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Who Are You?

The American Chemical Society manages for IUPAC the largest subset of subscribers to *Chemistry International*, including 3650 affiliate members, i.e., about half the readership. Each year, ACS produces an interesting demographic report, which indeed should tell us more about who you are. The data include age group, year of service, major and degree, field of interest, nature of the business, job title, and activity. Overall the readership is evenly distributed with about 20% in each of the following age groups: 30 and younger, 31-40, 41-50, 51-60, and 61+. There is no way to tell if the youngest are those who joined most recently, but regardless, it is encouraging to see, for instance, that in 2001 alone, 684 affiliates joined the program, and in 2000, 733 joined. Roughly, 75% majored in chemistry and 5% majored in engineering, 40% have a PhD, 10% have a Masters, and 35% a Bachelors. According to the survey, the top 5 fields of interest are medicine/pharma (for 12%), analytical (11%), organic (10%), environmental (7%), and education (6%), while 18% of you are working in University or college and 25% are in a manufacturing business. The second half of the subscribers includes 30% from Europe, 9% from the Pacific Rim and Far East, 6% from Canada and South and Latin America, and 5% from the Middle East region and Africa. For more numbers, visit <www.iupac.org/news/archives/2002/01ACSdemo.html>.

Fabienne Meyers <fabienne@iupac.org>

Vice President's Column

IUPAC in a Changing World

We are constantly reminded of the fact that we live in a changing world. A number of experiences in our lives tell us so, and so do daily newscasts reaching us from all parts of the world. These influences affect us and, perhaps even without knowing it, we respond and adjust to the changing conditions to cope with new realities, to be able to deliver what is expected from us, or to feel more comfortable.

Organizations are not like human beings. That partly explains why most organizations, including international federations and unions, quite frequently do not respond to changing needs and demands as quickly as many would like. And that is also why most organizations have to be overhauled and revitalized every now and then to satisfy what the membership expects in return for the money and time spent year after year.

In this respect IUPAC is no exception to the rule (although some chemists still like to think it ought to be), so it is far from surprising that reorganization of the union became an informal topic for discussion decades ago. However, after the General Assembly in Lisbon in 1993, restructuring became gradually a formal item on IUPAC's agenda as well. Over the last 5-6 years the issue was the single most important subject dealt with by the union. As well-informed chemists will know, this process transformed IUPAC, from a union with appointed divisions and approved commissions with long lifetimes and rather static membership, to an organization with smaller, elected divisions and dynamic, short-lived project groups established after thorough international review of project proposals. The transition was complete by January 1st this year, so IUPAC is now operating in a restructured fashion, according to the so-called project-driven system.

. . . the future success of IUPAC depends on better communication between the union and its stakeholders . . .

Some chemists are saying that this restructuring looks good, but what are the future benefits from all these changes for the chemical sciences and the chemical community? That is a good question, which cannot be answered with certainty before we see how IUPAC develops in the years to come. However, we know one thing for sure: The restructured IUPAC will only be able to fulfil its objectives and the expectations of the global chemical community if chemists from around the world are actively engaged in addressing important global issues involving chemistry. The best guarantee for IUPAC success is, therefore, solid recruitment of good and dedicated chemists to all the union's activities.

Leiv. K. Sydnes
IUPAC Vice President

Successful recruiting is not done in a flash; planning and strategy are paramount to get the right group of competent volunteers involved year after year. A critical factor in this endeavour is good contact with the chemical community world wide, particularly with the countries that are members or associate members of IUPAC. This requires close and vivid communication with both the National Adhering Organizations (NAOs) and the chemical societies in these countries. A crucial question therefore surfaces: Is the communication, in particular with the NAOs, good enough? Overall, I am convinced the answer is no, and a few examples illustrate why. For instance, when the 45 NAOs are contacted by mail regarding a matter of importance to the union, it is rare to receive more than five replies. And when all the NAOs are asked and encouraged to nominate national representatives to various groups, the feedback is usually not much better. That is a pity, because the union's officers have been elected to serve the chemical community, not to replace its members.

Based on these observations I am sure that the future success of IUPAC depends on better communication between the union and its stakeholders, whether the matters under consideration are related to advancement of research in the chemical sciences, promotion of services of chemistry to society, improvement of education in chemistry, or initiatives to advance the public appreciation of chemistry. In fact I believe that the chemical community, including the chemical industry, will not benefit properly from IUPAC unless the two-way communication with the membership improves significantly. I have therefore decided to focus on communication in my vice-president critical assessment. The NAOs will hear more about that shortly. In the meantime I urge individuals to supply comments and ideas regarding how to improve the union's communication skills and efficiency. Challenging and inspiring response is most welcome!

Leiv K. Sydnes is the current IUPAC vice president and has been a member of the IUPAC Bureau since 1994. He is professor at the University of Bergen, Norway.

XML in Chemistry

by Antony N. Davies

Extensible Mark-up Language (XML) is a powerful alternative to conventional binary file storage and information exchange. As many scientific organizations and companies delivering scientific products have implemented or are looking at the use of XML, IUPAC decided to review and evaluate what could and should be its role in advancing the use of XML in chemistry. In January this year, the IUPAC Committee on Printed and Electronic Publications (CPEP) organized a two day Strategic Meeting to assess the Union's position and options. Hosted by the Unilever Cambridge Centre for Molecular Informatics in the University of Cambridge Department of Chemistry, delegates from all interested IUPAC Divisions gathered together with key players in the field.

XML can be regarded as an extension to the well known HTML or Hyper Text Mark-up Language, which is the language most frequently encountered when viewing web pages. XML is considered to be the universal format for structured documents and data on the Web.[1] As with a conventional Web page, it isn't the use of XML itself that is interesting or even particularly novel, but the content stored within the XML files. In chemistry and associated technical fields, various groups—commercial organizations, academic institutions, and government bodies—have been developing XML formats independent of each other. These formats have similar content but differing data dictionaries and conventions. This means they are not compatible with each other and, what is far worse, resources are being deployed to address problems already solved by other groups. In order to support standardization in this field for the benefit of the community, IUPAC has decided to actively explore ways in which it can help to unify the various dictionaries and publicize their availability.

It isn't the use of XML itself that is interesting or even particularly novel, but the content stored within the XML files.

IUPAC'S Role and Timeline

During the 2001 IUPAC General Assembly in Brisbane, an ad hoc group outlined the dos and don'ts [see box] of a possible IUPAC role in advancing the use of XML in chemistry and developed a timeline for further action. The strategic importance of these decisions was reflected in the presentation of Wendy Warr—CPEP chairman—to the IUPAC Council[2] and the subsequent comments by IUPAC's secretary general Ted Becker in his article in CI.[3]

It was very clear from the Brisbane meeting that there was an urgent need to address the issues that were raised there. Hence, by the end of December 2001 the issues of identifying glossaries, project team members, and contacts between divisions and standing committees had been addressed. By then, Professor Bobby Glen of the new

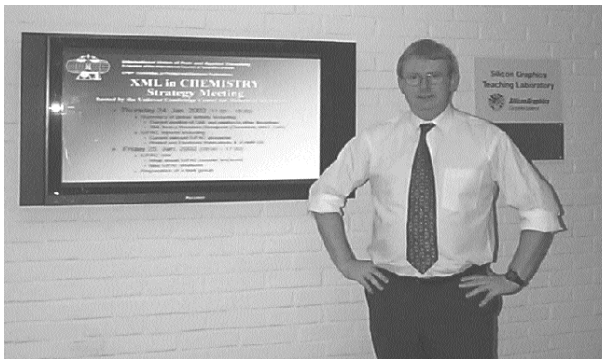
DOS AND DON'TS

IUPAC should not:

- Commence activities better left to the computer scientists
- Re-invent the wheel—the current activities at various locations should be invited to contribute to a standardization process through IUPAC as long as their efforts remain in the public domain
- Become formal members of World Wide Web Consortium (W3C), Object Management Group (OMG) or other similar organizations, however they should be informed of IUPAC activities in this area and we should continue to monitor their work.

IUPAC should:

- Establish "ownership" of the definition of standard terms in chemistry to be used in digital communications through formal IUPAC recommendations.
- Generate a glossary of standard terms in chemistry for use in applications involved in digital communications such as scientific data exchange or electronic publishing.
- Locate potential interested parties within IUPAC who "own" glossaries of terms or who are in the process of creating them
- Establish a method to identify and resolve problems in overlap of definitions (within IUPAC as well as with other scientific standards and other organizations)



Antony Davies

Unilever Centre for Molecular Informatics at the University of Cambridge, United Kingdom, agreed to host a follow-up meeting from 24-25 January 2002, as this type of initiative is of great interest to the fledgling center. Those invited to attend included IUPAC division and standing committee representatives and delegates from outside IUPAC who are active in establishing guideline for handling of chemical objects within their organizations. The IUPAC Analytical Chemistry Division was represented by its president David Moore; the Physical and Biophysical Chemistry Division represented by Jeremy Frey; and the new Chemical Nomenclature and Structure Representation Division, represented also by its president, Alan McNaught. In addition, I represented the IUPAC JCAMP-DX Working Party.

Meeting Overview

The meeting started with a welcoming address by Bobby Glen, who briefly explained the background of the Unilever Centre and provided a useful overview of the type of projects underway at the center.

Alan McNaught, Robert Lancashire, and I discussed IUPAC's intentions, current activities involving IUPAC glossaries, and the status of the JCAMP-DX file formats. Currently, within the eight IUPAC divisions there exist seven glossaries that are supervised by the Interdivisional Committee on Terminology, Nomenclature, and Symbols, which is responsible for ensuring conformity with existing IUPAC recommendations and consistency within and between each volume. These compendia, known as the IUPAC color books, cover chemical terminology, quantities, units, and symbols in physical chemistry, inorganic, organic, macromolecular, and analytical nomenclature, as well as the terminology and nomenclature of clinical laboratory sciences.[4]

Jeremy Frey pointed out that one difficulty encountered during the revision of the "green book" (which covers quantities, units, and symbols in physical chemistry) was the accommodation of different definitions, which originated from different fields of chemistry, for single entries in the data dictionary. Steve Heller offered an even broader example of the problem: although nm is widely recognized as nanometers in the scientific community, there is a significant body of opinion that feels that the letters obviously refer to nautical miles!

The International Union of Crystallographers (IUCr), represented at the meeting by Brian McMahon, has a very special interest in mark-up language because it has developed a standard format—the Crystallographic Information File (CIF)—for the deposition, storage, and distribution of crystallographic data with the publication

Crystallographic Information File (CIF)

by Brian McMahon

Commissioned by the International Union of Crystallography (IUCr), CIF consists of a very rich set of descriptors, allowing a file to contain raw and processed experimental data, a detailed experimental log, information about subsequent structure solution and refinement cycles, and a complete description of crystal and chemical structure and connectivity. A small excerpt from the standard example file for submissions to Acta Crystallographica Section C is presented here; the complete file can be viewed at ftp://ftp.iucr.org/pub/example.cif.

```
data_99107abs
_chemical_name_systematic
; 3-Benzo[b]thien-2-yl-5,6-dihydro-1,4,2-oxathiazine 4-oxide
;
_chemical_name_common          ?
_chemical_formula_iupac        'C11  H9  N  02  S2'
_chemical_formula_moiety       'C11  H9  N  02  S2'
_chemical_formula_sum          'C11  H9  N  02  S2'
_chemical_formula_weight       251.31
_chemical_compound_source      'synthesized by the authors,
see text'
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_U_iso_or_equiv
_atom_site_adp_type
S4      S 0.32163(7) 0.45232(6) 0.52011(3) 0.04532(13) Uani
S11     S 0.39642(7) 0.67998(6) 0.29598(2) 0.04215(12) Uani
O1      O -0.00302(17) 0.67538(16) 0.47124(8) 0.0470(3) Uani
O4      O 0.2601(2) 0.28588(16) 0.50279(10) 0.0700(5) Uani
H5A     H 0.1284 0.4834 0.6221 0.060 Uiso
H5B     H 0.1861 0.6537 0.5908 0.060 Uiso
```

of peer-reviewed papers. As McMahon explained, CIF was commissioned by IUCr following long-standing interest in the need for an open standard for data and information exchange. CIFs are divided into blocks, with each block consisting of individual labels or tags whose definition is stored elsewhere. Key points are that the semantic content is kept separate from the syntax of data representation, and that different dictionaries are used for different topic areas. McMahon concluded that one thing was abundantly clear from experience with CIF: "The design of a file format is an essential step, but it is only one component (and in many ways the least difficult) in the process of devising a feature-rich exchange mechanism. Far more difficult is the detailed definition of the tags that will be used within the file to ensure that applications attribute exactly the same meaning to the same item of information. The experience of the expert committees who undertake this work to extend CIF is that years of painstaking effort and discussion may be needed to define a few dozen tags, which are accepted across the community." As a contribution toward the establishment of content-rich XML applications in related areas of chemistry, the IUCr will make available its CIF-based definitions to the IUPAC groups working to establish XML-based applications. The scientific community said McMahon is looking forward to the day when effective chemical information exchange standards, widely accepted by the community, should complement and interoperate with CIF or its successors.

Peter Murray-Rust summarized other global activities surrounding the use of XML in science—see page 9 for a review of his work, co-authored with Henry Rzepa. At the meeting, Murray-Rust explained some of the benefits of using XML-based documents, including the ability to "validate" documents for correct or complete content, to create better electronically linked publications, and to significantly simplify information harvesting from such documents. According to Murray-Rust, for XML to function effectively for the sciences there needs to be agreement on the vocabularies or "ontologies" in use. He noted that the W3C expects that "domains" will create domain-specific tools and protocols for different subject areas such as chemistry. He also explained how the XML files differentiate between content, which has often been specified at different locations. Individual XML files may contain content from different ontologies such as a structure as defined by Chemical Markup Language (CML), a spectrum as defined by JCAMP-DX or SPECTROML, and a mathematical relationship as defined by MathML. This can be regarded as a powerful bonus, but again poses the question about reliability of the links the content needs to be put. This is currently leading to situations where "<element> carbon" might need to be handled differently, such as "<cml:element> carbon". The key is in the

. . . for XML to function effectively for the sciences there needs to be agreement on the vocabularies or "ontologies" in use.

The same file may be transferred from diffractometer to computational workstation to molecular graphics software, with each program in the chain importing and adding data. Authors using text editors or more complex editorial tools to create a full commentary and discussion of the structure may further extend the same file. Consequently the journals of the IUCr require all supplementary files recording crystal structure data to be in CIF format, and two of its journals will only accept papers submitted in this format. Such submissions are not only accepted and transformed by typesetting software into formatted research publications, but their embedded data are extracted and subjected to a battery of analytical and diagnostic calculations that provide referees with an objective assessment of the quality and consistency of the reported results.

The consequence of adopting such a standard is that data exchange becomes more efficient, computation is facilitated, transcription errors are removed from the publication process, and the quality of published data tends to improve. Overall, publication of structural reports journals becomes more efficient, onward transmission of the results to databases is also simplified, and readers may see any published crystal structure in three dimensions (and interact with the structure, generating stereo pairs, packing plots, and hydrogen bond networks ad libitum with the appropriate browser plug-ins or helper applications).

CIF has a somewhat different and rather simpler structure than XML. This is largely because it was developed at a time when SGML, the precursor of XML, was expensive and unwieldy to work with. Nevertheless, it is clear that automatic transformation between CIF and suitably devised XML formats is entirely feasible. Since its earliest days the CIF community has worked with pioneers in the chemical information field to work towards interoperability with emerging chemical information standards.

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explanation of the data dictionary associated with the defined name space "cml."

Namespaces do not have to be registered and so it is simple for any group or company to define their own version of "element." For example, although they could quite correctly claim to be using XML for data storage and transfer, the files generated would be as limited to their own internal applications as if they were using 17-bit binary encoded files. One way in which IUPAC could play a significant role in furthering XML for chemistry explained Murray-Rust is by ensuring that dictionaries are future safe and don't vanish from the Internet when a particular professor retires or a software or publishing house is bought out or goes bankrupt.

Goodman and McMahon agreed that IUPAC needed to identify the customers who would benefit from XML projects.

Jonathan Goodman, of the Unilever Centre, presented an amusing view from an academic and educational standpoint. His group has developed several databases that could lend themselves to being made available in an XML format. But, Goodman asked, what would be the immediate benefit? Quite simply, there would be none he stated. Should IUPAC take a clear lead in laying down guidelines on the presentation of chemical information in XML then it would be worthwhile to take this additional step as then other chemists and projects would be able to access and use the information more easily.

To conclude, Goodman said "there is a long way to go before XML is used routinely to improve and enhance chemical communication. However, XML friendly structures are already in place, and this should mean that a lot of data can easily be moved to this marked-up language. If an XML-based standard is accepted, then this process could be very rapid and data could be shared and reused much more easily than is now possible."

This supported the views of McMahon, who had commented that to generate an XML file from CIF would be a simple enough task, but questioned whether this would be "good" XML and "fit for purpose." Goodman and McMahon agreed that IUPAC needed to identify the customers who would benefit from XML projects. This includes clearly identifying stakeholders who will make the effort to implement whatever is developed.

Other presentations dealt with XML from various information providers' standpoints. Bill Town from ChemWeb and Sandy Lawson from MDL Information Systems pointed out the difficulties in achieving the uptake of technical developments in large organizations. Efforts have been made across the publishing industry to establish electronic submission and presentation of published papers, but authors still are unhappy about changing their habits. A general discussion was also held on the lack of decent authoring tools.

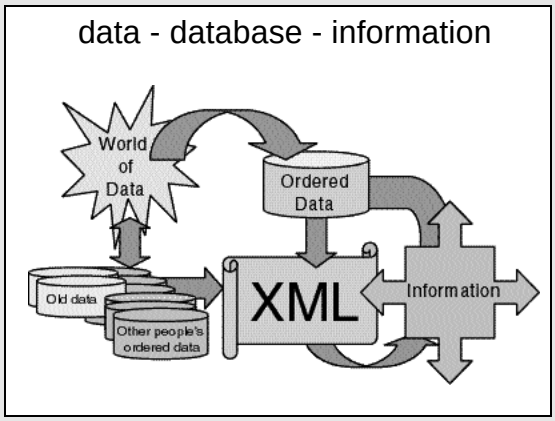
Kirk Schwall summarized the views of the Chemical Abstracts Service (CAS). According to Schwall, CAS has a collection of highly integrated data that have been organized using SGML since 1994. Since 1997, XML has been used for some data that have required frequent updating and interchangeability. Both the document and authority data collection concepts at CAS have XML as

Some of the attendees at the IUPAC Strategic Meeting on XML in Chemistry: (from left to right) Robert Lancashire, Bill Town, Jonathan Goodman, Sandy Lawson, Peter Murray-Rust, Kirk Schwall, Brian McMahon, Alan McNaught, Gary Mallard, Steve Stein, David Moore, Steve Heller, Bobby Glen, Kirill Degtyarenko, Richard Cammack, Peter Lampen, and Tony Davies.

How Well Are We Using XML in Chemistry?

by Jonathan Goodman

From an academic and educational viewpoint, one could say, unfortunately, not too well right now. Here are some reasons. One of the reasons is the complexity of XML. It may well be as simple as it can be, but it is not simple, and it requires substantial effort to master the syntax and restrictions of its structure. For example, <xsl:number count="paragraph" format="а"> is an instruction to number paragraphs in old Slavic, a powerful feature, but probably not frequently used, nor immediately comprehensible to the casual reader. Despite its complexity, the structure of XML relates well to the thought processes of most chemists and to the process of using marked-up text. For example, entering a name in the author search box of the World of Science, or other chemical database, is becoming so obvious as to require almost no thought. It could be suggested that, even though the details of XML syntax are not widely known, the structure that it imposes on documents is both understood and expected.



Successful Examples

A number of databases have been developed in our research group and made available on the Web. The general process we have followed is first to gather data from the huge and disordered sources and put them in an ordered and focused form. We then take this collection and find a way of presenting it so that it is useful information. For example, we have explored the Web for university chemistry departments, collected their URLs and names in text files, which we do not make available, and used these text files to create HTML and Java programs, which can be queried through the Internet. This final product is valuable information and it is created by a two-step process: order information and then present it. The database is available at <www.ch.cam.ac.uk/c2k/>.

We could introduce another step into the process: ordered information to XML before creating the simplified and beautified form, which is then made available. However, this extra step requires additional effort, which brings no immediate benefit. The potential of the XML form in chemistry is that it could relate well to other people's XML data and to old data from related projects in the group. However, this stage is an advantage for the future, and not the present, unless a clear community consensus is to recognize the preferred structure of XML for chemists; then, this extra step should become worthwhile.

While marking-up, ordering, and sharing data, one success of our department is our **list of colloquia**. Six different subject-groups within the department regularly invite external speakers to give lectures, while many other lectures are arranged on a less predictable basis. How can all of this information be put in a consistent form and used effectively to produce current information and a searchable and logical archive? The information comes from a wide variety of people, who usually run the colloquium program for only a short time before handing the responsibility on. The entire process achieves the unification of disparate information. Today's lectures are available on the Web at <www.ch.cam.ac.uk/today/>, a page that is automatically updated. Historical lists and current lists of lectures are available in a consistent format. Information is flowing freely and available to be used and reused in different ways, both automatically and by individuals. A restricted subset of HTML is used to order the information. The restrictions mean it could easily be converted by computer to a pure XML form. This is a successful data-handling project in chemistry, which has not been a trivial problem to solve. However, it is much simpler than the more general issues of chemical information.

Lecture handouts are also shared well, not because they are produced in a consistent and reusable form, but because of the high standard of our undergraduates' ability and industry. Exam papers also work effectively, because a very precise format is required and enforced. We do not have the option of turning to another publisher who might be more relaxed about presentation and the precise way in which diagrams are constructed. **Compound databases** and **experimental data** are shared much less effectively, even within the department of chemistry, and the situation gets worse when communication is attempted with other departments.

Conclusion

There is a long way to go before XML is used routinely to improve and enhance chemical communication. However, XML friendly structures are already in place, and this should mean that a lot of data can easily be moved to this marked-up language. If an XML-based standard is accepted, then this process could be very rapid and data could be shared and reused much more easily than is now possible.

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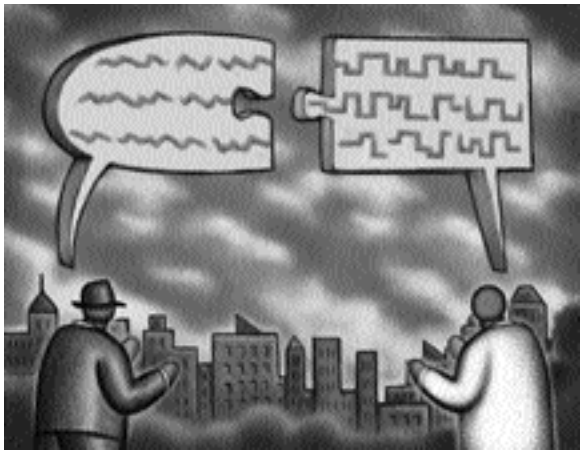

an element of their design. The vast complexity of their operation meant that they were forced to handle about to every possible mode of information delivery with only a small minority of their information suppliers delivering content in an XML format. Even when it is available it is not used, as the tags are stripped before being regenerated at the end of the document handling process. CAS does have an extensive thesaurus, but this is not publicly available. It was agreed that there is a need for CAS and IUPAC to discuss common ontologies.

Gary Mallard from the U.S. National Institute of Standards (NIST) summarized XML activities within that organization. According to Mallard, NIST uses XML for standardizing the delivery of the following types of scientific information: numerical data, exchange of instrument/reference data, materials property, and reactions design. The wide range of experience gained by NIST in different fields of scientific information delivery have placed it in a unique position to advise on the strengths and weaknesses of XML in chemistry. Quite often difficulties have arisen over rather banal problems such as unit names not being standardized internationally (e.g., meter vs metre vs mètre), symbols requiring special fonts and characters (e.g., unit °C, prefix μ, and quantity Vemf) or cases in which symbols are not available (or are not standardized internationally) for all units or quantities. Mallard, was, however, quick to point out some of the drawbacks of XML. He highlighted the problems associated with files that are essentially uninterpretable if the explanations of the individual labels used are not open and freely available. According to Mallard, he had created a nice presentation of the various XML efforts underway, but a problem arose when it turned out that several of the reference Web sites essential for the understanding of the ontologies no longer existed.

A Project for IUPAC

At the conclusion of this very successful meeting, Steve Stein of NIST was appointed to draft a project proposal to IUPAC on "Standard XML Data Dictionaries for Chemistry." In addition, a group of volunteers was established for a task group to support this project. The group plans to give a presentation at the coming CAS/IUPAC Conference on Chemical Identifiers and XML for Chemistry to be held in Columbus Ohio on 1 July 2002.[5]

The Future

The future is always difficult to predict and those who are brave or foolish enough to attempt it are usually proved wrong—often before their predictions go into print. However, I would like to put one point at the end of this summary: IUPAC is in an excellent position to provide a vital service to the scientific community by assisting in the development of information technology in chemistry and associated sciences. This is probably a unique situation in the history of IUPAC because those championing this work clearly understand the need to work fast, but also the inherent limitations of working within an IUPAC framework, as shown by the dos and don'ts list from the Brisbane meeting. I wish them all the best and hope to see all of you at the IUPAC/CAS conference in July.

Acknowledgements

I would like to thank Ian Michael, for permission to use my original column published in *Spectroscopy Europe*,[6] as the basis for this extended report, and Henry Rzepa, Peter Murray-Rust, Jonathan Goodman, Brian McMahon, Gary Mallard, and Kirk Schwall for their contributions. Also, I would like to thank Bobby Glen for hosting the conference and all those who attended the meeting, whether it was just to learn and report back to their IUPAC bodies or whether it was to assist with the drive for standardization of scientific IT. It is a hard road we tread and one with few rewards. After all, no one ever won a Nobel Prize for enabling communication among scientists!

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For more general information on XML:
www.isgmlug.org/n3-1/n3-1-18.htm
www.oasis-open.org/cover/xml.html#overview

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www.iupac.org/standing/cpep.html

Markup Languages—How to Structure Chemistry-Related Documents

by Peter Murray-Rust and Henry S. Rzepa

Although the use of markup languages in publishing goes back to the 1960s when IBM introduced GML (Generalized Markup Language), which subsequently evolved into the standard SGML, most authors are nowadays more familiar with the more recent implementation, referred to as HTML (HyperText Markup Language). The rapid rise in the use of HTML in conjunction with the growth of the World Wide Web was in large measure due to its ease of use for achieving presentational and visual effect. However, its limitations as a mechanism for expressing precisely defined data and meanings were not always adequately recognized. These limitations meant that in areas such as molecular sciences where precise meanings are essential, a variety of often proprietary solutions continued to be used to define and manipulate molecular "data" and information. The publishing processes were seen as quite separate and the process of translating data, information, and knowledge into a published entity remained an activity requiring much human perception. It is also worth noting that the reverse process of converting the published materials back into usable data remained equally human intensive and hence expensive.

The need to reconcile these two extremes was recognized at the first World Wide Web conference in 1994. A solution gelled shortly after the conference as a remarkable communal effort resulted in the specification of extensible markup language or XML. The ultimate vision of XML , as described by Berners-Lee, is the creation of a "Semantic Web."[1] The rationale for this impressive effort included the following:

- Provision of a more universal infrastructure for publishing
- Recognition that the use of XML will require subject-specific vocabularies called "ontologies" Ontology is defined as a description—such as a formal specification of a program—of the concepts and relationships that can exist for a software agent or a community of agents.
- Provision of a mechanism for enhancing quality ("validation")
- Promotion of the creation of dynamic hyper-documents
- Recognition of the need to be able to reuse components of documents for other purposes
- Provision of a mechanism for creating *smart archives*, in which the re-usable components (information objects) can be readily identified
- Creation of an infrastructure for underpinning the emerging areas of e-business

The extension to chemistry included, therefore, the creation of a new generation of ontologically rich, primary publication and a clear division of the respective roles of humans and software agents (robots). Thus, humans should be able to:

- Publish all their data automatically
- Eliminate *errors* from publications
- Use the published literature as a database
- *Understand* information from other domains

Robots should be able to:

- Analyze publications (on whatever scale)
- Create secondary publications
- Purchase chemicals
- Synthesize chemicals from literature

To achieve this, we argue that a number of prerequisites must be in place:

- Automatic data capture, especially from instruments. We note that in 30 years we have moved from using instruments that captured data often only in analogue form (chart paper) to using standard computers to capture and process data to most recently an increasing tendency for placing these computers online and connecting them to centralized data stores.
- Common ontologies for a specific community (e.g., molecular science)
- Ontologically guided authoring.

Issues Involved in "Capturing" Chemistry

The following extract[2] from a typical science journal illustrates both how precisely data and information must be represented, but also how much human perception is required to translate this information (e.g., to a reproducible experiment or a mechanistic interpretation):

> "Thiamin phosphate synthase catalyzes the formation of thiamin phosphate from 4-amino-5-(hydroxymethyl)-2-methylpyrimidine pyrophosphate and 5-(hydroxyethyl)-4-methylthiazole phosphate. The reaction involves . . . dissociative mechanism . . . carbenium ion intermediate . . . and pyrimidine iminemethide observed in the crystal . . ."

Note the profusion of chemical structure information, concepts, and terms, which only a trained human chemist could easily process. Quantitative concepts and units are also ubiquitous:

"A 500 µl aliquot of 0.8 µM TP synthase in 50 mM Tris-HCl (pH 7.5) and 6 mM $MgCl_2$ incubated at room temperature with 50uM CF_3HMP-PP."

An even greater degree of human perception is required when handling graphical chemical representations, which may contain many, often fuzzy and dangerous, human-only semantics (e.g., 2-D representations of 3-D properties, relative stereochemistry, aromaticity, hydrogen and other "weak" bonding, use of generic and "R" groups, reaction arrows, and mechanisms, etc.). The challenge, therefore, is to develop an infrastructure that can be routinely used to capture, store, and appropriately filter and display such information.

The Current Position of XML

As it is in 2002, XML offers a general, powerful, and extensible mechanism for handling both the "capture" and the publication of chemical information. In particular, XML allows for the first time this process to operate equally well in both directions. Our basis for stating this derives from the following observations:

- XML is increasingly accepted as an information infrastructure.
- The protocols are all public and many of the tools are open source.
- XML is vendor neutral, but with heavy vendor involvement.
- There is a large communal investment in generic tools (e.g., business2business, e-commerce).
- XML has a modular approach; an application is built from components.
- Domains are expected to create domain-specific XML protocols and tools.
- XML is increasingly universal in back-ends, middleware, and servers.
- Support for XML from database vendors is rapidly increasing.
- XML has close interoperability with other informatics standards such as UML, OMG/CORBA, etc.
- There is increasing support for "XML over the net" and from browsers (e.g., Internet Explorer, Netscape 6, etc).
- XML is very well supported by books, tutorials, etc.

Global Open Activity in Scientific XML

So how has the scientific community adopted these concepts? As noted above, the first World Wide Web conference specifically identified mathematics and chemistry as requiring specific markup languages. With this spark, CML (Chemical Markup Language) evolved between 1995-1997 to become the first scientific extended markup language. A concurrent effort lead to MathML becoming formalized as such in 1998.[3] We estimate that by 2002, perhaps 50 specifically scientific applications have been described in some degree. For example, 37 scientific applications are quoted at <www.xml.com/pub/rg/Science> and a more general listing is at <www.oasis-open.org/cover/xml.html#applications>. The Science Citation Index shows around 570 references to the keyword XML, and SciFinder retrieves 38 references to the term "XML in chemistry."

XML offers a general, powerful, and extensible mechanism for handling both the "capture" and the publication of chemical information.

We also emphasize that XML is designed to allow markup languages to be combined, at whatever level of granularity, so that documents can contain any number of components deriving from specific XML languages. HTML, which we noted above, has evolved into one such language (XHTML), but in its latest development has been modularized into smaller, more easily implemented components (e.g., XFORMS, a data-entry and validation component can be implemented separately from other, more display-oriented components). XHTML can co-exist in a document with languages such as SVG (a scalable vector graphical language), MathML, and CML. We elaborate this when discussing namespaces (*vide infra*).[4]

Some Essentials of an XML System

The following tasks will have to be accomplished in order to implement an XML solution to publishing chemical information:

- Creation of documents from both legacy sources of data and *de novo* by humans
- Creation and capture of metadata (dictionaries of terms, tables of contents, codes, etc.)
- Specification of namespaces (a reserved addressing scheme for information)
- Human validation of the system (conformance to agreed specifications)
- Machine validation of documents (according to a specified and agreed upon schema)
- Document transformation (XSLT)
- Rendering and display (XSL-FO, domain-specific such as molecular representations)

The design of an XML-based markup language should provide for the following:

- A *simple*, extensible document type definition (DTD) or schema (modular and not over-complicated)
- Agreed semantics
- One or more agreed and published ontologies
- Agreed examples and conformance tests
- A community of critical mass

Appropriate tools for accomplishing this should be identified. These might include the following:

- XML writers
- XML readers (more difficult than readers since the XML may not be normalized to a single form)
- Legacy converters (difficult because of variation and ambiguity in the original data which may require some degree of perception for an accurate conversion)
- Validators
- Dictionaries
- Editors

Custom-written XSLT style sheets and generic editors will accomplish some of these, but a document object model (DOM), which represents a syntax free abstraction of the data in memory, is probably essential for many subjects.

Ontologies of Relevance to Chemistry*

An overview of the types of ontologies required is shown in Table 1. Of the chemically specific information types, support should be included for:

- Molecules and substances
- Reactions
- Analytical information, especially spectra
- Computation and simulation (QM, mechanics, dynamics, etc.)
- "Data-centric" concepts (numbers, units, arrays, matrices, etc.)
- Specialist software for display, editing, searching, etc.
- "Adjoining" disciplines such as bio areas, materials science, etc.

Creating Valid XML Documents

Generic tools and protocols already exist to create valid XML documents. In particular, the use of DTDs (Document Type Definitions) and Schemas can bring enormous benefits, including eliminating/reducing software failure due to the use of invalid data and reducing difficulty of (human) understanding due to invalid publications. The DTD is a concept rooted in SGML, and is still used in XML to constrain the Markup vocabulary (i.e., the basic elements used for markup) and to some extent the (sub)structure of documents (i.e., what element can be a parent or child of another). Schemas are a more recent development, and unlike DTDs, are themselves expressed using XML. Of particular relevance to chemistry, they provide advantages over DTDs in that they can also be used for:

- Datatyping: numbers and user-defined types
- Enumeration (for example to specify the list of chemical elements)
- Lexical patterns
- Inheritance

Moreover, schemas allow for additional user-created rules (schematron/XSLT), and with dictionaries, support the conversion to software (e.g. CML-DOM), authoring (e.g., in editors), validation of the data on entry by the user.

Table 1: Types of Ontologies Relevant to XML in Chemistry and *Tasks for the Chemical Community*

General Non-Chemical Informatics	
Business and commerce, government, regulatory, academic, publishing, etc.	*Reuse existing or emerging approaches.*
Domain-Specific Non-chemical	
Mathematics (MathML), healthcare (HL7/XML), genomics (GeneOntology), etc.	*Collaborate to reuse existing or emerging approaches.*
Chemical-Specific but Generic Information Types	
Numeric data, descriptive prose, safety	*Create ontologies and reuse generic tools.*
Chemical-Specific Information Types	
Chemical substances, molecules, analytical and spectroscopic, reactions, computational chemistry	*Build the complete tool set.*

Namespaces—The Key to Making *It* Unique

Each information object must be uniquely named to avoid collision and ambiguity. This is achieved using XML namespacing.

The example below shows a paragraph of text (derived from XHTML, which inherits the default namespace), within which components of CML are

*In this context, the term ontology refers to a machine readable set of definitions that create a taxonomy of classes and subclasses and relationships between them. Ref: <www.w3.org/2001/sw/WebOnt/charter>

embedded, including prefixes using the defined namespaces:

```
<html  xmlns="http://www.w3.org/1999/xhtml"
xmlns:cml="http://www.xml-
cml.org/schema/cml2/core">
<p>We can supply the following set of mol-
ecules:</p>
<ul>
<li>
<cml:molecule id="p1" title="phosphine">
<cml:atomArray>
<cml:atom elementType="P"
hydrogenCount="3"/>
</cml:atomArray>
</li>
<li><cml:molecule id="p2" title="pen-
guinone"/></li>
</ul>
</html>
```

A proposal[5] for domain-independent components for Scientific-Technical-Medical information, or STMML, contains key elements such as units, dictionary, metadata, item, array, and matrix and which supports datatypes such as numbers, max/min, ranges, errors, etc. The next example illustrates how CML can be used in conjunction with the STMML namespace[5] to specify units and their constraints:

```
<molecule id="m1">  <crystal
spacegroup="Fm3m" z="4">
<stm:scalar title="a" errorValue="0.001"
units="angstrom">5.628</stm:scalar>
<stm:scalar title="b" errorValue="0.001"
units="angstrom">5.628</stm:scalar>
<stm:scalar title="c" errorValue="0.001"
units="angstrom">5.628</stm:scalar>
<stm:scalar title="alpha"
errorValue="0">90</stm:scalar>
<stm:scalar title="beta"
errorValue="0">90</stm:scalar>
<stm:scalar title="gamma"
errorValue="0">90</stm:scalar>  </crystal>
<atomArray>    <atom id="a1"
elementType="Na" formalCharge="1"
xyzFract="0.0 0.0 0.0" xy2="+23.2 -21.0"/>
<atom id="a2" elementType="Cl"
formalCharge="-1" xyzFract="0.5 0.0 0.0"/>
</atomArray></molecule>
```

A more extended example of this concatenation of namespaces[6] contains up to eight namespaced components and illustrates how a complete publication in XML/CML could be achieved. The use of namespaces can be seen in a more general context in Figure 1, which illustrates how the various specific XML components might relate to each other.

In particular, we note how the original CML specification[7] can be extended by modularization into a core namespace, and extended via other schemas into the following:

- **CMLReact**. A reaction, containing reactantLists, productLists and links between them.
- **CMLComp**. A container for computational and simulation input and results.

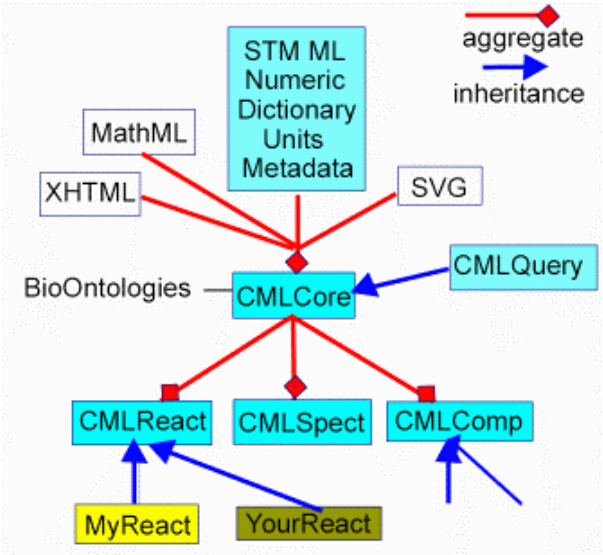

Figure 1: The use of namespaces in CML.

- **CMLQuery**. A generic query language.
- Hooks for other Schemas, such as **SpectHook**, for spectral parameters and data and links to molecular details (assignment).

Dictionaries and Schemas

It is useful to separate the domain ontology from the Schema/DTD, which allows the schema to be more abstract and which helps extensibility. Thus, with the instance document referring to NAMESPACE dictionaries, a three- or four-level hierarchy can be envisaged:

- The data instance
- The XMLSchema describing the instance
- The dictionary/ies describing the instance
- The schema describing the dictionaries

Such hierarchy and referring processes add semantics and ontology. An overview of this process is shown in Figure 2, where, for example, units are themselves verified by the UNITS dictionary.

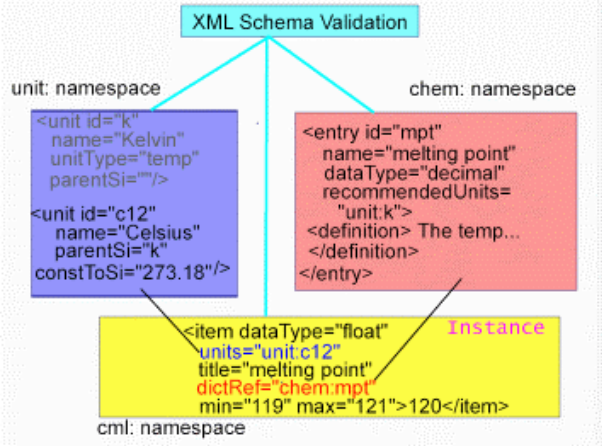

Figure 2: Validation scheme using dictionaries.

Document Structure and Metadata

Common dictionaries and compendia usually have some of the following features:

- Dictionaries consist of curated entries and many are "flat" (e.g., the IUPAC GoldBook).
- Dictionaries are compiled within a single hierarchy:
  - — **generic** ("is A"):

    eukaryote <-- vertebrate <-- mammal <-- human
  - — **partitive** ("has A"):

    body <-- leg <-- foot <-- toe
- Dictionaries can now be associated with a namespace for uniqueness and navigation.
- Dictionaries must have curatorial information.
- Dictionaries should support versioning.

Metadata is an important component of a document or information object and it can serve a number of purposes:

- **Navigational/Discovery**—How is a piece of information to be discovered (e.g., Dublin Core and GILS)?
- **Descriptive**—What does the information mean and how is it to be used?
- **Constraining**—What constraints are there on the structure and content of the information? Is it valid? This would be accomplished using mainly XML Schemas.
- **Supplementary**—Additional (hyper-) data added from metadata
- **Algorithmic**—Deductions can be made from metadata (e.g., using Schematron, XSLT, and RDF).
- **Chemical-descriptive**—For example, medicinal, physical organic chemistry, Gold Book, stereochemistry.
- **Chemical-constraining**—For example, theoretical chemistry and CIF.
- **Chemical-supplemental**—For example, tables of atomic weights, dictionaries of compounds, etc.
- **Chemical-algorithmic**—For example, theoretical chemistry and CIF.

Communally agreed-upon schemas for defining such metadata are again seen as an essential component of the XML-infrastructures.

The existing IUPAC compendia provide a natural foundation for creating XML-based machine processible resources. They fall into three broad categories: descriptive (e.g., medicinal chemistry, physical organic chemistry, stereochemistry, etc.), validating (e.g., theoretical chemistry) and supplemental (e.g., atomic weights). Their availability for XML-based processes would be a considerable asset.

Conclusions

In this brief review of the application of XML in chemistry, we have summarized the essential advantages of adopting the XML approach. We have discussed in particular the benefits in creating reusable namespaced information components or objects, how these can be created and validated using subject-specific ontologies and dictionaries, and then how they can be enhanced with appropriate metadata. The role of communities and global organizations, such as IUPAC, is crucial to this endeavour. The use of such XML-based documents opens the prospect of creating avenues for the reversible flow of data and information between the scientific publication processes and the discovery, research, and learning processes in molecular sciences; a reversibility that has hitherto only been achieved with considerable human effort and expense.

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http://cml.sourceforge.net

A Preprint Server for Chemistry

As the concept of preprint servers for the scientific community in general continues to be debated, *CI* has asked Bill Town, managing director of ChemWeb.com, to review for us the development and status of the initiative to provide a preprint server for the chemistry community.

by Bill Town

Before the advent of the Internet, scientists would typically only publish their work as research articles in standard peer-reviewed journals. In this process, an article is submitted to a board of editors and occasionally, the article is accepted in the state in which it was submitted. However, articles are often returned to the authors with a list of corrections that should be made before publication. In the field of chemistry the duration of the entire submission process—from completion of first draft to publication—can often extend to one year or more.

Authors within different scientific communities have for some time discussed their research by exchanging articles—"preprints"—amongst themselves before formal publication. Some authors choose to do this by posting articles to their own Web site. The alternative, which is growing in popularity, is to submit to"preprint servers"—permanent and freely available databases on the Internet. This process does not involve any peer review.

Perhaps the most successful example of a preprint server is the arXiv server,[1] covering high-energy physics and mathematics. Founded in 1991 by Paul Ginsparg, the arXiv server is now host to more than 300 000 preprints with just under 3 000 new preprints being submitted every month. Other disciplines have been slower to follow this trend. Recently, similar services have been set-up, including Cogprints[2] (for psychology and biology) and the Chemical Physics Preprint Database hosted at Brown University.[3] In August 2000, ChemWeb.com launched the Chemistry Preprint Server (CPS),[4] which is the first preprint server to cover the entire field of chemistry. The CPS was officially launched at the fall ACS National Meeting on 21 August 2000 in Washington, D.C.[5] By the launch date, 20 preprints had already been submitted.

Whether a chemistry preprint server will prove to be as successful as the arXiv server is for physics and mathematics is a question that will be answered by chemists themselves. The CPS was set up as an experimental service to examine the response of the community. ChemWeb.com believes that preprint servers have many advantages for researchers. For example, articles submitted to the CPS may take any format from an initial draft to a complete article ready for publication. Authors may continually revise the original version of the article and any number of supporting files may be added. In this way, scientific information is disseminated very rapidly and is archived permanently in electronic format. Furthermore, all preprints submitted to the CPS have their own discussion group where all users may discuss the article online.

Critics have raised concerns regarding the use of preprint servers for the dissemination of chemical information.[6,7] One such concern is the possible poor quality of information hosted online without any formal peer review in place. In other words, how do you extract the signal from the noise?

In general, the CPS received a positive response at the ACS meeting, where there was a plenary presidential event and Webcast entitled "The Impact of Preprint Servers in Scholarly Publishing."[8] The opinions expressed at this event were mixed. Again, the primary concerns were issues relating to prior publication and the possible lack of quality control. This debate has been discussed comprehensively in *Science*: "Chemists Toy with the Preprint Future."[7]

Preprint servers are permanent and freely available databases on the Internet.

To counter the concerns there are comprehensive searching and browsing facilities available on the CPS which allow the user to rapidly find an article of interest. All articles are screened to ensure that they do genuinely contain scientific content related to chemistry. Authors also must write in a standard format. In addition, the preprint discussion groups could provide an environment where an article is truly reviewed by one's peers. Every article accepted on the CPS is given a unique identifier—this supports the position of the CPS as a permanent Web archive and distribution medium.

Whether peer review really does guarantee the quality of a published article is another question. For printed media, the number of articles being submitted to peer-reviewed journals is growing so rapidly that editors and publishers now face an increasingly difficult task. In principle, they should ensure that the work is original and based on true scientific research. The introduction of preprint servers, as an additional step before formal publication, may in fact aid this process. Further information may be found in the recent article "Chemical E-Prints: The Ostriches" by Ray Dessy, published in *Trends in Analytical Chemistry*.[9]

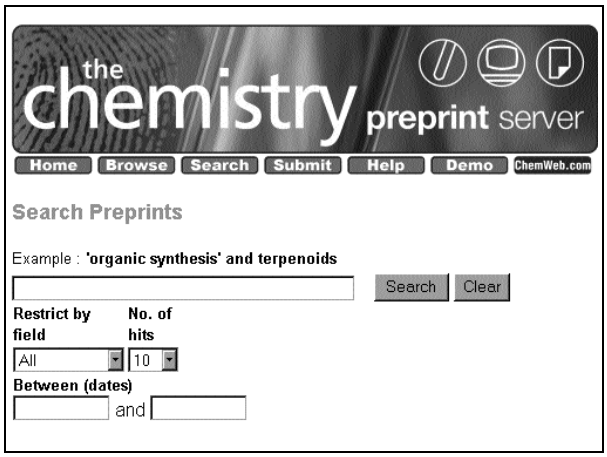
Perhaps the most important concern at the present time involves the prior-publication policies of all publishers within the field of chemistry. Currently, there is significant confusion over which publishers will publish preprinted articles. For example, *Elsevier Science*, the *Royal Society of Chemistry*, *Nature*, and many physics publishers will accept preprinted articles for publication in their journals. However, the American Chemical Society released a policy statement[9] stating that articles that have previously been made available on a preprint server will not be considered for publication. This problem arises from the policies of individual publishers and should not be confused with the issue of copyright or prior art issues for patents. For example, all authors must retain the article copyright to submit to the CPS. Furthermore, all preprints are stamped with the time of upload and a unique citation reference.

Politics aside, the CPS has been set up as an experiment in scientific communication for the worldwide chemistry community, and its success will be determined by its acceptance within the community. Although early signs do indicate a positive response, time will tell if researchers in the field of chemistry will adopt the CPS in the same way physicists and mathematicians have the arXiv preprint server.

The CPS was modelled on the arXiv preprint server, described above, to provide the first preprint server to cover the entire field of chemistry. In setting up the service, ChemWeb.com has constantly referred to the Open Archive Initiative[11] (OAI) for e-print archives. The CPS is now a compliant data provider for the OAI. The general purpose of the OAI is to set standards for the transfer of information between different Web servers. In this way, users of remote preprint servers are able to search through all of the information hosted on the CPS.

From the outset, an advisory board was set up for the CPS so that its independent status is maintained. The advisory board also ensures that the server develops and adapts to meet the needs of the chemical community. Some of the community's most respected names have shown their support for the CPS by becoming founder members of the advisory board, including Professor Pieter Steyn, current president of IUPAC. Other members include Professor Peter Atkins, Oxford University; Dr. Steve Bachrach, *Internet Journal of Chemistry*; Dr. Ad Bax, National Institutes of Health; Professor Ray Dessy, Virginia Tech; Dr. Jonathan Goodman, Cambridge University; Dr. Bill Milne, JCICS; Professor Paul Schleyer, University of Erlangen-Nuremberg; Dr. Edlyn Simmons, The Procter & Gamble Company; and Dr. Engelbert Zass, ETH Zürich.

Since the CPS was launched in August 2000, almost 500 preprints have been uploaded and made available for browsing, review, and discussion. The topics encompass all areas of chemistry, from computational and physical chemistry to biochemistry. To date, submissions have been made from 51 different countries. The largest number have been from the United States, but significant numbers have also come from the United Kingdom, Western and Eastern Europe, Russia, and India.



It is important to note that the CPS is still very much an experiment in scientific communication for the chemistry community. However, usage analysis of the service during its first two years of operation does indicate that it is receiving a very positive response. As the CPS becomes better known within the academic and industrial communities, the number of submitted papers will continue to grow. The CPS will develop and adapt to meet the needs of the chemical community.

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IUPAC Forum

On the Reality of Virtual Libraries

by Paul Erhardt

During one of the activities of the Chemistry and Human Health Division, namely a medicinal chemistry subsection meeting directed toward harmonizing nomenclature in the area of combinatorial chemistry, we became aware of a movement to obtain patent protection of virtual libraries. Such patents have been sought most often on the basis that a library has been pre-selected to be "drug like" in its make up. Along these same lines, it appears that Chemical Abstracts Service CA Registry numbers are now being sought for the compound members within virtual libraries. Concerned about these developments for the reasons mentioned below, we welcome the views of the readership to clarify what position might actually be best to advocate as we all continue to proceed into the rapidly evolving future of drug discovery.

Since its formalization as a discipline nearly 100 years ago, medicinal chemists have contemplated what structural features a new therapeutic agent ought to contain in order to exhibit the most desirable pharmacological profile. Simply drawing such conceptions on paper, however, has never been regarded as an adequate basis for a patent even when the conceived family of structures is new and novel. This is because the patenting process has traditionally also emphasized a reduction to practice (e.g., actual synthesis of a number of representatives so as to encompass the breadth or "scope" of the proposed family of structures) along with a demonstration of potential utility by at least a real, if not the preferred, embodiment of the concept (e.g., positive responses from the synthesized members upon their study in a biological model indicative of the anticipated response being sought in humans).

Today, it is possible with the aid of computers, to draw huge numbers of "virtual compounds" that can be thought of as drug like in their overall character based upon our notions of what types of parameters are generally required for such behavior. While this might constitute conception relative to a particular molecular scaffold to be deployed for a given therapeutic indication, it does not constitute either a reduction to practice or an actual demonstration of utility. In some ways, this situation is reminiscent of issues raised within the *Journal of Medicinal Chemistry* several years ago. In the midst of the so-called "heyday of rational drug design," this audience stepped forward to express its reluctance to engage in the wholesale publication of proposed new drug molecules that had not actually been synthesized. This is because it was recognized that this type of public disclosure could bar the patenting of such structures at a later point and could thus serve to discourage, rather than to encourage, the true pursuit of compounds deemed to be of therapeutic value. Finally, it might also be suggested that for similar reasons, prudence ought to be exercised relative to the potential assignment of CA Registry numbers to virtual compounds whether or not patents are being pursued.

Paul Erhardt is a professor at the University of Toledo, Ohio, USA, and is the director of the University Center for Drug Design & Development. He is also the current vice president of the IUPAC Chemistry and Human Health Division.

IUPAC News

The Analytical Chemistry Division

It seems extremely arrogant and naïve to assume that 10 individuals can possibly keep up with and do their part to drive forward a field as large and diverse as analytical chemistry. Yet that is the task of the IUPAC Analytical Chemistry Division Committee. To accomplish it, these 10 analytical minds work as a team, apply their own quality control (QC)/quality assurance (QA) procedures, and adopt new managerial strategies and organizational initiatives. In this article, we have asked the new Division president, David Moore, to explain what the Analytical Chemistry Division (ACD) does and how its members are selected.

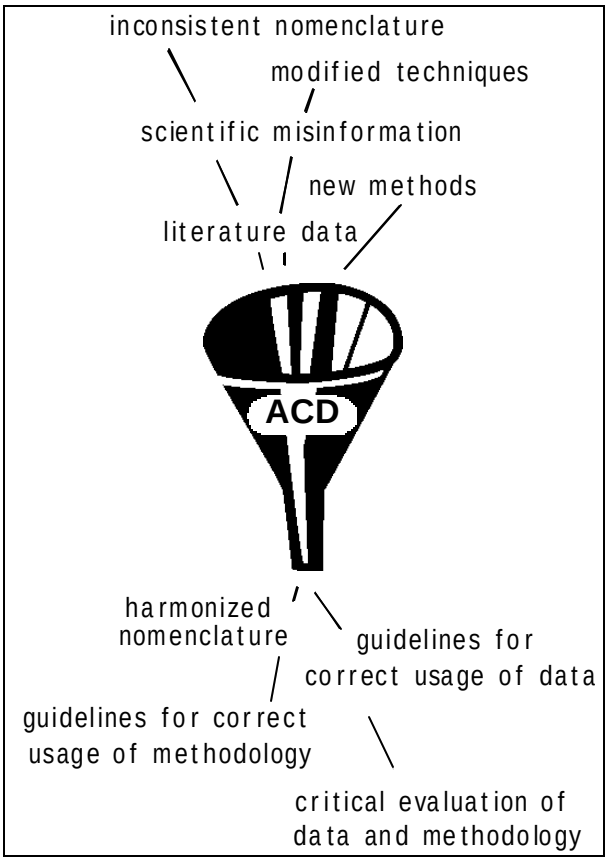
David Moore

Analytical Chemistry—A Discipline At the Heart of IUPAC

by David Moore

Analytical chemistry is a scientific discipline that develops and applies methods, instruments, and strategies to obtain information on the composition and nature of matter in space and time, as well as on the value of these measurements (i.e., their uncertainty, validation, and/or traceability to fundamental standards).

For more than 50 years, the role of the IUPAC ACD has been to catalyze interactions between the scientific community and users of analytical methodology and data and between the scientific community and beneficiaries of analytical results, such as international organizations (IAEA, OECD, WHO), accreditation bodies (ISO), standards bodies (BIPM, NIST), chemical societies, and society as a whole. The process involves taking input, such as literature data, information about sources, inconsistent nomenclature, newly developed or modified methods and techniques, and scientific misinformation, and then performing harmonization of nomenclature, critical evaluation of data and methodology, formulation of guidelines for correct usage of data and methodology, and promotion of analytical chemistry to society in general.



Where Role and Structure Define an Organization

In response to the recent IUPAC reorganization, the ACD also reorganized—through a phased process over the past four years—into a smaller structure with well-defined roles for committee members. These roles cover the various fields within analytical chemistry: methods (general aspects, separations, spectrochemical, electrochemical, nuclear chemical) and applications (particularly to environmental and human health problems). To enable analytical chemists to choose the methods best suited for specific applications, the roles of the ACD encompass:

- the critical and comparative evaluation of established and emerging analytical methods (including the harmonization of associated terminology, proficiency testing, and other inter-laboratory comparisons);
- the recommendations for sample collection, preparation, storage, and handling;
- the compilation of data used in analytical chemistry and their critical evaluation; and
- the definition of recommended methods and proper application of QC and QA procedures.

To optimally perform its required duties under a smaller structure, the division committee established several new managerial and organizational initiatives. Roles and responsibilities were established for each category of division committee membership. Each titular member (TM) of the division committee is encouraged to organize an advisory group in order to help them develop and/or select projects in response to pressing needs in a given area. An advisory group should therefore have a global view and experience in a specific area, in order to aid in identifying and soliciting new projects. Associate members of the committee are to provide focused representation in a particular area of analytical chemistry or to establish a tight link to other IUPAC committees, such as the Committee on Chemistry Education, the Interdivisional Committee on Terminology, Nomenclature and Symbols, or the Committee on Printed and Electronic Publications. National representatives are nominated by IUPAC National Adhering Organizations that are not otherwise represented on the committee (up to six are appointed). Each national representative is linked to a TM according to their expertise, with the goal of ensuring they participate and are tutored in project proposal reviews and ACD planning activities.

A shortcoming and criticism of IUPAC has been its lack of internal and external communication as well as relevance to the community. We have addressed the internal communication issue by establishing a regular e-mail newsletter (“Teamwork”) to keep members apprised of their responsibilities, upcoming events, new project proposals, and deadlines. As discussed below, initiatives to improve relevance have begun with a fresh review and selection process for new projects. External communication has been improved by better dissemina-

tion of project results. Moreover, we are establishing a directory of expertise database to allow us to locate experts according to a set of keywords related to their own field of expertise. Each person that has served the IUPAC ACD on a commission or project task group in the past decade or more will be recorded. New task group and division committee members, as well as experts involved in project review, will be added.

Electing *the* 10 ACD Committee Members

The smaller size of the division membership has also increased the difficulty in maintaining continuity over many years. We have addressed this problem by establishing a revolving election, whereby half of the committee is elected each biennium to facilitate four-year terms.

New ACD committee members are elected through a process defined in the IUPAC Bylaws. Nominees are selected by a Nominating Committee composed of five members: two from the ACD and three other well-known external analytical chemists, one of whom is appointed to be the chair. It is necessary for the Nominating Committee members to be very active to ensure a supply of fresh blood to the division committee, to ensure geographical diversity, and complete representation of the different branches of analytical chemistry. After the slate of nominees is complete, the IUPAC Secretariat handles the election itself via e-mail ballot. The electorate consists of the division committee titular members, associate members, and national representatives; project and task group leaders of current projects and projects scheduled to be completed during the current biennium; and nominating committee members not otherwise eligible.

Selecting the Most Relevant Projects

The ACD has a limited project budget, and yet, there are pressing needs within the international analytical chemistry community. The ACD therefore established a selection process for funding project proposals, based on a set of priorities.

After ensuring that a project proposal is complete, the Division president assigns one or two TMs to check the financial feasibility and practicality of the project. If needed, the proposed task force leader (or Task Group Chairman [TGC]) is asked to modify and resubmit the proposal. The Division president then recommends at least two external reviewers (either as suggested in the project proposal form or others as deemed appropriate) and transmits their names to the Secretariat, which handles the correspondence. Upon receipt of the reviewers comments, the Division president either accepts the reviews or asks the TGC to modify and resubmit the proposal.

A complete and annotated model project proposal is available on the ACD Web site. To be approved, projects should demonstrate clear evidence of advance planning and should describe the process that will be used to complete the project. Appendix A of the model proposal provides an example of such advance planning.

Following the initial review, and twice a year, the division committee carries out the selection and funding of projects, giving priority to pressing needs in given areas. The ACD committee is, however, concerned that all the different subject areas in analytical chemistry are covered in as equitable a fashion as possible. April 30 and October 31 are the deadlines for submitting completely reviewed proposals and initiating the selection process. The projects that are considered good, but cannot be funded, are then carried forward for the next selection, if so desired by the TGC.

The ACD has adopted the following general guidelines for project priority:

- IUPAC objectives met
- Task group membership complete with appropriate expertise and diversity
- Funding amount appropriate and justified
- High scientific value to user groups per cost
- Subject area coverage balance
- Cost sharing with other funding agencies so that funds are leveraged
- High visibility and usability of product
- Dissemination plan complete and appropriate

Monitoring Projects

Individual TGCs are responsible for the implementation of their projects and the management of their project budgets. Practically, a TM of the division committee is assigned to track a given project, as soon as funding is approved. Each TGC is asked to send a progress report to the Division vice president semi-annually (at the end of June and December), stating the completion of milestones, indicating whether any difficulties have been encountered, and stating whether the project is likely still to meet its completion date. All these reports are collated and forwarded to all ACD members so that they can add comments when needed. The expenditures are handled and tracked by the Secretariat.

Completing a Project

The final product of a project—usually a manuscript—is sent to the Division secretary (a copy also goes to the Division president), who then sends it to two or three ACD members for internal review, and also to three external reviewers named by the TM monitoring the project. The Division secretary then collects the reviews and returns them to the TGC for incorporation into a revised camera-ready manuscript. If the project involves nomenclature or terminology, an additional review process through the ICTNS is then initiated to further ensure consistency with previous publications, as well as worldwide consultation.

Does it Just End There?

No, the next stage is the dissemination plan, one of the most important parts of any IUPAC project. This is how terminology recommendations, for instance, are made known to practitioners or to the intended audience. Therefore, the implementation of the dissemination plan will be monitored. Again, an assigned TM will liaise with the TGC. As each step in the dissemination plan is executed, the TGC is asked to notify the assigned TM. This tracking system is to supplement the semi-annual progress reports and to help the ACD to improve on external communication.

What Does the Future Hold?

A major undertaking that looms just over the horizon is the revision of the Orange Book (Compendium of Analytical Nomenclature), which is being posted on the IUPAC Web site. Each chapter is slated to be systematically updated over the next few years according to the latest recommendations in each field. In the future, each project that recommends terminology will also provide for a mechanism to update the relevant entries in the Orange Book.

Project proposals are always welcome. In addition, ideas for projects and/or pressing needs within the analytical chemistry community can be communicated to anyone on the division committee so that a task force can be organized.

Dr. David Moore is a technical staff member at the Los Alamos National Laboratory, New Mexico, USA, and is the current president of ACD. He has been involved in the Analytical Division since 1988, and a member of the division committee since 1998.

www.iupac.org/divisions/V

2002 Winners of the IUPAC Prize for Young Chemists

On 14 May 2002, IUPAC today announced the winners of the IUPAC Prize for Young Chemists, an award for the best Ph.D. thesis in the chemical sciences, as described in a 1 000-word essay. The winners are:

- Jeroen J. L. M. Cornelissen, University of Nijmegen, The Netherlands (currently at IBM Almaden research Center, San Jose, CA);
- Jinsang Kim, Massachusetts Institute of Technology, Boston, MA, USA (currently at the California Institute of Technology, Pasadena, CA);
- Stefan Lorkowski, University of Münster, Germany;
- Simi Pushpan, Indian Institute of Technology, Kanpur, India.

The four winners will each receive a cash prize of USD 1 000 and a free trip to the IUPAC Congress, 10-15 August 2003, Ottawa, Canada. Each prize winner will also be invited to present a poster at the IUPAC Congress describing his/her award winning work.

Applications for the 2003 Prize are now being solicited, as described on the IUPAC Web site.

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

- Dr. Cornelissen, "Polymers and Block Copolymers of Isocyanopeptides—Towards Higher Structural Order in Macromolecular Systems;"
- Dr. Kim, "Supramolecular Assemblies of Conjugated Sensory Polymers and the Optimization of Transport Properties;"
- Dr. Lorkowski, "Differential Gene Expression in Human Macrophages During Foam Cell Formation;"
- Dr. Pushpan, "Core Modified N-confused and Expanded Porphyrinoids: Syntheses, Characterization and Photodynamic Activity."

There were 40 applicants from 20 countries. The Prize Selection Committee was comprised of Members of the IUPAC Bureau with a wide range of expertise in chemistry. The Committee was chaired by Dr. Alan Hayes, IUPAC Past President.

In view of the quality of many applications, the Committee decided also to give four Honorable Mention awards to:

- Christopher J. Kuehl, University of Utah, USA (currently at Los Alamos National Laboratory, NM);
- Gábor Lente, University of Debrecen, Hungary;
- Shinsuke Sando, Kyoto University, Japan (currently at Stanford University, CA, USA);
- Izabela Tworowska, Polish Academy of Sciences, Lodz, Poland (currently at Rice University, Texas, USA).

The Honorable Mention Award winners will receive a cash prize of USD 100 and a copy of the Compendium of Chemical Terminology, the IUPAC "Gold Book."

The awards to the four winners of the IUPAC 2002 and those of 2003 will be made during the Opening Ceremony of the IUPAC Congress in Ottawa, Canada.

www.iupac.org/news/prize/2002_winners.html

IUPAC Projects

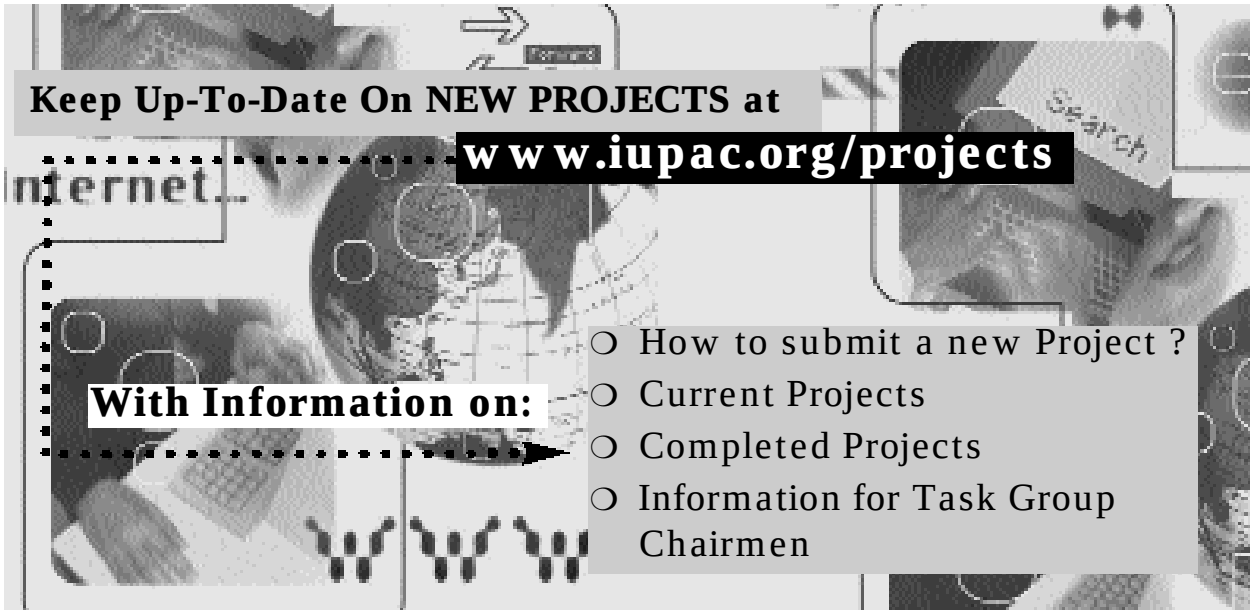
Pest Management for Small-Acreage Crops: A Cooperative Global Approach

The pesticide industry is global, with seven companies dominating world markets. The primary crops for which the industry develops pesticides are those that occupy large acreages such as grain and oilseed commodities. Fruits, vegetables, and other smaller-area crops receive attention in proportion to their area. However, such minor crops constitute a major portion of most region's economies and are often a region's best protection against the negative effects of globalization. With a relatively small market potential for any individual crop, pesticide manufacturers need cooperative assistance—with the expense of registration and liability control—from growers and governments. Thus, national minor-use pesticide registration programs are in various stages of development worldwide. There is a need for communication and data-sharing between these programs and for technology transfer to countries that are initiating them. The IUPAC Chemistry and the Environment Division is supporting an information exchange project to address this need. R. Donald Wauchope is Task Group chairman of the project.

The project methodology includes the (1) comparison of minor-use procedures between countries; (2) proposal of harmonization and data-sharing approaches; (3) examination of minimum data requirements for minor uses; (4) examination of extrapolation possibilities:

from major to minor crops, from major crops to crop groups, and between climatological zones; and (5) mining available crop residue data for development of a food crop pesticide residues predictive model. We propose to develop an open information system, and we invite participation from all interested parties, with the expectation that improved global consistency in minor use registration procedures will benefit consumers, agriculture, and the environment.

www.iupac.org/projects/2001/2001-039-1-600.html



Provisional Recommendations

IUPAC Seeks Your Comments

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

There are currently two documents available for review:

Quantities, Terminology, and Symbols in Photothermal and Related Spectroscopies
Comments by 31 July 2002
Chem. Int. 2002, Vol 24, No 2, p. 19

Thermochemistry of Chemical Reactions: Terminology, Symbols, and Experimental Methods for the Determination of Bond Energies
Comments by 30 September 2002
Chem. Int. 2002, Vol 24, No 3, p. 16

If you would like to comment, please visit the IUPAC Web site, where the full texts are available for downloadings as draft pdf files.

www.iupac.org/reports/provisional

Highlights from Pure and Applied Chemistry

Presenting recently published IUPAC technical reports and recommendations

Critical Evaluation of Proven Chemical Weapon Destruction Technologies (IUPAC Technical Report)

by Graham S. Pearson and Richard S. Magee
Pure and Applied Chemistry, Vol. 74, No. 2, pp. 187-316 (2002)

The Chemical Weapons Convention (CWC), which entered into force on 29 April 1997, prohibits the development, production, transfer, acquisition, stockpiling, and retention of chemical weapons and their use and requires all State Parties to undertake "to destroy chemical weapons it owns or possesses, or that are located in any place under its jurisdiction or control, in accordance with the provisions of this Convention." The CWC opened for signature in January 1993 and, as of May 2002, had 145 State Parties—states which have ratified or acceded to the Convention.

The Requirement for Destruction

Article IV of the Convention requires that:

> "Each State Party shall destroy all chemical weapons. . . Such destruction shall begin not later than two years after this Convention enters into force for it and shall finish **not later than 10 years after entry into force of this Convention.**" [Emphasis added]

Consequently, the deadline for destruction of chemical weapons is 29 April 2007. However, the CWC's Verification Annex includes a provision allowing a State Party to apply to the Executive Council for an extension of the deadline if it believes that it will be unable to ensure destruction of all chemical weapons within the 10-year timeframe. The Convention states that "any extension shall be the minimum necessary but in no case shall the deadline for a State Party to complete its destruction of all chemical weapons be extended beyond 15 years after entry into force of this Convention."

Five years left to destroy chemical weapons

The destruction requirements are further elaborated in Part IV(A) of the Verification Annex which *inter alia* require that the "chemicals are converted in an **essentially irreversible** way to a form unsuitable for production of chemical weapons, and which in an **irreversible** manner renders munitions and other devices unusable as such." [Emphasis added]

This report, published in *Pure and Applied Chemistry*, Vol. 74, No. 2, February 2002, pp. 187-316 is intended to provide policymakers and decisionmakers concerned with the destruction of chemical weapons with information about technologies proven to destroy chemical

weapons. The IUPAC Working Party that prepared this report recognized that each country faced with destruction of chemical weapons will need to consider the quantity and nature of their weapons, the CWC requirements, and its own national laws and regulations in deciding where and how to destroy them safely with minimal impact on public health and the environment. Consequently, the report is designed to provide appropriate and relevant information on the proven and available destruction technologies in order to help countries arrive at informed national decisions appropriate for their circumstances.

As already noted, the CWC requires that all declared chemical weapons be destroyed within 10 years after its entry into force, with a possible extension, should that be necessary, for up to five years, which would be until 29 April 2012. The CWC also sets out requirements for the destruction of old and abandoned chemical weapons, which will continue to be found for decades in countries where chemical weapons have been produced, tested, stored, and used. There are, thus, two principal categories of chemical weapons:

1. **Stockpiled chemical weapons**, which have to be destroyed by 29 April 2007 with a possible extension to 29 April 2012; and
2. **Old and abandoned chemical weapons**, in unknown types and quantities, which will be found from time to time and will need to be destroyed also by 29 April 2007 unless the Executive Council decides to modify the provisions on the time limit.

The report starts by addressing in its first chapter the mandate for destruction. The second chapter provides a historical perspective on the type of chemicals that have been used in chemical weapons during the past century and then the third chapter addresses the nature of the problem. The report notes that many chemical weapons have been destroyed or disposed of by methods that are no longer accepted. Indeed, the CWC specifically prohibits "dumping in any body of water, land burial, and open pit burning." During the past 40 years, over 20 000 agent-tonnes of chemical weapons have been destroyed; more than 70% by incineration and the remainder by neutralization. As of October 2001, the United States had destroyed over 20 percent of its stockpiled chemical weapons—around 6 700 agent-tonnes—using incineration. [Note: the unit used in the IUPAC Technical Report for the quantities of chemical weapons destroyed is agent-tonnes and **not** the weight of munitions.]

According to the Organization for the Prohibition of Chemical Weapons (OPCW), as of 30 June 2001, 69 862 agent-tonnes of chemical weapons have been declared and 5 734 agent-tonnes of chemical weapons have been destroyed under OPCW supervision since the CWC entered into force. The principal contributors to the global stockpile are the United States and the Russian Federation. The United States has declared its stockpile to be some 31 495 agent-tons (short tons), which corresponds to 28 570 agent-tonnes. The Russian Federation has declared its stockpile to be about 40 000 agent-tonnes. As India and one other country, known from non-OPCW information to be South Korea, have also declared chemical weapons, the combined stockpiles for these two countries can be deduced to be about 1 500 agent-tonnes.

In addition to stockpiled chemical weapons, there are also quantities of old and abandoned chemical weapons in several countries around the world. The following State Parties to the CWC have made declarations of old and abandoned chemical weapons:

- Belgium
- Canada
- China
- France
- Germany
- Italy
- Japan
- Panama
- Slovenia
- United Kingdom
- United States

The old and abandoned weapons in Europe are primarily from World War I and in China from World War II.

The quantity of chemical weapons that have been destroyed during the past 40 years in a number of countries has been in excess of 20 000 tonnes. The majority, over 16 000 tonnes, has been destroyed by incineration, while 4 000 tonnes have been destroyed by neutralization. Yet, there remain some 64 000 agent-tonnes of declared weapons to be destroyed by 29 April 2007.

Destruction Technologies

It is important to recognize that the destruction technology is only one part of the overall process of safely disposing of chemical weapons. The technology destroys the chemical agents and decontaminates their containers, while creating residual effluent streams of gas, liquid, or solid. The treatment of these effluent streams so they can be discharged to the environment with minimal impact on public health and the environment is as important as the destruction technology itself.

Because these chemical agents were produced to cause harm, steps were never taken to ensure that they were particularly pure. The original considerations were simply that the agent should be effective and should have sufficient stability to be stored for a number of years. Destruction and disposal are consequently made more complex because the agents are likely to contain impurities and materials such as solvents that were present when originally produced, as well as degradation products generated during storage. Many stockpiled chemical weapons are over 40-years old and the nature of their contents is variable and uncertain. Therefore, destruction technologies and effluent treatments must be robust to handle a wide range of impurities and agent compositions.

The fourth chapter of the IUPAC Technical Report addresses the transportation of chemical weapons and bulk agent from storage depots or other locations where chemical weapons have been found to sites at which they are destroyed. In the following chapter, the various options for the removal of the agents from weapons are considered. The next two chapters examine the high-temperature and low-temperature technologies that have been used—or are being considered for use—to destroy chemical agents. The report identifies the following processes as having been sufficiently and successfully demonstrated with actual chemical warfare agents to be considered for use within the timeframe of the CWC requirement.

High-Temperature Destruction of Chemical Agents

- Incineration
- Plasma Pyrolysis
- Molten Metal Technology
- Hydrogenolysis
- Destruction of Arsenical Agents

Low-Temperature Destruction of Chemical Agents

- Hydrolysis of Mustard Agent
- Hydrolysis of Mustard and Nerve Agents using Aqueous Sodium Hydroxide
- Reaction of Mustard and Nerve Agents using Amines and Other Reagents
- Electrochemical Oxidation
- Solvated Electron Technology

It should be noted that there is wide variation in the technical maturity of these technologies. The additional development required for some of these technologies makes it highly problematic that they will be sufficiently advanced to use within the CWC treaty timelines. These technologies may, however, have application for the destruction of old and abandoned chemical weapons. Again, it may be possible for the CWC treaty timeline for these weapons to be modified should the State Party concerned make such a request.

A separate chapter of the report addresses the treatment of gas, liquid, and solid effluent. A subsequent chapter considers how to deal with abandoned chemical weapons, which will be found intermittently in unknown types and quantities in many countries for decades to come. References are provided throughout the report to assist those seeking additional detail.

National Decisions and National Circumstances

A final chapter considers the technologies and constraints that have to be considered by a country faced with making informed decisions about destruction of chemical weapons. The IUPAC Working Party recognized that chemical agents are highly toxic chemicals that primarily became available for use in chemical

weapons programs from ongoing work in chemistry. There is thus a sense in which chemical agents are merely members of a vast array of chemicals of varying toxicity. Consequently, there is a logic in considering the destruction of chemical agents as being no different from the destruction of other highly toxic chemicals. **Chemical agents, therefore, need not be regarded as being a special class of materials whose destruction demands unique precautions—they are merely members of the vast family of chemicals and their destruction, as that of any chemical, requires appropriate precautions to safeguard worker safety, public health, and the environment.**

The working party is acutely aware that much of the information presented in the report is based on U.S. experience. Indeed, one member of the IUPAC Working Party (Richard S. Magee) was chairman of the U.S. National Research Committee's 1996 Panel on "Review and Evaluation of Alternative Chemical Disposal Technologies." However, this is hardly surprising as the United States and the Russian Federation had by far the largest stockpiles of chemical weapons and agents anywhere in the world. The United States has made much progress in destroying its stockpile of chemical weapons and agents and has also done more work than any other country to examine alternative technologies for the destruction of chemical weapons and agents. The report, therefore, drew heavily from the U.S. experience. **However, the decisions to be made by countries faced with the destruction of chemical weapons and agents need to be made in light of the particular national conditions and standards—and thus may well result in a decision to use different approaches from those adopted by the United States.** Other countries will need to consider the size and nature of their chemical weapons in deciding both where and how to destroy

them in accordance with CWC requirements and how to do this safely with minimal impact on public health and the environment. The aim of the IUPAC Technical Report is to provide information on the available destruction technologies in order to help countries arrive at appropriate, informed decisions.

Graham S. Pearson was chairman of the IUPAC Working Party which prepared this Technical Report and is a professor of international security in the Department of Peace Studies at the University of Bradford, Bradford, West Yorkshire, United Kingdom. Prior to 1995, he was director-general and chief executive of the Chemical and Biological Defence Establishment at Porton Down, United Kingdom.

Richard S. Magee is vice president of Carmagen Engineering, Inc., Rockaway, New Jersey, USA. He was previously associate provost for Research and Development at the New Jersey Institute of Technology.

www.iupac.org/publications/pac/2002/7402/7402x0187.html

Definitions of Basic Terms Relating to Polymer Liquid Crystals (IUPAC Recommendations 2001)

by M. Barón and R. F. T. Stepto
Pure and Applied Chemistry, Vol. 74, No. 3, pp. 493-509 (2002)

This document provides definitions of the basic terms that are used in the field of liquid-crystalline polymers. It is the result of extensive discussions and evaluations by the former Commission of Macromolecular Nomenclature. It was produced with the cooperation and advice of representatives of the International Liquid Crystal Society.

The recommendations concern terminology relating to the structure of liquid-crystalline polymers. In view of the rapid growth of the field, the terms defined have been restricted to those presently in common usage. They have been selected from the recently published comprehensive document "Definitions of Basic Terms Relating to Low-Molar-Mass and Polymer Liquid Crystals" [(*Pure and Applied Chemistry*, 73(5) 845-895 (2001)].

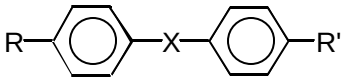
The recommendations are intended to form a readily usable guide for the reader interested in the structural description of polymer liquid crystals. The more comprehensive document (vide supra) should be used for terminology associated with mesophases and the optical textures and physical characteristics of liquid-crystalline materials. The numbering of terms in the document is consistent within itself and cross-references are made to the numbering of terms in the more comprehensive document.

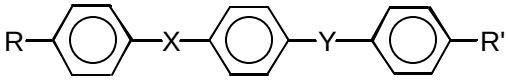
The document contains the following sections: introduction, general definitions, and liquid-crystalline polymers. It also contains a reference list and an alphabetical index of terms that serves as a subject index. The general definitions section gives the definitions of 27 principal terms and some subsidiary terms concerned mainly with the types of mesophase and types of mesogen; one example is reproduced below. The section dealing specifically with liquid-crystalline polymers defines 12 terms and gives 21 structural examples.

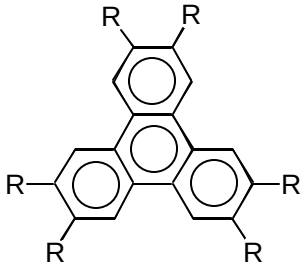
2.7 [2.10] mesogenic group, mesogenic unit, mesogenic moiety
A part of a molecule or macromolecule endowed with sufficient anisotropy in both attractive and repulsive forces to contribute strongly to mesophase or, in particular, LC mesophase formation in low-molar-mass and polymeric substances.

Notes:
1."Mesogenic "is an adjective that in the present document applies to molecular moieties that are structurally compatible with the formation of LC phases by the molecular system in which they exist.
2.Mesogenic groups occur in both low-molar-mass and polymeric compounds.
3.A majority of mesogenic groups consists of rigid rod- or disc-like molecular moieties.

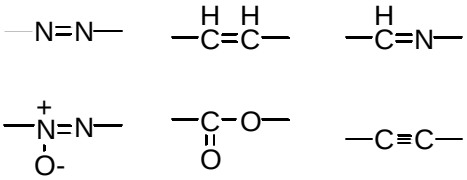
Examples







where X and Y are covalent bonds or linking units such as:



www.iupac.org/publications/pac/2002/7403/7403x0493.html

Dos and Don'ts—Tips of ICTNS

On Quantity Calculus

Each symbol of a quantity (single letter italic) in an equation stands for the value of the quantity, which is

$$(\text{quantity}) = (\text{numerical value}) \times (\text{unit}) \qquad (1)$$

In this way the equations hold for any units as we believe the laws of nature should. Units are a matter of human choice, and no law in nature should depend on it.

Thus

$$\text{force} = \text{mass} \times \text{acceleration}$$

or with symbols

$$F = m\,a \qquad (2)$$

irrespective of what units we choose.

Equations should be written in a form not implying certain units.

In applications with many repetitive calculations it is often convenient to write equations with numerical values in certain units. Then, however, different symbols should be used.

Equation (2) can for a certain purpose be written in the form

$$\{F\}_{\mathrm{N}} = \{m\}_{\mathrm{kg}} \cdot \{a\}_{\mathrm{m\,s^{-2}}}$$

or

$$\frac{F}{\mathrm{N}} = \frac{m}{\mathrm{kg}} \cdot \frac{a}{\mathrm{m\,s^{-2}}} \qquad (3)$$

where $\{F\}_{\mathrm{N}} = F/\mathrm{N}$ is the numerical value of the force in newtons, etc. Eq. (3) can be derived from (2) by division of both sides by $\mathrm{N} = \mathrm{kg\ m\ s^{-2}}$.

If we measure the mass in pounds and acceleration in inches per second squared and we are still interested in the force in newtons, we can divide equation (2) by $(\mathrm{lb\ in\ s^{-2}}) = 0.545\ \mathrm{kg} \cdot 0.0254\ \mathrm{m\ s^{-2}} = 0.0115\ \mathrm{N}$ obtaining

$$\frac{F}{0.0115\mathrm{N}} = \frac{m}{\mathrm{lb}} \cdot \frac{a}{\mathrm{in\ s^{-2}}}$$

or in a more convenient form

$$\frac{F}{\mathrm{N}} = 86.7\,\frac{m}{\mathrm{lb}} \cdot \frac{a}{\mathrm{in\ s^{-2}}} \qquad (4)$$

This is also the way in which we would write computer programs. However, this does not mean that we are allowed to write

$$F = 86.7\ m\ a$$

which obviously only holds if the symbols denote numerical values of quantities in a special choice of units. Even worse, if mass happens to be 1 lb always in our experiments, this does not allow us to write

$$F = 86.7\ a$$

See also: *Quantities, Units and Symbols in Physical Chemistry*, 2nd edition (The Green Book), I. Mills, T. Cvitas, K. Homann, N. Kallay, and K. Kuchitsu, Blackwell Science, 1993 [ISBN 0-63203-5838]

www.iupac.org/standing/ictns/quantity_and_percents.html

New Books and Publications

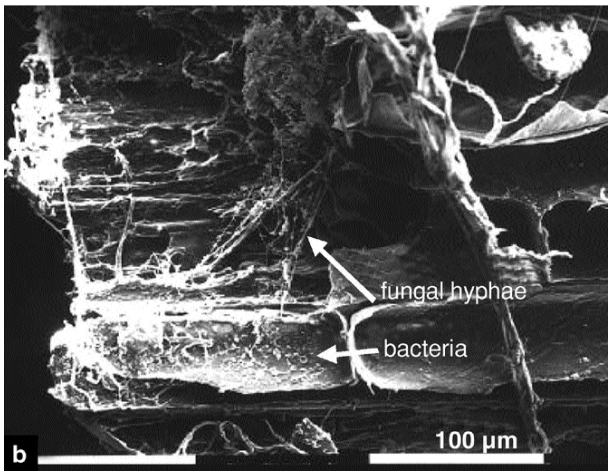
Interactions Between Soil Particles and Microorganisms: Impact on the Terrestrial Ecosystem

P. M. Huang, J. M. Bollag, and N. Senesi
Series on Analytical and Physical Chemistry of Environmental Systems, Vol. 8
John Wiley & Sons, New York, 2002
(ISBN 0-471-60790-8)

The three major (solid) components of soil—minerals, organic components, and microorganisms—together profoundly affect the physicochemical and biological properties of terrestrial systems. To date, there have been major scientific accomplishments in individual sub-disciplines (i.e., in the chemistry of soil minerals, the chemistry of soil organic matter, and soil microbiology). However, minerals, organic matter, and microorganisms should not be considered as separate entities but rather as a united system, with the components constantly in close association and interaction with each other in the terrestrial environment. These interactions have an enormous impact on terrestrial processes critical to environmental quality and ecosystem health around the globe. *Interactions Between Soil Particles and Mircroorganisms* provides the scientific community with a critical evaluation of state-of-the-art research on the subject matter, with the goal of advancing the understanding of reaction and processes at the interface between chemistry and biology of soil and related environments.

Key features:

- The first book to provide a comprehensive review of current research into the interactions of minerals, organic components, and microorganisms in the soil, at molecular and microscopic levels
- Defines the impact that these interactions have on environmental quality and ecosystem health
- Provides a unique insight into the effects of mineral-organic component-microorganism interaction on pollutants in the soil
- Provides a stimulus for further research into the dynamics and mechanisms of environmental processes in nature



Electron microscopy of bacteria and fungi attached to wheat straw surfaces; C. Chenu and Recous, from chapter one.

This volume will be an essential reference for chemists and biologists studying environmental systems, as well as for earth and soil scientists, environmental geologists, and environmental engineers. It will also serve as a useful reference for professionals/consultants in microbiology and ecology.

www.iupac.org/publications/books/author/huang02.html

Non-Conventional Polymer Dispersions

I. Capek, Symposium Editor
Macromolecular Symposium, Vol. 179, Wiley-VCH, 2002, pp. 1-358
(ISBN 3-527-30469-x)

The 15th Bratislava International Committee on Polmers, Non-Conventional Polymer Dispersions, held 25-28 June 2001in Smolenice, Slovakia continued the series of Bratislava meetings organized by the Polymer Institute of the Slovak Academy of Sciences (SAS). The Symposium was sponsored by IUPAC and supported by the Slovak Grand Agency of SAS and participants themselves. The meeting took place at the fairy-tale-like castle of Smolenice located about 65 km north of the Slovakian capital, Bratislava.

The main topics of the Symposium included.

- Microemulsion, miniemulsion, and multiple emulsion polymerizations
- Association and polymerization behavior of amphiphilic macromonomers, graft copolymers, and macroinitiators in polar media
- Novel and non-conventional polymer products and polymer dispersions, prepared by radical polymerization

The Symposium included invited plenary lectures, contributed lectures and poster presentations. This meeting was a international one: lectures and posters

were presented in English by scientists from the Czech Republic, France, Germany, Hungary, Italy, Japan, Russia, Turkey, Taiwan, and Slovakia. The plenary and contributed lectures were presented by eminent scientist and by well-known active researchers of younger generations. The Symposium featured a dynamic poster section which included presentations by many participants, especially young scientists, and was accompanied by very lively discussions. A short account on the materials presented at the Symposium was published in the *Book of Abstracts*. Regrettably, this volume does not cover all the new and interesting results presented at the Symposium since not all the authors were able to present their lectures for publication in this volume (some of the material had been published earlier or submitted elsewhere). However, it provides a good representation of the scope of the meeting and the main topics of the discussion.

The symposium focused on current developments in the radical polymerization in the micellar media and synthesis of novel (surface-active) polymer products. It attracted an excellent attendance, reflecting the strong and wide-spread interest in the field of preparation of non-conventional polymer dispersions and stimulated mutual interactions between researchers working on similar display technologies. Both an interesting venue of the conference and well-organized scientific and social program added to the success of the event as quoted by participants.

This brief review of the materials of the Symposium including those presented in this volume shows that the main interest in the investigation of the preparation of non-traditional polymer dispersions and polymer products lies in the nature of the reaction loci, particle nucleation, and particle-growth events.


www.iupac.org/publications/macro/2002/179_preface.html

Solubility of Ethyne in Liquids

Peter G. T. Fogg, Sim-wan Annie Bligh, M. Elizabeth Derrick, Yuri P. Yampol'skii, H. Lawrence Clever, Adam Skrzecz, and Colin L. Young
IUPAC-NIST Solubility Data Series. 76.
Journal of Physical and Chemical Reference Data, Vol. 30, No. 6, pp. 1693-1875, 2001

Ethyne was probably first made in the laboratory by Edmund Davy in 1836. It was rediscovered nearly a quarter of a century later by Berthelot who gave it the name acetylene. Since that time ethyne has become a cheap raw material for the synthesis of organic materials and an important industrial fuel. A summary of the available solubility data for ethyne was published by Miller in 1965 [S. A Miller, *Acetylene—Its Properties, Manufacture, and Uses* (Academic, New York, 1965), Vol. I]. Many more data are now available in a wide range of research papers and patent applications. These data vary in their reliability. In this work, the data for systems included in Miller's book have been reassessed and complemented by data published more recently. Literature has been surveyed to 1999. Data for a system may be unreliable unless two or more groups of workers have published values in close agreement. Where possible, values of the mole fraction solubility at a partial pressure of 101.3 kPa have been tabulated. Equations have been given for the variation of mole fraction with temperature in cases in which values over a temperature range are available. The greater the number of independent sources of the data, the greater the reliability of the utility of the resulting equation. Extrapolation of such equations beyond the temperature range of experimental measurements can lead to errors. In many of the systems it may be assumed that approximate values of the mole fraction solubility, x_1, at a partial pressure of 101.3 kPa may be obtained by linear extrapolation of values for lower partial pressures, p_1, on the assumption that x_1/p_1 is approximately constant. However, a similar linear extrapolation of solubilities at pressures appreciably higher than 101.3 kPa to give mole fraction solubilities at 101.3 kPa can lead to gross errors. For the purpose of evaluation of data, use has been made of the Krichevsky—Il'inskaya equation to obtain approximate values of solubilities at 101.3 kPa from measurements at higher pressures. These values were then compared with measurements made at or near to 101.3 kPa.


www.iupac.org/publications/sds/2001/76_abstract.html

IUPAC Handbook 2002-2003

IUPAC (2002), pp. viii + 1-360.
(ISBN 0-9678550-3-9), USD 25.00

The new edition of the *IUPAC Handbook*, available for sale now from the Secretariat and also posted on the IUPAC Web site at www.iupac.org, contains updated listings and information on all aspects of IUPAC's organization. Included in the new *Handbook* are current listings of organization and membership for all IUPAC Divisions, Commissions, and Committees. Also included are recently revised lists of IUPAC National Adhering Organizations, Associate National Adhering Organizations, IUPAC Officers, and Projects. The *Handbook's* appendixes list recently published IUPAC reports and IUPAC-sponsored symposia and conferences, describe procedures for publication of IUPAC technical reports and recommendations, provide guidelines for drafting IUPAC technical reports and recommendations, and outline IUPAC copyright policies.


www.iupac.org/handbook.html

Handbuch für die Systematische Nomenklatur der Organischen Chemie

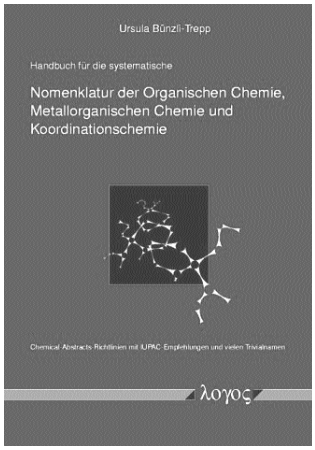
U. Bünzli-Trepp
Metallorganischen Chemie und Koordinationschemie, Logos Verlag, Berlin, 2001. 559 pages, A4 format. (ISBN 3-89722-682-0), EUR 89.50

This book gives a description of organic nomenclature in the German language, and is intended to be used by those who have had at least a few years of chemistry. In the book, Chemical Abstract names are favored, but differences with IUPAC names, when there are any, are pointed out. The book starts with instructions as to its use. In chapter two, one finds an alphabetical list of nomenclature "jargon," richly illustrated with examples; the conventions regarding parentheses and brackets; and a discussion of whether or not vowels are subject to elision in the construction of a name. Chapter three covers the general procedure for naming a compound (priority rules), the different kinds of nomenclature (substitution, addition, etc.), determination and numbering of the parent compound, and the order of prefixes and substituents. The different parent compounds (acyclic, monocyclic and polycyclic), with and without heteroatoms are introduced in chapter four. A short chapter five deals with prefixes that include compounds, such as carbon- and hetero-chains, rings, and more complicated compounds. Chapter six, the longest chapter at 278 pages, gives the nomenclature of different classes of compounds by order of priority (radicals, cations, neutral coordination compounds, anions, acids, etc.). The appendices deal with the nomenclature of special classes of compounds and with special conventions, such as the λ-convention. Very useful are the Internet addresses where one can find more information.

The book contains thousands of examples. The corresponding parts of names and structures of these examples are often printed in the same color. For instance, in the name '2-Mercaptobenzoesäure' (2-mercaptobenzoic acid) 'Mercapto' is in green, '2' and 'benz' are in red, and 'oesäure' is in blue; the corresponding parts of the structure carry the same colours. This is very helpful to the reader, and makes the book more accessible in principle than the Blue Book.* The examples often also contain explanatory notes that refer to other parts of the book. In many instances, the English name is given as well. The index at the end of the book leads the reader quickly to the relevant page.

Cramming all of this information into 559 pages required the use of a lot of small print that will send readers over 45 to their ophthalmologists if they have not been there yet. The pages look overly busy due to the use of color, bold print, and boxes. However, the information is there, one just has to take the time to find it. It should be stressed that this book is not for beginning chemistry students.

The names in this book follow Chemical Abstracts guidelines, which differ somewhat from IUPAC recommendations. Where necessary, differences with IUPAC rules are indicated, as in: "*N*,*N*-Diethylethanamin, IUPAC: nur Triethylamin." There is a deviation from German nomenclature rules in that the author has added an "o" to prefixes like "chlor." As a consequence of concentrating on the Chemical Abstracts guidelines, various attempts of the now-extinct IUPAC nomenclature commissions to make nomenclature rules more systematic are not found in this book. For instance, PH_3 by Chemical Abstracts rules is named "phosphine," although the IUPAC-preferred name is, and has been for quite a while, "phosphane." In parts, the book deviates from inorganic nomenclature guidelines. The systematic names of inorganic anions, for instance, trioxosulfate(2-) for sulfite, are not used in the derivation of names of organic molecules that contain such groups. Chapter 6 starts with "Freie Radikale." As no one these days uses the word "radical" for a substituent group, we do not speak about "free radicals" anymore, just "radicals." Some of these criticisms are more aimed at the differences between inorganic and organic nomenclature than at the book.



According to the title, organometallic chemistry and coordination chemistry are also covered. These topics are, however, confined to Chapter 6.34 and 10 pages in Appendix 6, taking up only 42 pages; further, the treatment of organometallic nomenclature does not reflect current IUPAC guidelines.

This book is clearly the result of many years of work and the author deserves praise for putting it all together in such a systematic way. However, English has become increasingly the language of chemistry since this project was apparently undertaken, a trend that is unlikely to be reversed, and the general usefulness of a German-language compendium is to be questioned. I would, thus, argue that such a book in the English language, especially one that is more accessible to students and other nomenclature novices, would make a more useful addition to the chemistry bibliography.

Reviewed by Prof. Willem H. Koppenol, ETH Hoenggerberg, Zuerich.

www.logos-verlag.de

*The so-called Blue Book is the *IUPAC Nomenclature of Organic Chemistry*, J. Rigaudy and S.P. Klesney, Pergamon, 1979 [ISBN 0-08022-3699], and most recently, the *Guide to IUPAC Nomenclature of Organic Compounds* (recommendations 1993), R. Panico, W.H. Powell, and J.C. Richer, Blackwell Science, 1994 [ISBN 0-63203-4882].

Reports from Conferences

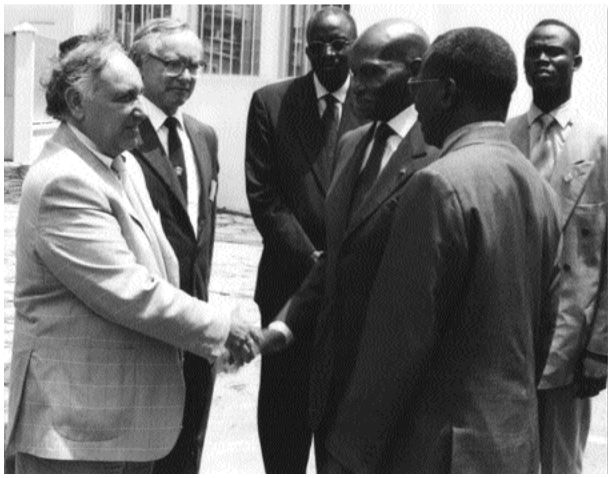
Chemistry and Quality of Life

by Stanley S. Langer

Almost 150 people attended the 8th International Chemistry Conference in Africa (8 ICCA) held 30 July-3 August 2001 at the Université Cheikh Anta Diop in Dakar, Sénégal. Fifteen African countries and ten other countries were represented at the conference, the latest in a triennial series. The meeting was opened by the President of Sénégal, H.E. Abdoulaye Wade, who flew in specially from meeting his counterpart in Côte d'Ivoire. His inspiring address was much appreciated by all those present. Over 250 people attended the opening ceremony, including Professor M Sourang (Minister of National Education) and Professor A. K. Boye (Chancellor of the University).

The major theme for the conference centered on Chemistry and the Quality of Life, with 10 plenary talks dealing with environmental issues, health and agriculture, water quality, natural products, chemical education, and African chemistry in a societal context. In addition, there were many short talks and excellent poster sessions that provoked much animated discussion. As might be expected, anti-malarial chemistry and AIDS were two of the predominant areas for discussion, both within the main sessions and at informal gatherings. All the plenary lectures were published in the July 2001 issue of *Pure and Applied Chemistry* (*PAC*, Vol. 73, No. 7, pp.1147-1223).

Associated with the meeting was a three-day workshop organized by the ACS in cooperation with ICCA and the African Association for Pure and Applied Chemistry (AAPAC). The workshop, which dealt with environmental chemistry, specifically exploring collaborative opportunities to improve water quality, attracted almost 50 attendees.



Shaking hands are Stanley Langer (left) and President Abdoulaye Wade. On the left side of Langer is Prof. Trevor Letcher and on the left side of the President is Prof. M. Sourang.

The hospitality accorded to the participants at the conference was much appreciated and the success of the meeting was due largely to the organizational skills of Libasse Diop and Abdoulaye Samb. Thanks for financial and other support are also extended to the Université Cheikh Anta Diop, the Government of Sénégal, the American Chemical Society, the Royal Society of Chemistry, and UNESCO. It is hoped that the many positive outcomes will be reflected in the programme for the next conference in the series to be held in 2004 in Tanzania.

Stanley S. Langer is secretary, UK NAO to IUPAC, Royal Society of Chemistry, London, England.

Macromolecules-Metal Complexes

by Y. Okamoto

The 9th International Symposium on Macromolecules-Metal Complexes (MMC9) was held 19-23August 2001 at the Polytechnic University's campus in Brooklyn New York, USA. The symposium was organized by the Polytechnic University's Polymer Research Institute and was sponsored by IUPAC and by the American Chemical Society's Division of Polymer Chemistry.

The honorary chairman of the conference was Professor Eishun Tsuchida and the chairmen of the meeting were Kalle Levon, director of PRI, and Professor Yoshi Okamoto. The symposium focused on the role of metal ions, complexes, and clusters in macromolecular systems. These macromolecular complexes play a pivotal role in a wide range of technologies including sensors, fuel cells, batteries, medical devices, toxic material recovery, and fiber optic amplifiers.

There were 40 oral presentations in addition to a poster session at the conference, which attracted over 150 attendees, including 75 international scientists. Professors Eli M. Pearce, Victor Kabanov, Eishun Tsuchida, and Alan G. MacDiarmid, the Nobel Laureate 2000, were the plenary speakers. The 10th Macromolecular Metal Complexes (MMC-10) will be held in Moscow in May 2003.

Y. Okamoto is a professor at Polytechnic University, Brooklyn, New York, USA.

Ionic Polymerization

by StanislawPenczek

The IUPAC International Symposium on Ionic Polymerization (IP' 01) was held 22-26 October 2001 at the Kreta Maris Hotel in Crete, Greece. The Symposium had the support of IUPAC, the Ministry of Education of Greece, the European Polymer Federation, the Greek Polymer Society, the Greek Chemists Association, and the University of Athens. The sponsors of the Symposium were the Ministry of Education and Religious Affairs, ExxonMobil Research and Engineering Company, USA; ExxonMobil Chemical, European Science and Engineering Programme; BASF; MALVA Ltd-WATERS; Techline S.A.; Agmartin; INTERCHEM; Analytical Equipments/K.Vamvakas; HELLAMCO A.E.; and ASTERIADIS S.A.

Dr. Andrew Lovinger of the National Science Foundation, USA, was the honorary chairman of the Symposium. Professor Nikos Hadjichristidis of the University of Athens was the chairman of IP' 01. Dr. Hermis Iatrou chaired the Local Committee—of which Drs. Marinos Pitsikalis and Stergios Pispas were members—that organized this superb Symposium.

During the Opening Ceremony, Professor R.F.T. Stepto, President Elect of the IUPAC Macromolecular Division presented the role of IUPAC and, more particularly, the recent work of the Macromolecular Division.

The International Symposia on Ionic Polymerizations have a long history. Started in the late 40s/ early 50s by Professors David Pepper of Dublin, Ireland, and Peter Plesch of Keele, Great Britain, the symposia dominated the field of cationic polymerization at that time. Then in 1956, after the discovery of the processes of "living polymerization" by Professor Michael Szwarc, founder and "father" of modern ionic polymerizations, a series of more or less formal meetings were organized in the field of anionic polymerization. Two decades later (in 1975) the first IUPAC Symposium on Ring-Opening Polymerization was organized by this author in Warsaw, Poland. Finally, the concerted efforts of a group of scientists—working in anionic, cationic, and ring-opening polymerisations—converted these separate meetings into a chain of Symposia, unifying all of the fields of ionic polymerizations.

The Crete Symposium was the fourth (after Istanbul, Paris, and Kyoto) of this new series. However, the organizers of the Crete Symposium went even further, rightly adding several lectures on topics related to the living radical polymerizations, metathesis, metal coordination, template and enzymatic polymerizations, polymer physical chemistry, and the physics of materials made by these processes, and by doing so, created a scientific program of outstanding quality.

There were over 240 active participants from 30 countries at the Symposium. In total, 68 invited lectures, 29 oral lectures, and 91 posters were presented. All of the research centers contributing to the synthesis of macromolecules with well-controlled structures were represented at this Symposium. The presenters comprehensively described the methods of preparation of miscellaneous block and graft copolymers, including the miktoarms star-shaped macromolecules, originally developed in Professor Hadjichristidis' laboratories. Several groups of physicists discussed morphologies of these and related polymers, showing sophisticated structures in which complicated geometrical structures of or two polymers are imbedded in the matrix of another polymer. Several of these materials of the future have unusual anisotropic properties.

Papers presented at that conference are being prepared for publication in a coming volume of *Macromolecular Symposia.*

Stanislaw Penczek is a Titular Member of the Macromolecular Division.

Polymer Characterization

by Michael Hess

This year's Polychar World Forum on Polymer Application and Theory was held 7-11 January 2002 in Denton, Texas, USA. This was the 10th conference in the series on relationships between characterization, synthesis, processing, manufacturing, and properties of polymer systems. The Chancellor of the University of North Texas, Warren Burggren, opened the conference, which featured 48 participants from 19 countries and comprised 8 special speakers, 6 invited speakers, 23 normal speakers, and 28 posters.

The number of participants and speakers at the conference was lower than in previous years because of the particular difficulties in travelling these days. The number of registrations was initially much higher, but because of the aftermath of September 11 and unexpected weather problems, many registered participants could not attend. Therefore, the conference suffered from many unexpected gaps in its time schedule. Despite these problems—which were professionally handled by the experienced local crew of the Department of Materials Science and other supporting departments of the University of North Texas—the conference provided an impressive overview of current developments in polymer science.

The conference presenters included a number of well-known scientists, but consisted mainly of those who are at the front line of science-diploma- and doctoral students who presented their results as oral presentations or as posters. For many of the young scientists, this conference is the first occasion to present their work in front of a larger international audience.

The day before the official conference starts, there is a tutorial on analytical methods in polymer characterization, which is presented by notable specialists. This event is very useful for advanced and doctoral students to get an overview of the most important techniques available to characterize polymers in theory and application.

The areas covered by the conference were:

- Predictive Methods
- Polymerization
- Polymer Liquid Crystals
- Mechanical Properties and Performance
- Dielectrical and Electrical Properties
- Surface, Interfaces, and Tribology
- Rheology, Solutions and Processing
- Characterization and Structure-Property Relations
- Recycling

Presentations covered a range of subjects, such as Combinatorial Methods for Polymer Science, Alleviation of Environmental Pollution by Converting Polystyrene Waste into Nonionic Surfactants, Processing and Performance of Polymer-Based Shape Memory Alloy Adaptive Composite, and Biobased Polymeric Flocculants for Industrial Effluent Treatment.

In addition, a number of awards and prices were announced at the conference:

- The Paul Flory Polymer Research Prize was shared by Ronald Koningsveld, Sittard, The Netherlands, and Moshe Narkis, The Technion Israel Institute of Technology, Haifa, Israel.
- The Prize for the Best Lecture of the Tutorial was awarded to Dirk Schubert, Freudenberg Forschungsdienste, Weinheim, Gemany.
- The Bruce Hartmann Award (for a young polymer researcher) was given to Sirina Putthanarat, University of Akron.
- The Carl Klason Award (for the best student paper) went to Ricardo Simoes, University of North Texas, Denton, U. S. A.
- Diplomas of Distinction (for a student's presentation) went to Frederic Dreux, University of Rouen, France; Kwan Yee Lau, Hong Kong University of Science and Technology, China; Joanne Yip, Polytechnic University of Hong, China; and Rice University, Houston, U. S. A.

The next World Forum on Polymer Application and Theory (POLYCHAR 11) will be held in Denton, Texas, 7-10 January 2003 with the Short Course on Polymer Characterization on 6 January 2003.

Michael Hess is a professor at the Gerhard-Mercator Universität, in Duisburg, Germany and is chairman of the Subcommittee on Macromolecular Terminology.

Heterocyclic Chemistry

by Thomas T. Tidwell

The 3rd Florida Heterocyclic Conference was held at the University of Florida in Gainesville, Florida, USA from 6-8 March 2002. The conference was organized by the Florida Institute of Heterocyclic Compounds directed by Alan Katritzky, Kenan Professor of Chemistry at the University of Florida. The audience of 100 was distinguished by extensive industrial participation and four of the lectures, by Peter Wuts of Pharmacia (Kalamazoo, Michigan), Graham Johnson of Bristol-Myers Squibb (Wallingford, Connecticut), Joseph Sisko of GlaxoSmithKline (Philadelphia), and Nicolas Bodor of Ivax Corporation and the University of Florida dealt with industrial themes. The topics included the discovery and development of new drugs for the treatment of Parkinson's disease, HIV treatment, and dopamine agonists.

Other lecturers included Ronald Grigg (Leeds University, UK) on cascade reactions for heterocyclic synthsis, William Pearson (University of Michigan) on alkaloid synthesis, Jose Baruenga (Universiy of Oviedo, Spain) on heterocyclic synthesis using metal carbene complexes, Dennis Curran (University of Pittsburgh) on fluorous techniques in organic synthesis, Ernst Anders (University of Jena, Germany) on the synthesis of novel heterocycles, Joachim Schantl (University of Innsbruck, Austria) on synthesis of cyclic azomethine imines, and Nicos Petasis (Universit of Southern California, Los Angeles) on heterocyclic synthesis using organoboron compounds.

From left to right: Ronald Grigg, Alan Katritzky (the conference organizer), and Jose Barulenga.

A feature of the conference was an initial full day short course on the fundamentals of heterocyclic chemistry. The Florida Heterocyclic Conference is also used to support ARKIVOC (Archive for Organic Chemistry), a free on-line refereed journal covering all aspects of organic chemistry, available at http://www.arkat.org .

Thomas T. Tidwell, University of Toronto, is president of the IUPAC Organic and Biomolecular Chemistry Division.

On the Web

Co-Operation on International Traceability in Anaytical Chemistry (CITAC)

CITAC arose out of an international workshop held in association with the Pittsburgh Conference in Atlanta in March 1993. The aim of this workshop was to discuss how analytical activities could be developed to meet the needs of the 21st century. It identified a wide variety of issues to be addressed to ensure that analytical measurements made in differencountries or at different times are comparable. For several years, CITAC has maintained a website containing programs and reports from events, publications (including a yearly newsletter-the latest being February 2002), contact details, and more. For more informations about CITAC or its Web site contact Ioannis Papadakis, CITAC Secretary at citac@irmm.jrc.be.

www.citac.ws

The International Network for the Availability of Scientific Publications (INASP)

INASP is a co-operative network of partners aiming to improve world-wide access to information and knowledge. Established in 1992 by the International Council for Science, its mission is to enhance the flow of information within and between countries, especially those with less developed systems of publication and dissemination. Its three immediate objectives are the following:

- To map, support and strengthen existing activities promoting access to and dissemination of scientific and scholarly information and knowledge
- To identify, encourage and support new initiatives that will increase local publication and general access to quality scientific and scholarly literature
- To promote in-country capacity building in information production, organization, access and dissemination.

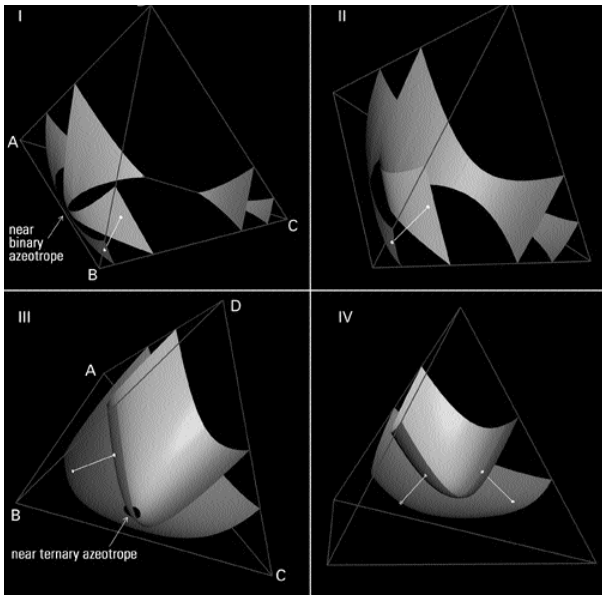
The INASP Web site contains sections on events, links, publications, African Journals Online, program information, and more. An archive of INASP newsletters, including the February 2002 edition, are also available on the site.

www.inasp.org.uk

Visualized Thermodynamics

For many years, K.R. Jolls et. al. have developed computer visualization techniques for application to thermodynamics. The results (i.e., methods, software, and images) can be used in teaching thermodynamics at a variety of levels. For example, the tutorial program "Phase" produces fixed and movable three-dimensional phase diagrams of pure, binary, and ternary systems in the vapor-liquid phase-change regions (See "An Eye for the Abstract," *Science*, Oct. 15, 1999, p. 430).

More recently, the group has created the Gibbs Models Web site, that is a hierarchical collection of drawings of various surfaces depicting 3-dimensional, parametric sections of thermodynamic fundamental and state functions for pure, binary, and ternary systems.



Vapor-liquid equilibrium in the quaternary system acetonitrile (A), benzene (B), ethanol (C), and acetone (D) at T " 348K. Light (inner) surfaces denote dew-point states, dark surfaces bubble-point states. Random white tie-lines are drawn. The originals are in color. Views I-IV are at successively higher pressures. View I is at a pressure intermediate to the A-B and A-C binary azeotropes while view II is above the A-C but below the B-C azeotrope. View III is at a pressure just below the A-B-C ternary azeotrope, and IV is in the range where simple VLE persists up to the vapor pressure of acetone.

These images were generated by "Animate," software for visualizing higher-dimensional VLE. Concept and programming by Eric Cochran and Kenneth R. Jolls, Chemical Engineering Department, Iowa State University. Coexisting states were calculated from the Peng-Robinson equation using common mixture rules. Computations were performed using ASPEN PLUS.

www.iastate.edu/~ch_e/faculty/jolls.html
www.public.iastate.edu/~jolls

Conference Announcements

 *designates IUPAC sponsorship*

Purchasing, Servicing and Maintenance of Scientific Equipment 5-8 November 2002, Cameroon

The International Foundation of Science (IFS) is holding a meeting from 5-8 November 2002 in Cameroon on purchasing, servicing, and maintenance of scientific equipment. The meeting is being organized in collaboration with the International Science Program in Uppsala (ISP), the Third World Academy of Science (TWAS), the International Organization for Chemical Sciences in Development (IOCD), and the Buea University in Cameroon, which is also hosting the meeting. The Institut de Recherche pour le Développement (IRD) also has expressed interest in being involved in the meeting.

Although the lack of funds has been identified as the main constraint to scientific research being carried out in developing countries, the lack of functioning scientific equipment comes a close second. Technical infrastructure and well functioning instrumentation play a crucial role in the successful execution of research projects, but are often less than optimal at universities and research institutions in developing countries.

The purpose of the meeting is to bring together stakeholders in the region who are involved in the purchasing, and servicing and maintenance of scientific equipment (eg policy makers at government level, management from institutions and universities, and the technical staff, teachers, and researchers who are ultimately responsible for the utilisation and repair of the instruments/equipment) with organisations with experience in the maintenance of scientific equipment, and potential donors for future activities.

The discussions at the meeting will be focused on the particular situation in the region. Topics to be discussed are as follows:

- Reviewing the problems that various parties have experienced regarding the purchasing, servicing and maintenance of scientific equipment;
- Reviewing previous approaches that have been made to address the identified problems;
- Identifying new approaches that might be taken to address the identified problems;
- Reviewing the activities of organisations and networks that are tackling these issues;
- Preparing strategies, involving the various parties in the region, to tackle the identified problems;
- Discussing and developing policies for scientific equipment at the university or institutional level;
- Providing an e-mail discussion group.

Contact: Dr. Cecilia Öman
International Foundation for Science
Grev Turegatan 19, SE-114 38 Stockholm, Sweden
Tel.: +46 8 545 818 07
Fax: +46 8 545 818 01
E-mail: cecilia.oman@ifs.se

www.ifs.se

2nd European Symposium on Clinical Laboratory and In Vitro Diagnostic Industry 6-7 February 2003, Barcelona, Catalonia, Spain

The objective of this symposium, jointly organized by the Catalan Association of Clinical Laboratory Sciences (ACCLC) and several companies, is to discuss how clinical laboratories and the in vitro diagnostic industry may develop a common strategy to share the production of physiological reference values for the biological quantities having medical interest.

This symposium, to be held 6-7 February 2003 in Barcelona, Spain, will bring together experts on reference values and other interested professionals to answer and debate a set of questions on practical aspects of physiological reference values production and adoption. Examples of the questions to be answered and debated are as follows: Who should produce reference values, the clinical laboratories or the in vitro diagnostic companies?, How we can verify the sustainability of reference interval for a specific measurement procedure?, and How should the reference intervals be described in books? This symposium will help the in vitro diagnostic industry and clinical laboratories to reach a consensus on the interpretation and fulfilment of some controversial requirements of the European Directive 98/79-CE and EN-ISO 15189 standard dealing with reference values.

Contact: Dr. X. Fuentes-Arderiu
Servei de Bioquímica Clínica
Ciutat Sanitària i Universitària de Bellvitge
08907 L'Hospitalet de Llobregat
Catalonia, Spain
E-mail: xfa@csub.scs.es

Conference Announcements in Brief

Green Solvents for Catalysis
13-16 October 2002
International Symposium on Green Solvents for Catalysis (DECHEMA e.V.)
Conference Secretariat, Attn.: Barbara Feißt
Theodor-Heuss-Allee 25
D-60486 Frankfurt am Main/Germany
Tel: +49 69 7564 333
Fax: +49 69 7564-441
E-mail: feisst@dechema.de
<www.dechema.de/gsfc2002>

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2002

Macromolecules
7–12 July 2002
39th International Symposium on Macromolecules—IUPAC World Polymer Congress 2002, Beijing, China.
Prof. Fosong Wang, The Chinese Academy of Sciences, Beijing 100864, China
Tel: +86 10 62563060
Fax: +86 10 62573911
E-mail: fswang@mimi.cnc.ac.cn

Solid-State Chemistry
7–12 July 2002
5th Conference on Solid-State Chemistry, Bratislava, Slovakia.
Prof. P. Sajgalik, Slovak Academy of Sciences, Dubravska c. Bratislava, SK-842 36 Slovakia
Tel.: +421 7 59410400
Fax: +421 7 59410444
E-mail: ssc2002@savba.sk

Organometallic Chemistry
7–12 July 2002
20th International Conference on Organometallic Chemistry, Corfu, Greece.
Dr. C. G. Screttas, National Hellenic Research Foundation, Institute of Organic and Pharmaceutical Chemistry, 48 Vas. Constantinou Avenue, 11635 Athens, Greece
Tel.: +30 1 7273876
Fax: +30 1 7273877
E-mail: kskretas@eie.gr

Carbohydrates
7–12 July 2002
XXIst International Carbohydrate Symposium, Cairns, Queensland, Australia.
Prof. R. V. Stick, University of Western Australia, Department of Chemistry, Nedlands, 6007, Western Australia
Tel.: +61 8 9380 3200
Fax: +61 8 9380 1005
E-mail: rvs@chem.uwa.edu.au

Polymers and Organic Chemistry
14–18 July 2002
Polymers and Organic Chemistry 2002, San Diego, California, USA.
Prof. Spiro Alexandratos, Office of Academic Affairs, City University of New York, 535 East 80th St., New York, New York 10021, USA
Tel.: +1 212 794 5470
Fax: +1 212 794 5706
E-mail: sdabh@cunyvm.cuny.edu

Organic Synthesis
14–19 July 2002
14th International Conference on Organic Synthesis, Christchurch, New Zealand.
Prof. Margaret A. Brimble, Department of Chemistry, University of Auckland, 23 Symonds St., Auckland, New Zealand
Tel.: +64 9 373 7599, Ext. 8259
Fax: +64 9 373 7422
E-mail: m.brimble@auckland.ac.nz

Photochemistry
14–19 July 2002
XIXth IUPAC Symposium on Photochemistry, Budapest, Hungary.
Prof. H. D. Roth, Rutgers University, Department of Chemistry and Chemical Biology, 610 Taylor Road, New Brunswick, NJ 08854-8087 USA
Tel.: +1 732 445 5664
Fax: +1 732 445 5312
E-mail: roth@rutchem.rutgers.edu

Electrical Properties of Polymers
15–18 July 2002
21st Discussion Conference and 9th International ERPOS Conference on Electrical and Related Properties of Polymers and Other Organic Solids, Prague, Czech Republic.
Prof. Dr. Drahomir Vyprachticky, Institute of Macromolecular Chemistry, Academy of Sciences of the Czech Republic, Heyrovského nám. 2, 162 06 Praha 6, Czech Republic
Tel.: +420 2 20403251 or +420 2 20403332
Fax: +420 2 35357981
E-mail: vyprach@imc.cas.cz or sympo@imc.cas.cz

Solubility Phenomena
21–26 July 2002
10th International Symposium on Solubility Phenomena, Varna, Bulgaria.
Prof. Christo Balarew, Institute of General and Inorganic Chemistry, Bulgarian Academy of Sciences, BG-Sofia 1040, Bulgaria
Tel.: +359 (2) 9793925
Fax: +359 (2) 705 024
E-mail: balarew@svr.igic.bas.bg

Coordination Chemistry
21–26 July 2002
35th International Conference on Coordination Chemistry (35-ICCC), Heidelberg, Germany.
Prof. Roland Krämer, Chairman Anorganisch-Chemisches Institut Universität Heidelberg Im Neuenheimer Feld 270 D-69120 Heidelberg, Germany
Tel.: +49 (0) 6221 548438
Fax +49 (0) 6221 548599
E-mail: roland.kraemer@urz.uni-hd.de

Chemical Thermodynamics
28 July–2 August 2002
17th IUPAC Conference on Chemical Thermodynamics, Rostock, Germany.
Prof. A. Heintz, FB Chemie, Universitat Rostock, Hermannstr. 14, D-18051 Rostock, Germany
Tel.:+49 381 498 1852
Fax: +49 381 498 1854
E-mail: andreas.heintz@chemie.uni-rostock.de

Natural Products
28 July–2 August 2002
23rd International Symposium on the Chemistry of Natural Products, Florence, Italy.
Prof. B. Botta, Dip. Studi Chimica e Tecnologia Sostanze, Biologicamenta Attive, University "La Sapienza", P.le A. Moro 5, 00185 Roma, Italy
Tel.: +39 06 49912781 or +39 0649912783
Fax: +39 06 49912780
E-mail: bruno.botta@uniroma1.it

Boron Chemistry
28 July–2 August 2002
XIth International Meeting on Boron Chemistry (IMEBORON XI), Moscow, Russia.
Prof. Yu. N. Bubnov, A. N. Nesmeyanov Institute of Organoelement Compounds of the Russian Academy of Sciences, Vavilov str. 28, Moscow V-334,

GSP1, 119991 Russian Federation
Tel.: +7 095 135 6166 or +7 095 135 7405
Fax: +7 095 135 5085
E-mail: imeboron@ineos.ac.ru

Polymer Synthesis NEW
29 July–1 August 2002
Macro Group UK International Conference on Polymer Synthesis, Coventry, UK.
Dr. D. M. Haddleton
Department of Chemistry, University of Warwick, Coventry, CV4 7AL, UK
Tel: +44 (0) 2476 523256
Fax: +44 (0) 2476 524112
E-mail: D.M.Haddleton@warwick.ac.uk

Crop Protection
4–9 August 2002
10th IUPAC International Congress on the Chemistry of Crop Protection (formerly International Congress of Pesticide Chemistry), Basel, Switzerland.
Dr. Bernard Donzel, c/o Novartis CP AG, WRO-1060.3.06, CH-4002 Basel, Switzerland
Tel.: +41 61 697 22 67
Fax : +41 61 697 74 72
E-mail: bernard.donzel@cp.novartis.com

Physical Organic Chemistry
4–9 August 2002
16th International Conference on Physical Organic Chemistry: Structure and Mechanism in Organic Chemistry, San Diego, California, USA.
Prof. Charles L. Perrin, Department of Chemistry, University of California at San Diego, La Jolla, California 92093-0358, USA
Tel.: +1 858 534 2164
Fax: +1 858 822 0386
E-mail: icpoc@ucsd.edu

Chemical Education
6–10 August 2002
17th International Conference on Chemical Education—New Strategies for Chemical Education in the New Century, Beijing, China.
Prof. Xibai QIU, 17th ICCE c/o Chinese Chemical Society, P.O. Box 2709 Beijing 100080, China
Tel.: +86 10 62568157, 86 10 62564020
Fax: +86 10 62568157
E-mail: qiuxb@infoc3.icas.ac.cn

Bioorganic Chemistry
11–14 August 2002
6th International Symposium on Bioorganic Chemistry (ISBOC-6), Toronto, Ontario, Canada.
Dr. Ronald Kluger, Department of Chemistry, University of Toronto, Toronto, Ontario, Canada M5S 3H6
Tel.: +1 416 978 3582
Fax.: +1 416 978 3482
E-mail: rkluger@chem.utoronto.ca

Polymer Networks 2002
2–6 September 2002
Polymer Networks 2002, Autrans, France.
Prof. E. Geissler, Université J. Fourier de Grenoble, Laboratoire de Spectrométrie Physique, B.P. 87, F-38402 St Martin d'Heres cedex, France
Tel: +33 476 635823
Fax: +33 476 514544
E-mail: erik.geissler@ujfgrenoble.fr

Physical Chemistry of Liquids
6–15 September 2002
European Molecular Liquids Group (EMLG) Annual Meeting on the Physical Chemistry of Liquids. Novel Approaches to the Structure and Dynamics of Liquids: Experiments, Theories, and Simulations, Rhodes, Greece.
Prof. Dr. Jannis Samios
Tel.: +30 1 7274534 or +30 1 7274751
Fax: +30 1 7274752
E-mail: isamios@cc.uoa.gr

Polymer Science and Technology
2–5 December 2002
IUPAC Polymer Conference on the Mission and Challenges of Polymer Science and Technology, Kyoto, Japan.
Prof. Seiichi Nakahama, Faculty of Engineering, Tokyo Institute of Technology, 2-12-1 Ohokayama, Meguro-ku, Tokyo 152-8552, Japan
Tel.: +81 3 5734 2138
Fax.: +81 3 5734 2887
E-mail: snakaham@polymer.titech.ac.jp

2003

Clinical Laboratory
6–7 February 2003
2nd European Symposium on Clinical Laboratory and In Vitro Diagnostic Industry, Barcelona, Spain
Prof. Xavier Fuentes Arderiu
Ciutat Sanitària i Universitària de Bellvitge Servei de Bioquímica Clínica L'Hospitalet de Llobregat, Catalonia, E-08907 Barcelona, Spain
Tel.: +34 93 260 7644
Fax: +34 93 260 7564
E-mail: xfa@csub.scs.es

Flow Analysis New Dates
17-21 February 2003
The 9th International Conference on Flow Analysis, Geelong, Victoria, Australia.
Dr. Daryl J. Tucker, School of Biological and Chemical Sciences, Deakin University, Geelong, Victoria 3127 Australia.
Tel.: +61 3 5227 2325
Fax: +61 3 5227 1040
E-mail: tucker@deakin.edu.au

100 Years of Chromatography
13–18 May 2003
3rd International Symposium on Separations in BioSciences (SBS '03), follow up to the International Symposia Series "Biomedical Applications of Chromatography and Electrophoresis," Moscow, Russia.
Prof. Vadim A. Davankov, Nesmeyanov Institute of Organo-Element Compounds, Vavilov str., 28, 119991, Moscow, Russia.
Tel.:/Fax: +7 095 135 6471
E-mail: davank@ineos.ac.ru

High Temperature Materials
19–23 May 2003
11th International Conference on High Temperature Materials Chemistry (HTMC XI), Tokyo Japan.
Prof. Michio Yamawaki, University of Tokyo, Department of Quantum Engineering and Systems Science, 7-3-1 Hongo, Bunkyo-ku, Tokyo 113-8656, Japan

Macromolecule Metal Complexes
20–24 May 2003
Xth International Symposium on Macromolecule Metal Complexes (MMC-X), Moscow, Russia.
Prof. Valerii V. Lunin, Department of Chemistry, Moscow State University, Leninskie Gory, Moscow, 119899, Russia.
Tel.: +7 095 939 5377
Fax: +7 095 932 8846
E-mail: kar@petrol.chem.msu.ru

IUPAC 42nd General Assembly
8–17 August 2003
Ottawa, Ontario, Canada.
IUPAC Secretariat
Tel.: +1 919 485 8700
Fax: +1 919 485 8706
E-mail: secretariat@iupac.org

IUPAC 39th Congress
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