effects of processing, food and feed fortification, supplementation, international legislation and standards, analytical developments, analytical quality assurance, and reference materials.

Over 200 participants, representing some 40 countries, joined the event. In addition to the 15 invited lectures, delegates from Europe, Asia, Africa, and North and South

America enriched the program with 20 oral and about 130 poster contributions.

The symposium was opened by Francesco Cubadda (symposium chair), Agostino Macrì (director of the Department of Food Safety and Veterinary Public Health at ISS), and Ryszard Lobinski (past president of the IUPAC Analytical Chemistry Division), who served as the IUPAC representative. The scientific program was organized in four sessions, summarized below.

# Advances in Trace Element Analysis in Food Matrices (Chairs: Kevin Francesconi and Ryszard Lobinski)

Joanna Szpunar reviewed state-of-the-art analytical techniques for element speciation studies in food and food supplements. Szpunar discussed advantages and drawbacks of the currently used analytical approaches, with a focus on selenium. Erik H. Larsen dealt with the detection and characterization of inorganic nanoparticles in life science studies. Larsen discussed the merits of field flow fractionation, coupled with multi-angle light scattering detection, for size determination and for use with on-line inductively coupled plasma mass spectrometry (ICP-MS). Alfredo Sanz-Medel addressed speciation and isotope pattern deconvolution (IPD) for ICP-MS quantitative studies of minerals metabolism and supplementation, showing how the multi-spike IPD approach can be used to differentiate and quantitate endogenous (natural) and exogenous (supplemented) elemental species.

A series of lectures dealt with recent developments in the speciation of iodine (Jose Luis Gomez-Ariza), of selenium (John Entwisle and Mihaly Dernovics), and of different metals in wine (Krystyna Pyrzynska). The isotopic and elemental fingerprints used to prove the

authenticity and origin of food and feed were addressed by Thomas Prohaska.

Finally, analytical quality in the determination of trace elements was discussed in regard to internal and external quality control procedures (Maria Beatriz de la Calle) and the reliability of published analytical data (Lars Jorhem).

At the end of this oral session, as with the other four, the chairs led a 15-minute plenary discussion with the aim of condensing the session's core message. The main focus was on summarizing the state of the art based on the lectures, and also on

trying to identify future challenges and subjects of research. The audience actively took part in the plenary discussions.

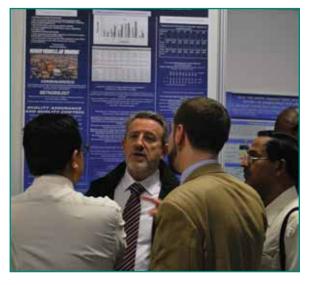


Francesco Cubadda opens

the symposium.

(Chairs: Alberto Mantovani and Barbara Szteke)

The session featured a series of interesting contributions on selenium, beginning with the invited lecture of Margaret Rayman that dealt with food chain selenium



A lively discussion during the poster session.

and human health, highlighting the complexity of optimal intake. Selenium uptake, bioaccessibility, and speciation were discussed in connection with plant (Anicke Brandt-Kjelsen and Darren Juniper) and animal (Qiuhui Hu and Espen Govasmark) farming.

In the second part of this session, biofortification of iron in genetically engineered rice (Christof Sautter) and of zinc through application of fertilizers (Ismail Cakmak) were treated. Finally, the effect of repeated annual applications of phosphorus fertilizers on the phytoavailability of cadmium was addressed (Cynthia Grant).



The chairs of the first session: Kevin Francesconi (left) and Ryszard Lobinski.

### **Toxicology and Risk Assessment** (Chairs: Philippe Grandjean and Erik H. Larsen)

The pitfalls in assessing the adverse health effects of methylmercury in seafood were discussed by Philippe Grandjean, whereas Marie Vahter treated the gender differences in susceptibility to cadmium in food.

The emerging topic of nanosized materials and nanotoxicology was addressed by Chunying Chen, who reviewed the application of nanotechnology in the food industry and the toxicological issues surrounding nanomaterials.

Arsenic speciation and toxicology were addressed in relation to seafood (Kevin Francesconi) and rice (Jörg Feldmann). The metabolism of metal(loid)s by intestinal microorganisms was discussed by Roland Diaz-Bone, who showed how gut bacteria are able to modulate metal(loid) speciation, bioaccessibility, and toxicity. He also described the identification of a number of species, including mixed Se/S, As/S as well as As/Se compounds through the use of GC with both EI-MS and ICP-MS detection. The intestinal absorption of the arsenic species with higher toxicity, as studied

by in vitro methods, was also dealt with (Vicenta Devesa).

Finally, the assessment of the risks and benefits of organic forms of trace elements as feed additives (Alberto Mantovani) and the effect of in vitro lead administration on porcine ovarian granulosa (Adriana Kolesarova) were discussed.

# Trace Elements in Nutrition and Human Health (Chairs: Marina Patriarca and Munehiro Yoshida)

The invited lecture of Bo Lönnerdal addressed the alternative pathways for iron absorption from food, and focused especially on ferritin. This iron-binding protein is present in meat, but also in low concentrations in a wide variety of plants (e.g., legumes), and it is possible to enhance the ferritin content of plants by conventional breeding or genetic engineering, and thereby increase the iron intake of populations consuming predominantly plant-based diets.

Susan Fairweather-Tait reported on the results of a human intervention study designed to establish the effect of selenium supplementation on selenium biomarkers and immune function, Ian J. Griffin reviewed the insights on trace mineral metabolism in children gained through stable isotopes studies. It was shown that fractional absorption is the main site of mineral homeostasis for some minerals (Ca, Mg) and faecal excretion is the main regulated site for others (Zn), and that the current Estimated Average Intakes for Ca and Zn may be too low for one- to four-year old children. The current perspectives on sustainable solutions to zinc deficiency in infants and young children were discussed by Nancy F. Krebs. Zinc in relation to metallothioneins and longevity was also addressed (Francesco Piacenza).

Other prominent topics of this session included the use of stable isotopes in in vivo studies by IPD-HPLC-ICP-MS (Maria Luisa Fernández-Sánchez), in vitro methods for assessing element bioaccessibility as influenced by breadmaking (Carmen Frontela), and the biomonitoring of iodine in the U.S. population by the U.S. Centers for Disease Control (Kathleen Caldwell).

### **Poster Sessions and Concluding Remarks**

The wealth of material covered at the poster sessions was remarkable.<sup>1</sup> Among many significant contributions, three works were selected for the poster awards. Katrin Löschner, Véronique Vacchina, and Tejo Prakash Nagaraja were awarded prizes for the posters entitled

"AFFF-MALS-ICP-MS and Electron Microscopy for the Characterization of Nanoparticles in Biological Studies" (Löschner et al.), "Determination of Selenomethionine and Selenocysteine in Edible Tissues of Animal Origin" (Bierla et al.), and "Total Selenium and Selenium Speciation in Food Crops from a Seleniferous Area of Punjab" (Cubadda et al.), respectively.

Overall, TEF-3 resulted in a lively interdisciplinary symposium where research and development efforts and emerging issues in the area of trace elements in food were thoroughly discussed in a enjoyable atmosphere. The success of this edition led to the deci-

sion to held TEF-4 in three years, most likely outside Europe.

#### References

 F. Cubadda, F. Aureli, S. Ciardullo, M. Patriarca (Eds.). 2009. 3rd International IUPAC Symposium on Trace Elements in Food: Abstract Book. ISTISAN Congressi 09/C2, pp 207 (downloadable from www.iss.it).

Francesco Cubadda <francesco.cubadda@iss.it> is a research chemist at the Istituto Superiore di Sanità (ISS), the Italian National Health Institute.

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

### Lavoisier's Better Half

Marie Anne Pierrette Paulze (1758-1836) was only 13 when she married a brilliant young member of the French Academy of Sciences, the chemist Antoine

Laurent Lavoisier (1743-1794), She later became the celebrated scientist's most important assistant and collaborator until his death at the height of the French Revolution. The extent of Marie Anne's contributions to her husband's career has often been underestimated and sometimes even completely ignored. However, it is clear that she played a key role in most of his research endeavors, from the critical experiments on combustion, respiration, and the composition of air and water to the development of chemical nomenclature and the law of conservation of mass. She translated from English to French Richard

Kirwan's *Essay on Phlogiston*, which Lavoisier and others systematically criticized, eventually leading to the demise of the infamous theory. She was a meticulous record-keeper and illustrator and singlehandedly produced the 13 plates contained in *Elementary Treatise* 

on Chemistry (1789), which presented an updated and unified overview of the subject and is usually considered the first modern chemistry textbook.

The stamp from the Republic of Maldives shown here was issued on 11 January 1990 to belatedly commemo-

rate the bicentennial of the beginning of the French Revolution (i.e., the storming of the Bastille on 14 July 1789). There is no obvious reason why the Maldive Islands, a former British protectorate in the Indian Ocean that gained its independence in 1965 and is today the smallest and least populated country in Asia, took such an interest in the French Revolution. In any event, the stamp features the double portrait of Monsieur and Madame Lavoisier painted in 1788 by Jacques-Louis David, one of the leading representatives of the French Neoclassical period. The iconic painting shows the

couple elegantly dressed next to a table with various pieces of contemporary glassware. It is now part of the permanent collection on display at the Metropolitan Museum of Art in New York.

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



# Where 2B & Y

# Challenges in Thermodynamics Applied to Materials World

1-6 August 2010, Tsukuba, Japan

The 21st IUPAC International Conference on Chemical Thermodynamics (ICCT-2010) will be held in Tsukuba, Japan, from 1–6 August 2010 under the theme "Role of Chemical Thermodynamics in the 21st Century." Nine exceptional plenary speakers from diverse fields of chemical thermodynamics will present their latest findings during this event. Participants at this conference will be able to:

• learn from internationally renowned researchers in a comprehensive and wide-ranging program

covering all aspects of chemical thermodynamics, such as pure and applied chemistry, biothermodynamics, pharmaceutical application, environmental issues, and education

- understand the current state of research and the challenges to future discovery/application
- present the latest research at oral or poster sessions

This IUPAC-sponsored conference is being organized by the Science Council of Japan, the Chemical Society of Japan, and the Japan Society of Calorimetry and Thermal Analysis.

See Mark Your Calendar on page 36 for contact information.



# Solubility Phenomena and Related Equilibrium Processes

25-30 July 2010, Leoben, Austria

The 14th International Symposium on Solubility Phenomena and Related Equilibrium Processes will be held 25–30 July 2010 in Leoben, Austria. The symposium will include a workshop called "From Chemical Equilibrium to Process Modelling, Inclusion of Kinetics into Thermodynamic Reasoning."

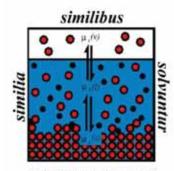
Phenomena related to the solubility of solids, liquids, and gases with one another, and the homogeneous

equilibria existing between the dissolved species, are of interest for scientists, technologists, and medical practitioners in a wide array of disciplines. Data from solubility and related equilibria are, for example, employed to determine thermodynamic quantities, to simulate chemical processes, and to assess the effectiveness of a given pharmacological treatment.

The 14th ISSP will put an emphasis on solubility aspects of aqueous salt solutions, molten salts, and ionic liquids. Particularly welcome are contributions to the solubility of lithium compounds in solutions and melts and its possible relevance for extraction, purification, and lithium battery technology.

The 14th ISSP will also stress the chemical basis of hydrometallurgy and the application of chemical concepts in industrial processes. An effort will be made to proceed beyond classical thermodynamics by including discussions on constrained equilibria, irreversible thermodynamics, and phase transformation kinetics. The symposium and workshop will bring together experts in chemical, metallurgical, and computational aspects of classical solubility phenomena and related equilibrium processes as well as dissolution and precipitation kinetics. The theme has significance to future key technologies in hydro- and pyrometallurgy as well as materials science.

See Mark Your Calendar on page 36 for contact information.



14th ISSP, Leoben, 2010

# Polymer Characterization

7-10 April 2010, Siegen, Germany

POLYCHAR 18: World Forum for Advanced Materials, will be held at the University of Siegen, Germany, from 7-10 April 2010. On 6 April, a short course on modern methods of polymer characterization will be held by experts in the field.

POLYCHAR 18 aims to bring together established polymer scientists from academia and industry, young

researchers and students. Synthesis, characterization, and application of polymeric materials and biorelated polymers will be discussed in two parallel sessions that will include plenary lectures, keynote lectures, regular oral contributions, and dedicated poster sessions.

See Mark Your Calendar on page 35 for contact information.

www.uni-siegen.de/fb8/polychar18/

### **EuCheMS Chemistry Congress**

29 August-2 September 2010 Nürnberg, Germany

The EuCheMS (European Association for Chemical and Molecular Sciences) 3rd Chemistry Congress in Nürnberg (Nuremberg) 2010 will present the latest research in the core topic areas of chemistry, feature multidisciplinary programming, and highlight chemistry's impact on society. The congress will bring together chemical and molecular scientists from industry, academia, and government from across Europe and from around the world. The vendor exhibition will include leading companies showing their latest innovations in chemistry and related fields.

This congress is organized under the auspices of the EuCheMS, which has 50 member societies representing 150 000 chemists. The German Chemical Society (Gesellschaft Deutscher Chemiker, GDCh) is the host of the Congress.





21st International Conference on Chemical Education

Chemical Education & Sustainability in the Global Age

> 8-13 August 2010 Taipei, Taiwain

http://icce2010.gise.ntnu.edu.tw/

# Biophysico-Chemical Processes in Environmental Systems Series



Sponsored by The Division of Chemistry and the Environment of the International Union of Pure and Applied Chemistry (IUPAC), the *Biophysico-Chemical Processes in Environmental Systems Series* addresses the fundamentals of physical-chemical-biological interfacial interactions in the environment and

the impacts on: the transformation, transport and fate of nutrients and pollutants; food chain contamination and food quality and safety, and ecosystem health, including human health. In contrast to classical books that focus largely on separate physical, chemical, and biological processes, this unique book series integrates the frontiers of knowledge on both fundamentals and impacts on interfacial interactions of these processes in the global environment.

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"This book is an important contribution to the literature on soil contamination by metals and its remediation."

— JOURNAL OF HAZARDOUS MATERIALS

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978-0-471-73778-0 ~ Hardcover ~ 658 pages ~ January 2008 US \$155.00 ~ CAN \$185.99 ~ £103.00 ~ €135.00

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### Mark Your Calendar

### **2009** (later than 15 September)



IUPAC poster prizes to be awarded

#### 28 September 2009-2 October 2009 • Frontiers of Polymers • Santiago, Chile

10th International Conference on Frontiers of Polymers and Advanced Materials Prof. Guillermo González, Department of Chemistry, Universidad de Chile, Las Palmeras 3425, Santiago, Chile Tel.: +562 978 7404, Fax: +562 271 3888, E-mail: ggonzale@uchile.cl

### 10-14 October 2009 • Molecular Environmental Soil Science • Hangzhou, China

International Symposium of Molecular Environmental Soil Science at the Interfaces in the Earth's Critical Zone Prof. Jianming Xu, Zhejiang University, College of Environmental & Resource Sciences, Hangzhou, 310029, China Tel.: +86 571-8697-1955, Fax: +86 571-8697-1955, E-mail: jmxu@zju.edu.cn

### 18-22 October 2009 • Novel Materials and Their Synthesis • Shanghai, China

International Symposium on Novel Materials and Their Synthesis (NMS-V) Prof. Yuping Wu, Fudan University, Department of Chemistry, Shanghai, 200433 China Tel.: +86 21 55 664 223, Fax: +86 21 55 664 223, E-mail: wuyp@fudan.edu.cn

### 9-12 November 2009 • Crop Protection • Rio de Janeiro, Brazil

3rd International Workshop on Crop Protection Chemistry in Latin America: Environment, Safety and Regulation See IUPAC Project 2007-057-1-600 or E-mail: secretariat@iupacrio2009.org

### 15-18 November 2009 • MacroMolecular Complexes • Termas de Chillán, Chile 🐺

13th International Symposium on MacroMolecular Complexes Prof. Bernabé L. Rivas. Universidad de Concepción, Facultad de Ciencias Químicas, Concepción, Chile Tel.: +56 412 204 109, Fax: +56 412 245 974, E-mail: mmc13-chile@udec.cl

#### 2010



### 6-9 March 2010 • Chemistry and Industry • Kuwait City, Kuwait 🎡

Kuwaiti Conference of Chemistry

Ms. Khalida M. Al-Dalama, Kuwait Institute of Scientific Research, Petroleum Research and Studies Center, P.O. Box 24885, Safat 13109, Kuwait, Tel.: + 965 398 0499, Fax: + 965 398 0445, E-mail: kdalama@yahoo.com

#### 7-10 March 2010 • Heterocyclic Chemistry • Gainesville, Florida, USA

11th Florida Heterocyclic and Synthetic Conference

Prof. Alan R. Katritzky, University of Florida, Department of Chemistry, Gainesville, FL 32611-7200, USA Tel.: +1 352-392-0554, Fax: +1 352-392-9199, E-mail: katritzky@chem.ufl.edu

### 7-10 April 2010 • Polymer Characterization • Siegen, Germany



18th International Conference on Polymer Characterization; World Forum on Advanced Materials Professor Werner Mormann, Universität Siegen, FB-8, Makromolekulare Chemie, Adolf Reichwein Strasse 2 D-57068 Siegen, Germany

Tel.: +49 271 740 4713, Fax: +49 271 740 2226, E-mail: mormann@chemie.uni-siegen.de

#### 5-11 June 2010 • Spectral Line Shapes • St. John's, Newfoundland, Canada

20th International Conference on Spectral Line Shapes

Prof. John K. C. Lewis, Memorial University of Newfoundland, Department of Physics and Physical Oceanography, St. John's, NL A1B 3X7, Tel.: + 709 737 8849, Fax: + 709 737 4569, E-mail: court@mun.ca

### 4-8 July 2010 • Pesticide Chemistry • Melbourne, Australia 🛣



12th IUPAC International Congress of Pesticide Chemistry

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

### 5-8 July 2010 • Polymer-Solvent Complexes • Strasbourg, France

8th International Conference on Polymer-Solvent Complexes and Intercalates

Prof. Jean-Michel Guenet, Université de Strasbourg, Institut Charles Sadron-CNRS, 23, Rue de Loess F-67034 Strasbourg, Tel.: + 33 038 841 4087, Fax: + 33 038 841 4099, E-mail: guenet@ics.u-strasbg.fr

### Mark Your Calendar

### 11-16 July 2010 • Macromolecules • Glasgow, UK 🏶

43rd International Symposium on Macromolecules—IUPAC World Polymer Congress (Macro 2010)
Prof. Peter A. Lovell, School of Materials, The University of Manchester, Grosvenor St. Manchester, M1 7HS, UK
Tel.: +44 (0) 161-306-3568, Fax: +44 (0) 161-306-3586, E-mail: pete.lovell@manchester.ac.uk

### 11-16 July 2010 • Photochemistry • Ferrara, Italy 🎡

XXIII IUPAC Symposium on Photochemistry

Prof. Franco Scandola, Dipartimento di Chimica, Università di Ferrara, Via L. Borsari 46, I-44100 Ferrara, Italy Tel.: +39 05 32 455 160, Fax: +39 05 32 240 709, E-mail: snf@unife.it

### 25-30 July 2010 • Solubility Phenomena • Leoben, Austria 🏶

14th International Symposium on Solubility Phenomena and Related Equilibrium Processes

Prof. Heinz Gamsjäger, Montanuniversität Leoben, Lehrstuhl für Physikalische Chemie,

Franz Josef Strasse 18, A-8700 Leoben, Austria

Tel.: +43 (0) 3842 402 4804, Fax: +43 (0) 3842 402 4802, E-mail: heinz.gamsjaeger@mu-leoben.at

### 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

### 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

### 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

### 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



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ICOS-18 Bergen, Norway August 1–6, 2010 www.ICOS-18.no

# 紫

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The Thieme–IUPAC Prize is presented every two years on the occasion of the International Union of Pure and Applied Chemistry – International Conference on Organic Synthesis (IUPAC–ICOS). The 2010 ICOS will be held in Bergen, Norway, on August 1–6. The prize is awarded to a scientist under 40 years of age whose research has had a major impact in synthetic organic chemistry.

**Prize € 5000** 

The Thieme–IUPAC Prize has been awarded to Stuart L. Schreiber in 1992, Paul Knochel in 1994, Eric N. Jacobsen in 1996, Andrew G. Myers in 1998, Alois Fürstner in 2000, Erick M. Carreira in 2002, John F. Hartwig in 2004, David W.C. MacMillan in 2006, and F. Dean Toste in 2008.

The prize will be awarded on the basis of scientific merit for independent research dealing with synthesis in the broadest context of organic chemistry, including organometallic chemistry, medicinal and biological chemistry, designed molecules, and materials. Candidates must be under 40 years of age as of January 1 of the year in which the prize is awarded.

Proposals must be accompanied by a biographical sketch of the nominee, a list of the candidate's ten most significant publications, and a statement of how the candidate's research has had a major impact on the field of synthetic organic chemistry. The material will be confidentially forwarded to an independent selection committee.

Nomination materials (8 copies)

should be submitted by December 7, 2009 to

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