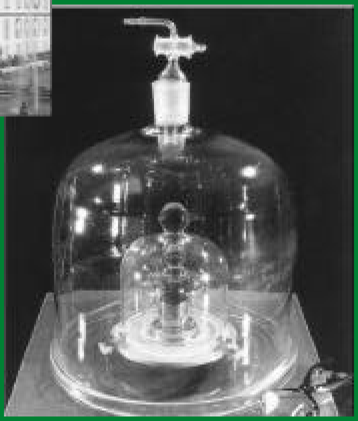
Chemistry International

The news magazine of the International Union of Pure and Applied Chemistry (IUPAC)

The Bureau International des Poids et Mesures: Establishing Standards in the Physical Sciences



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The Synthesis and Naming of Elements 110 and Beyond

Reliable Solubility Data in the Age of Computerized Chemistry: Why, How, and When?

IUPAC

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The news magazine of the International Union of Pure and Applied Chemistry (IUPAC)

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What Is Old Is New Again

Restructuring has been a key word for some time within IUPAC, as this 12-year old cartoon, previously published in *CI*, candidly testified. Over time, questions find answers, and good composition glue strengthens. My point of view is that the structure of the Union—the way it operates and the resulting benefits for the chemistry community—relies essentially on the people involved. My greatest privilege while working at IUPAC has not been working for the Union, but has been working with the volunteers that surround it. As it will be four years next month that my work ID became fabienne at iupac dot org, I feel it is time for me to say "thanks" to you—and I might add "thanks for sticking around."

Fabienne Meyers <fabienne@iupac.org>

Secretary General's Column

Broadening Active Participation in IUPAC Activities

After two years in transition from our traditional commission-based organization to the project-driven system, IUPAC is now operating fully in this new mode. Our eight divisions have been restructured, with the inclusion of National Representatives in the Division Committees. Several Standing Committees have also been reorganized, most notably the Committee on Chemistry Education.

The President's message in the January issue of *Chemistry International* laid out a list of activities for the current biennium. Among our priorities are broadening active participation in IUPAC activities. Several of the following initiatives are already underway, while others will be undertaken soon.

New Member Countries

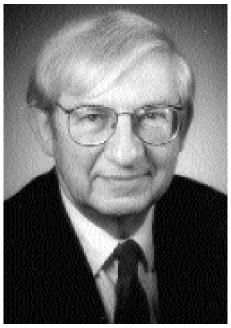
As reported previously in *CI*, a Membership Development Committee was formed in Brisbane. Committee members have visited organizations of chemists in several prospective member countries to describe the advantages of becoming a National Adhering Organization (NAO) and to try to help resolve the financial difficulties that membership in IUPAC entails. Mexico and Uruguay have recently become Associate NAOs. There are several promising prospects for countries upgrading to full NAO status.

Affiliate Member Program

The AMP was launched in 1986 to promote two-way communication between IUPAC and individual chemists throughout the world. After an initial surge in interest resulted in the enrollment of more than 7800 Affiliate Members in 1987, the program has declined to its present size of about 4800 in 65 countries. We will work with our NAOs and national chemical societies in many countries to reverse this trend and to revitalize the AMP. As described in the January 2002 issue of *CI*, we now offer a free sponsored affiliate membership to a chemist in a developing country for each new paid member. For many in the developing world, the AMP provides a communications "lifeline." Here is a way to help extend that lifeline.

Many readers of *CI* are already Affiliate Members. We want to hear from you about your ideas for new IUPAC activities, including formal projects, and your reaction to current activities. An e-mail message to <secretariat@iupac.org> will suffice, but we also welcome letters to *CI* to be published in the IUPAC Forum.

IUPAC Fellows



Edwin D. Becker
IUPAC Secretary General

While we are encouraging broader participation in IUPAC activities, we do not want to lose track of those chemists who have already contributed to the Union's activities and may well do so again. Our "alumni," designated as IUPAC Fellows in appreciation of their contributions, receive *CI* and other benefits. As a number of people have recently completed formal service in IUPAC bodies, the number of Fellows is expected to double from last year's size of about 450.

National Representatives

To broaden the geographic representation on each of our eight Division Committees, the IUPAC Council approved an amendment to the Bylaws that allows up to six NRs on each Committee and makes them full participants in the work of the Committee. In addition, I have invited each NAO to designate a specific contact to each Division Committee to facilitate communication and bring additional chemists into the mainstream of IUPAC activities. Also, the new Committee on Chemistry Education has a very large number of NRs—potentially involving every NAO in the IUPAC efforts in education and the public appreciation of chemistry.

Associated Organizations

IUPAC consists of about 40 international organizations, in various specialized fields or with specific geographic coverage, that have been formally recognized as IUPAC Associated Organizations (AOs). We have close ties with some AOs, especially those associations and federations that represent chemists or chemical societies in Europe, Asia, Africa, and Latin America. However, we should improve our interactions with many of the AOs in chemical specialties.

IUPAC Conferences

Each year IUPAC sponsors a large number of conferences, as readers of *CI* know from the conference calen-

> *If IUPAC is to be successful in representing worldwide chemistry, it needs to foster synergistic relationships with the global community of chemists.*

dar that was distributed with the January issue. We are planning stronger efforts to publicize IUPAC activities at these conferences and to encourage active involvement of conference attendees in proposing and participating in formal IUPAC projects.

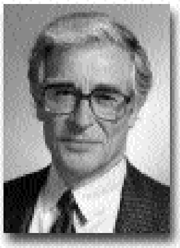
IUPAC Projects

A major objective in initiating the project system was to create within IUPAC a more dynamic environment, in which any chemist in the world can contribute. If IUPAC is to be successful in representing worldwide chemistry, we need to foster the synergistic relationship between the global community of chemists and the one organization that represents the chemical sciences worldwide. Let us hear from you!

Edwin D. Becker has been IUPAC Secretary General since 1996 and has been a member of various IUPAC bodies for almost 30 years. He is presently a scientist emeritus at the National Institutes of Health in Bethesda, Maryland, USA.

The Bureau International des Poids et Mesures: Establishing Standards in the Physical Sciences

by Ian Mills



Ian Mills

In a vault on the outskirts of Paris, a cylinder of platinum-iridium sits in a safe under three layers of glass. It is *the kilogram*, kept by the Bureau International des Poids et Mesures (BIPM), which is the international home of metrology. Metrology is the science of measurement, and it is of fundamental importance to us all. It is essential for trade, commerce, navigation, transport, communication, surveying, engineering, and construction. It is essential for medical diagnosis and treatment, health and safety, food and consumer protection, and for preserving the environment—e.g., measuring ozone in the atmosphere. Many of these applications are of particular relevance to chemistry and thus to IUPAC. In all these activities we need to make measurements reliably—to an appropriate and known level of uncertainty. The financial implications of metrology are enormous. In the United States, for example, some 15% of the gross domestic product is spent on healthcare, involving reliable quantitative measurements for both diagnosis and treatment.

BIPM is headquartered in the Pavillon de Breteuil, a historic and beautiful chateau overlooking the Seine at Sèvres, on the outskirts of Paris. Surrounding the chateau is a number of laboratories in which the world's measurement standards are maintained and researched, and in which results are collated between the National Metrology Institutes of the world. BIPM recently opened a new chemical laboratory, which specializes in the chemistry of the atmosphere.

The Convention of the Metre

The metric system was born at the time of the French revolution. At that time a Commission on Metrication was established (of which the mathematician Joseph Lagrange was the president and the chemist Antoine Lavoisier was a member) to consider the best way to define the base units. The commission recommended definitions for the metre as 10^{-7} of the distance from the pole to the equator, and the kilogram as the mass of a cubic decimetre of water at 4 °C. Two members of the commission were entrusted to "realize" the definition of the metre by measuring the distance from the pole to the equator. This they did, but it took them five years and led them through many adventures. By climbing church towers and measuring the angle to neighboring towers (with revolutionary battles taking place beneath them) and then walking on to the next tower, they surveyed and determined the distance over the ground from Dunkirk to Barcelona. Dunkirk is due north of Barcelona, and from the latitude of each city determined astronomically, they were then able to scale up this distance to obtain the arc distance from the pole to the equator. They returned with a metre stick, which they claimed was "according to the definition." The definition was never realized a second time!

The Bureau International des Poids et Mesures at Pavillon de Breteuil, Paris, France.

The definition of the kilogram as the mass of a cubic decimetre of water was easier to realize, but proved difficult to measure reproducibly, with accuracy comparable to that of comparing masses using a balance. Thus, neither of these definitions proved satisfactory.

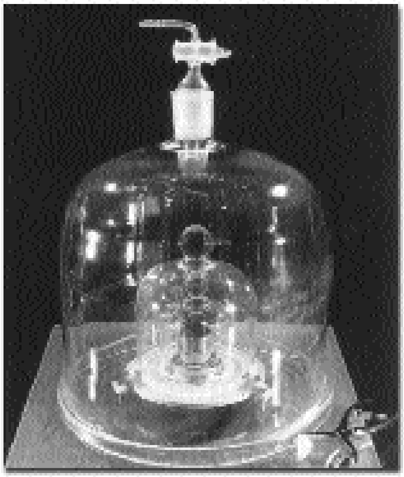
In 1875, the government of France invited every technologically advanced nation to send representatives to Paris to establish and to sign the Metre Convention, which is now the basis of our internationally agreed upon standards of measurement. The French government then presented the Pavillon de Breteuil, with the small park that surrounds it, as international land with the status of an embassy, for the use of the BIPM. In the years that followed, the kilogram and the metre were redefined in terms of platinum-iridium prototypes, which were kept at BIPM. Copies of these were distributed around the world. Thus the first lesson of establishing a standard was learned: it must be easy to reproduce, with an accuracy comparable to that with which the quantity can be measured.

There are now 51 countries that are signatories to the Convention of the Metre. They support and govern the BIPM through the Conférence Générale des Poids et Mesures, held once every four years. They appoint the Comité International des Poids et Mesures, the International Committee, which meets regularly to supervise the operation of the BIPM, and to appoint the Director—presently Dr. Terry Quinn from England. The International Committee also takes advice from 10 Consultative Committees with expertise in the various specialized fields. Members of the Consultative Committees are drawn from metrology institutes around the world, and the Consultative Committee for Units (CCU), in particular, has representatives from most of the international unions such as IUPAC. CCU is responsible for advising the International Committee on changes and developments to be made to the International System of Units (SI), and particularly on choosing the standards that define the base units of the SI.

Defining Our Units in Terms of Fundamental Physical Constants

The definitions of the base units are continually in need of revision as we develop more precise methods of measurement. The kilogram is, today, the only base unit still defined in terms of a material artifact. We now strive to define units in terms of fundamental constants or the properties of atoms, which—as an act of faith—we believe to be invariant. Thus, for example, the metre, defined in 1889 as the distance between two scratches on the prototype metre stick, was redefined in 1960 to be a multiple of the wavelength of the red krypton atomic line. This change was made because it was found that distances could be measured interferometrically in terms of the atomic wavelength more accurately and reproducibly than the distance between the scratches on the prototype stick could be measured. Similarly, the base unit of time, the second, used to be defined as 1/86,400 of the mean solar day. But even in the 19th century it was known that the rotation of the earth was slowing down due to tidal friction, and when quartz clocks and then atomic clocks were developed, other irregularities in the rotation of the earth were discovered. Thus, in 1967 the second was redefined as the duration of 9,192,631,770 periods of the hyperfine transition in the caesium atom. This was both more stable and easier to realize than the earlier definition, and it can be realized with much higher precision using an atomic clock. Finally, the metre was redefined again in 1983 to be the distance that light travels in 1/299,792,458 of a second, for exactly similar reasons.

The kilogram is, today, the only base unit still defined in terms of a material artifact.



The kilogram, kept by the Bureau International des Poids et Mesures.

Each of these changes was made because the precision with which we could make the measurements became greater than the precision with which we could realize, or make use of, the previous definition. Today, we choose definitions based on fundamental physical constants and atomic properties because they provide more stable and universally available standards. They may also generally be measured relatively easily and with high precision. Each change of definition is chosen to maintain unchanged the previous value of the standard, to the accuracy with which it had previously been known.

It is important to note that the effect of each new definition is to set a fixed value for some relevant constant. Thus, the present definition of the second sets the value of the frequency of the caesium transition to be exactly 9,192,631,770 Hertz, and the present definition of the metre sets the speed of light to be exactly 299,792,458 metres per second. The 1793 definition of the metre set the distance from the pole to the equator, but it is a definition that is difficult to realize! The 1889 definition of the metre set the distance between the scratches on the metre stick, and the 1960 definition set the wavelength of the red krypton line. The present definitions of the base units, and the general specification of the International System of units, is presented in the SI Brochure (*The SI Brochure*, 7th Edition, T.J. Quinn and I.M. Mills, BIPM 1998, ISBN 92-822-2154-7).

The present definition of the metre can be realized to approximately one part in 10^{12}, and the present definition of the second to approximately five parts in 10^{16}—which is equivalent to one second in 60 million years. You may well ask, what is the point? Why do we need all this precision? One answer is that you will never stop scientists from developing more accurate methods of measurement any more than you will stop men wishing to climb Mount Everest or travel to the moon. It then becomes necessary to develop standards that reflect the precision of our measurements. A more pragmatic answer is that more precise methods of measurement are invariably followed by new applications not previously foreseen. An example is the development of the global positioning system (GPS) based on signals from satellites. This is entirely dependent on the fact that each satellite carries an atomic clock, used to broadcast its position and time with the highest precision. From the difference between the time signals received by the observer, the differences between the distances from the satellites can be calculated, and from the known positions of the satellites the position of the observer can then be calculated.

> *. . . more precise methods of measurement are invariably followed by new applications not previously foreseen.*

Although our ability to make more precise measurements has been advancing rapidly in the last hundred years, metrology is not a new subject. Many of the foremost 19th century physicists concerned themselves with this subject. James Clerk Maxwell wrote in 1870, “If, then, we wish to obtain standards of length, time, and mass which shall be absolutely permanent, we must seek them not in the dimensions, or the motion, or the mass of our planet, but in the wavelength, the period of vibration, and the absolute mass of these imperishable and unalterable and perfectly similar molecules.” Today we accept the truth of this statement, but in making it Maxwell showed great foresight, because at that time we had not yet developed methods of measuring the wavelengths, frequencies, and masses of the atoms!

Tomorrow’s Kilogram

Today, the race is on to find an acceptable new definition of the kilogram. This is because we know that the prototype kilogram can change in mass at the level of a few parts in 10^{8}, due to surface chemistry and wear and tear, over a period of months. However, we can actually weigh the kilogram (i.e., compare the mass of two kilogram artifacts) with a precision of better than one part in 10^{11} using the best modern balances. A possible new definition would be to say that the kilogram is the mass of a specified number of carbon-12 atoms, which would set the value of the Avogadro constant. However, at present we cannot quite realize this definition (i.e., weigh the carbon atom, or determine the Avogadro constant) with the necessary accuracy. The present best estimate of the Avogadro constant is uncertain to about one part in 10^{7}, but this is obtained indirectly from other fundamental constants. Direct measurements are based on the silicon crystal density method, in which the spacing of the atoms in a single crystal sphere of silicon is determined by X-ray interferometry, and the mass and volume of the sphere is measured, so that the number of atoms in the sphere may be calculated. The uncertainty in the Avogadro constant needs to be reduced by at least one order of magnitude, and preferably two, before we adopt an atomic mass as the definition of the kilogram. There is also a possible electrical definition of the kilogram that may prove to be preferable, realized by a Watt balance, in which a mass is balanced against the force on a coil in a magnetic field, so that an electrical energy is balanced against a mechanical energy. The decision on a new definition of the kilogram will probably be made sometime in the next 10 years. The present best estimates of all the fundamental constants, and further information on this subject, may be found in the paper by Mohr and Taylor (P.J. Mohr and B.N. Taylor, *J. Phys. Chem. Ref. Data* **28**, pp. 1715-1852 [1999]).

In 1992, I was appointed to be the IUPAC representative on the CCU, and in 1995 I was appointed President of the CCU. It is a job that I find fascinating—meeting and discussing with some of the world’s best scientists and evaluating the latest experiments that improve our ability to make measurements. The results impact upon every activity of IUPAC, most particularly on the importance of making valid estimates of the uncertainty in the measurements upon which we all depend. Another aspect of the work is its international nature: the need for us all to speak the same language of science so that we understand one another without ambiguity and use internationally agreed upon names and symbols for the quantities and units involved. Like many of the activities of the BIPM, these are also problems that are close to the heart of IUPAC’s existence, so that IUPAC and the BIPM have strong common interests.

Ian Mills has been the IUPAC Representative on BIMP since 1996. He is a professor at the University of Reading, UK.

http://www.bipm.org

The Synthesis and Naming of Elements 110 and Beyond

by Herbert Kaesz

A Joint Working Party (JWP) of IUPAC and the International Union of Pure and Applied Physics (IUPAP) has published its analysis of the claims for the syntheses of elements 110, 111, and 112 (P.J. Karol, *Pure Appl. Chem.* Vol. 73, No. 6, pp. 959-9676, 2001).

The JWP has given credit for the synthesis of element 110 to a group at the Gesellschaft für Schwerionenforschung in Darmstadt, Germany. This laboratory has thus been invited to propose a name.

As to elements 111 and 112, the Joint Working Party did not feel that sufficient results have, as yet, been presented to assign credit for their discoveries. The difficulties in confirming syntheses of the heaviest elements is illustrated by the announcements in 1999 of the syntheses of elements 116 and 118, claims which were retracted this year. The earlier results could not be reproduced at the originating institution, Lawrence Berkeley National Laboratory, nor at other centers for heavy-element synthesis in Germany and in Japan (*Science*, 3 Aug. 2001, Vol. 293, pp. 777-778; *C&E News*, 6 Aug. 2001, p. 10; Darleane Hoffman, private communication).

The JWP's analysis followed a procedure that was earlier established for elements 101-109 because claims of the synthesis of heavy elements can be controversial. Until discoveries are confirmed, elements are provisionally designated in terms expressing their atomic numbers in Latin, for example “*ununnilium*” (one-one-zero for 110), “*unununium*” (one-one-one for 111), and “*ununbium*” (one-one-two for 112). To avoid confusion, discoverers are asked to use an atomic number rather than a name in the literature until approval of a proposed name is received from IUPAC. If a particular name has been used unofficially for a given element but a different name is ultimately chosen, then the first name cannot be transferred at a later time to designate a different element.

New Element?

▼ Analysis of the claim by IUPAC/IUPAP

▼ Publication of the analysis in *Pure and Applied Chemistry*

▼ Invitation to the credited group to propose a name

▼ Provisional recommendation presenting the proposed name

▼ Public review

▼ Final approval by the IUPAC Council

▼ Publication in *Pure and Applied Chemistry*

A review on the naming of new elements, with a summary of the recommended current procedures, has been prepared by W.H. Koppenol. This document is now available for public review. The steps for arriving at a IUPAC approved name of a new element are illustrated in the figure to the left.

Laboratories engaged in the synthesis of new elements are invited to submit claims and supporting evidence.

Herbert Kaesz is a professor at the University of California at Los Angeles, California, USA, and is a member of, among others, the Inorganic Chemistry Division Committee.

http://www.iupac.org . . .
/publications/pac/2001/7306/7306x0959.html
/reports/provisional/abstract01/koppenol_310302.html
/news/archives/2001/Z_greater_than_110.html

Reliable Solubility Data in the Age of Computerized Chemistry: Why, How, and When?

by John Rumble Jr., Angela Y. Lee, Dorothy Blakeslee, and Shari Young

IUPAC's *Solubility Data Series* (*SDS*), begun in the mid-1970s, is an exhaustive compilation and critical evaluation of all the world's published results of experimental determinations of solubility. Since 1979, over 70 *SDS* volumes have been published, including evaluated data on the solubility of gases in liquids, liquids in liquids, and solids in liquids. These volumes represent one of the largest collections of chemical property data ever produced and are the result of work of scientists throughout the world. Since 1998, and following an agreement with the National Institute of Standards and Technology (NIST), the *SDS* compilations have been published four times a year in the *Journal of Physical and Chemical Reference Data.* Since January 2002, a Subcommittee on Solubility and Equilibrium Data of the IUPAC Analytical Chemistry Division has continued the coordination of the *SDS*-related projects.

Although IUPAC has worked to maintain high scientific standards and a uniform approach for data compilation and evaluation throughout its existence, the evolution of personal computing and the rise of the Internet have substantially changed the ways that research is conducted and results are made available. In 1980, most communication between compilers, evaluators, and editors occurred through the mail, and most critically evaluated research data were published commercially in printed volumes. Only a few hundred libraries—virtually all in developed countries—maintained standing orders for the *SDS*. Today, collaboration is primarily via electronic means, with drafts passed around the world as e-mail attachments. Again with the help of NIST, and as described in this article, the computerization of the entire collection is being considered as a Web-accessible database.

Introduction

Every aspect of chemistry is being affected by the growth of chemical informatics and the Internet/Web explosion. The once tedious task of building databases and disseminating them widely has become much easier. Today, some data gateways point to hundreds of Web sites that provide some type of chemical information. The accessibility of these data is part of a larger effort both to improve the quality of scientific data and to make them as widely available as possible. Before examining the details of computerizing IUPAC solubility data, it is useful to examine some of the broader aspects of scientific data.

Modern computers are profoundly changing the nature of 21st-century chemistry research. Already, industrial development and innovation flow primarily from computer-aided design, model-based processing and manufacturing, and virtual testing. The confluence of increased computer power, advances in applied mathematics, and a new generation of highly computer-proficient scientists and engineers makes the move to model-based research inevitable.

Data Evaluation and Reliability

Modeling, regardless of the discipline, has one common feature: *Reliable* data are an essential element. Model-based science and engineering cannot function properly without a large data collection of known quality. The expression "garbage in, garbage out" applies in every instance. The generation and dissemination of reliable data is a complex process. Most scientific and technical data are generated in the course of research not specifically focused on data measurement and quality. In fact, most data are scattered throughout the technical literature and are poorly documented. Data users are not usually experts in how data were generated. Consequently, even if they find needed data, they cannot easily determine the quality of those data.

Several organizations collect and evaluate data so that researchers and others may use measurement results more confidently. The process of critically evaluating data involves four key steps:

- collecting the data from the published literature;
- reviewing and evaluating data by experts;
- designing databases and publications to meet user needs; and
- disseminating those data collections widely.

The evaluation of scientific data proceeds from three viewpoints. First, the data are evaluated with respect to how well their generation is documented. Have all independent variables affecting the measurement been identified? Have they all been controlled during the measurement? And how have these facts been demonstrated and documented? The second viewpoint is how do the data follow the known laws of nature. The third viewpoint is how do the data compare with other measurements that purport to look at the same phenomena.

> *Modeling, regardless of the discipline, has one common feature: Reliable data are an essential element.*

The mixture of these viewpoints depends on the maturity of the discipline and the existence of previous data evaluation efforts. In areas such as chemical thermodynamics and atomic spectroscopy, in which knowledge of the measurement technology is quite developed, the independent variables understood, and previous evaluations exist, the emphasis in new evaluations is on the latter two viewpoints. In areas in which measurements are fairly new, or the phenomena are quite complex and not totally understood, the emphasis must be on the first viewpoint.

The NIST Data Programs

NIST has long been interested in data evaluation. Beginning with the International Critical Tables[1] in the 1920s, the National Bureau of Standards, which was renamed as the National Institute of Standards and Technology in 1987, operated a large number of data evaluation activities.[2] Why is NIST interested in data evaluation? As the U.S. national laboratory concerned with advancing measurement science and technology, NIST considers data to be a fundamental result of measurements, both experimental and calculational. Data collections summarize previous measurement experience, and data evaluation therefore assesses the quality of current measurement technology.

NIST has unique, broad expertise in measurement technology, and the knowledge and experience necessary to perform data evaluation. NIST measurement experts are neutral (i.e., they do not favor any particular method except on merit). Data projects often involve partnerships on a national and international scale, and NIST has much experience in such partnerships in terms of sharing responsibility, costs, and outputs.

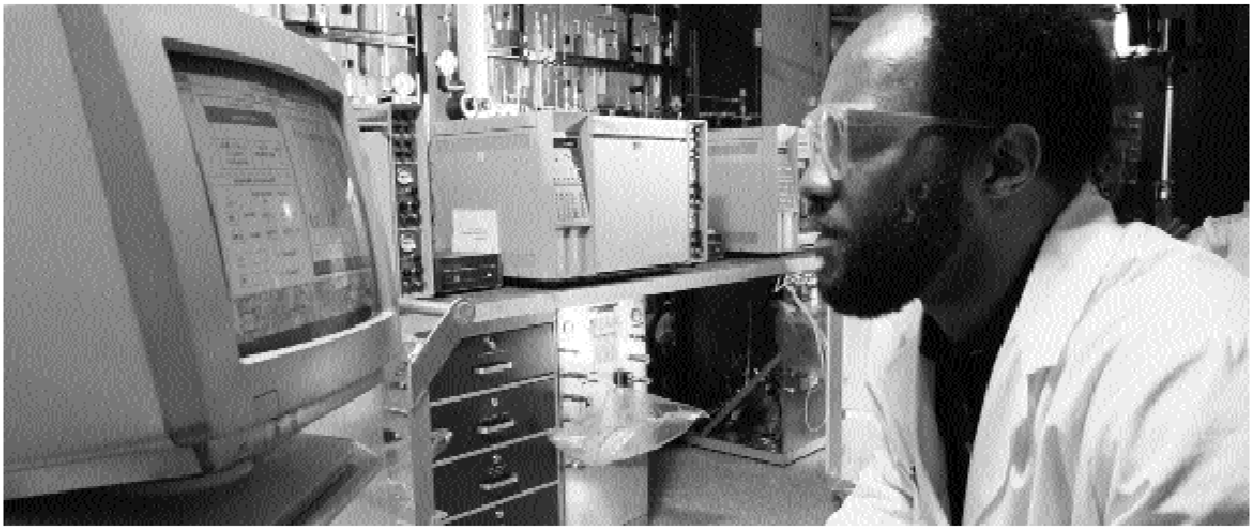
Today, NIST operates the Standard Reference Data Program, a network of data centers and projects covering about 40 scientific and technical disciplines. NIST operates 15 online data systems, available at no charge over the Web.[3] It also sells about 45 individual use databases, usually installable on PCs.

For many years, NIST and the American Institute of Physics (AIP) have published the *Journal of Physical and Chemical Reference Data*. NIST and AIP are now committed to creating an electronic journal and, since 1 January 2000, an online, full-text version of the *Journal* has been available to subscribers. NIST is building a complementary database, which will contain important data from the tables and graphs of various articles. Eventually, we anticipate that the printed and online full-text version of the *Journal* will be greatly reduced in size, and the majority of data will be available through the *Journal* database.

NIST and IUPAC Solubility Data

In 1998, NIST and IUPAC signed an agreement to publish four volumes per year of the *IUPAC SDS* in the *Journal of Physical and Chemical Reference Data.* NIST is providing some help with respect to manuscript preparation, but the bulk of the work is still performed by the individual volume editors with funding raised from their own sources.

With the explosion of Web-based chemical information resources, IUPAC and NIST began discussions about how best to make the contents of the entire *SDS* available online. In 1999, NIST and IUPAC concluded an agreement to achieve this. Over the next five years, it is hoped that all data still valid will be made available



via the Web at no charge. The remainder of this paper discusses these plans and the planned system. Because over 70 printed volumes have been printed, many of which are not available in computerized formats of any type, a subset has been selected to determine the best approach to important issues. The first subset deals with the solubility of halogenated hydrocarbons in water and covers four volumes: SDS 20 “Halogenated benzenes, toluenes and phenols with water” (1985), SDS 60 “Halogenated methanes with water” (1995), SDS 67 “Halogenated ethanes and ethenes in water” (1999), and SDS 68 “Halogenated aliphatic compounds C_3- C_{14} with water” (1999).

Building the NIST-IUPAC solubility data systems involves many activities, including the following:

- data entry (for volumes not computerized)
- data uniformity, including translation from old formats
- data verification, that the numbers are entered or translated correctly
- database design
- interface design
- search strategies
- display formats

During the next few years, these issues will be explored using the subset of four volumes identified above as a test bed. A prototype database design has already been developed and data entry is proceeding for Vol. 20. While NIST is performing this work, IUPAC keeps playing an important role in giving advice, reviewing the proposed design, and checking the data.

The proposed system will contain compiled experimental data as well as the critically evaluated recommendations. The printed volumes do have a limited number of expressions and formats for the data. It is NIST’s experience, however, that printed text often contains subtle inconsistencies and ambiguities that are identified only upon computerization.[4] Additional problems exist in making computerized data uniform, especially if the definitive publication of the data is via printed page. For example, it is common practice for small changes to be made directly onto page proofs without alteration of the computer files that were input into an automated typesetting system. Documentation of such changes is usually nonexistent, which means that every number must be compared with the printed page, and discrepancies investigated.

In spite of the diverse data expressions, the search strategies are remarkably simple. As is widely recognized, the solubility of substance A in substance B can also be viewed as the solubility of substance B in substance A. Therefore, there is no need to designate uniquely the solute and solvent in designing the underlying database that stores the data, nor to constrain search strategies unreasonably.

The three search strategies that will definitely be supported are as follows:

- find data on the solubility of substance A in substance B;
- find data on the solubility of A; and
- find data on the solubility of substances in substance B.

At first, searching on the solubility data themselves will not be supported, but depending on user needs, such as for liquid-liquid separations, this capability could be added later. To support these searches, methods for handling uncertainties need to be worked out. However, display of data in different units will be supported. In the future, additional features may be added, as requested by users, including performing calculations and generating plots.

For this project to be successful, NIST and IUPAC will have to work closely together on several issues, including system priorities, additional search strategies, interface design, data quality, system functionality, and display of results. The partnership is working successfully, as evidenced by the smooth transition to publication of new volumes of the *SDS*. Both parties look forward to a long relationship in order to make solubility data readily available via the Web.

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[2] T.E. Gills et al., “NIST mechanisms for disseminating measurements,” submitted for inclusion in *NIST Journal of Research*, 102, no.1 (2001).

[3] http://www.nist.gov/srd

[4] J.H. Westbrook. *J.Chem.Info.Comput.Sci*. 33, 6-17 (1993).

John Rumble Jr. is Chief of the NIST Standard Reference Data Program, Gaithersburg, Maryland, USA.

Further information about the *SDS*, including a list of volumes published and in preparation, is available on the *SDS* Web site (see below). This site also contains e-mail addresses of David Shaw, Heinz Gamsjäger, and Mark Salomon, members of the IUPAC Subcommittee on Equilibrium Data, who will gladly receive comments, questions, and proposals for future volumes.

This article was originally published in *Pure and Applied Chemistry*, Vol. 73, No. 5, pp. 825–829, 2001 as part of the lecture presented at the 9th IUPAC International Symposium on Solubility Phenomena, Hammamet, Tunisia, 25–28 July 2000.

http://www.iupac.org/publications/sds/index.html
http://www.iupac.org/publications/pac/2001/7305/7305x0825.html

IUPAC Forum

Two National Adhering Organizations reacted to Dr. Pryzbylowicz's essay published in the previous issue of CI (Vol. 24, No. 1, pp. 7-9, January 2002), regarding the U.S. Young Observer Program. The Japanese NAO describes how the programs can challenge an old stigma, and invites young scientists to attend IUPAC General Assemblies. On a somewhat different note, the Canadian NAO favors young participation in broader IUPAC-related activities by offering travel awards to IUPAC-sponsored conferences. Please send your comments to <edit.ci@iupac.org>.

Breaking Away from the Old Three Ss

by Hitoshi Ohtaki

The contributions of Japanese scientists to various international communities became quite significant in these decades. At almost all international conferences, the names of Japanese scientists are listed as plenary and invited lecturers. They often appear in organizing committees and advisory boards. Their presentations at conferences are usually quite satisfactory and the standard of their science is high enough to be at the world-leading level.

In contrast to their significant contributions to, and involvement with, international scientific communities, Japanese scientists at international meetings are often said to behave according to the three Ss: *smile*, *silence*, and *sleep*. The reasons for such behavior are varied. For one, it may be rather difficult for many Japanese members to join debates among Europeans and Americans because of a language barrier and their traditional philosophy that "Silence is Golden." Therefore, it is often difficult for them to present new proposals at international meetings, and in most cases they gently smile and say "I agree." Since the contributions of Japan to IUPAC, as well as to other international organizations, are very important, we would like to remove the barrier of the three Ss from international meetings.

When we look at the involvement of Japan in IUPAC, more than 50 Japanese chemists are Titular and Associate Members and National Representatives in various committees and commissions. The national subscription of Japan is the second largest after that of the United States. However, it is sometimes critically commented that Japanese members are rather quiet, do not easily join discussions, and scarcely propose new issues. However, such problems caused by the language barrier can be solved in the near future by young scientists of Japan.

IUPAC members have occasionally criticized the role, importance, and visibility of the IUPAC organization and the General Assemblies (GAs). However, the increase in the activities of IUPAC, supported by the improved financial situation after the movement of the Secretariat to North Carolina, USA, makes the contribution of IUPAC to individual countries and members more visible than before. The IUPAC prize for young chemists and the financial support program for international conferences organized in developing and economically disadvantaged countries are just some of the examples.


Hitoshi Ohtaki

The GAs are essential forums for chemists to learn about the latest ideas and developments in the field. The problem is that the financial support for participation in the GA is not adequate for all people who wish to contribute to the meeting. Associate Members and National Representatives do not usually receive financial support when they attend the GAs.

> *Since the contributions of Japan to IUPAC, as well as to other international organizations, are very important, we would like to remove the barrier of the three Ss from international meetings.*

In order for all members to play their necessary roles in IUPAC and other international organizations, they need to have face-to-face discussions at meetings, something that can help to establish mutual understanding among members. From this point of view, the National Committee for Chemistry of the Science Council of

Japan, which is a National Adhering Organization of IUPAC, developed a program about 10 years ago through which financial support is given to chemists under 45 years old, to attend commission meetings of divisions at the GA. Financial support is also extended to Associate Members, National Representatives, and chemists who want to attend the GAs as observers.

The budget of the program has been supported by the Company Associates of IUPAC in Japan through the efforts of Japanese Committee on Chemistry and Industry (COCI) members. The selection of awardees is made by the Subcommittee of International Relationship of the National Committee for Chemistry. After careful consideration of applicant’s scientific activities, four young chemists are chosen for each GA. Efforts are made to evenly distribute the awards through different areas of chemistry. The award amount is usually enough to cover their travel. The subcommittee requires awardees to submit their reports after coming back from GA meetings. Through this program we believe that the contribution of Japanese chemists to IUPAC will be improved and their participation in meetings will be much more active and significant. We expect that Japanese scientists will establish a new philosophy of the Three Ss: *speak* at meetings, be *sincere* in behavior, and *serve* the world.

Hitoshi Ohtaki is a professor at Ritsumeikan University, Bureau Member and the Chairman of the Committee for Conferences in Developing and Economically Disadvantaged Countries, Chairman of the Membership Development Committee, and Chairman of the Subcommittee on International Relationship of the National Committee for Chemistry of Japan.

Young Chemists Travel Far with Canadian National Committee Awards

by Vedene Smith

In 1982, the Canadian National Committee for the International Union of Pure and Applied Chemistry (CNC/IUPAC) established a program of Travel Awards whose purpose is to help young Canadian chemists and chemical engineers (within 10 years of gaining their PhDs) present papers at IUPAC-sponsored conferences outside continental North America.

The annual awards are financed by a trust fund and funding from CNC/IUPAC’s Company Associates. The criteria used in making these awards include evidence of an independent research program, a high-quality publication record, and the ability to attract high-quality research funding.

Normally, five or six of these awards are given each year, but an individual can only receive an award once. Although the amount of an award covers only a portion of total travel costs, it can help to catalyze additional support. Within the chemistry community, the CNC/IUPAC Travel Awards are considered prestigious. Numerous past winners are now established and prominent researchers.

Vedene Smith is a professor at Queeen’s University in Kingston, Ontario, Canada, and is a member of CNC/IUPAC.

http://www.sao.nrc.ca/sims/upac_e.html

IUPAC News

Chemical Nomenclature and Structure Representation

by Alan McNaught

This year sees the birth of a new division of IUPAC. Its conception dates from a survey carried out in 1998 for the Organic Division, in which the chemistry community was asked for opinions on future nomenclature requirements. Comments received highlighted the increasing need for a body to oversee IUPAC nomenclature development across all disciplines, to ensure compatibility with previous work, and to coordinate related activities. The resulting report[1] drew attention in particular to the need to integrate nomenclature standards with computerized facilities, and to push ahead with efforts to define for each unique structure a single preferred IUPAC name, correlated with other names in common use.

This report stimulated further consultation. A strategy roundtable in March 2000, involving people from many professions with a need for standard chemical identifiers, reinforced the views from the original survey and added some important new items.[2] In particular, the need for a IUPAC standard for computerized representation of a chemical structure was recognized.

The roundtable recommendations led IUPAC’s Executive Committee to establish a temporary Committee on Chemical Identity and Nomenclature

Systems,[3] which developed plans for future management of IUPAC's nomenclature work and launched the IUPAC Chemical Identifier project.[4] The work of this *ad hoc* Committee culminated in a proposal for a new IUPAC division. The IUPAC Council endorsed this proposal, stressing the continuing importance to IUPAC of nomenclature and related activities. And so, the Division of Chemical Nomenclature and Structure Representation[5] was established on 1 January 2002.

Alan McNaught

So What Will the New Division Be Doing?

Most importantly, it will bring together work on nomenclature of chemical compounds with development of other methods of designating chemical structures. The Chemical Identifier project is a first step in this direction. It will also be tackling interdisciplinary issues that have been difficult to deal with hitherto. For example, we have a project group considering divergent recommendations arising from the development of preferred names for organic compounds in parallel with revision of the inorganic nomenclature rules. Also, we will study the applicability of naming systems developed for polymers with particular reference to macrocycles, rotaxanes, and catenanes. Additionally, we will be assessing to what extent recent developments in conventional organic nomenclature and phane nomenclature can allow us to deal conveniently with these and other structures.

Other areas of activity will include the following:

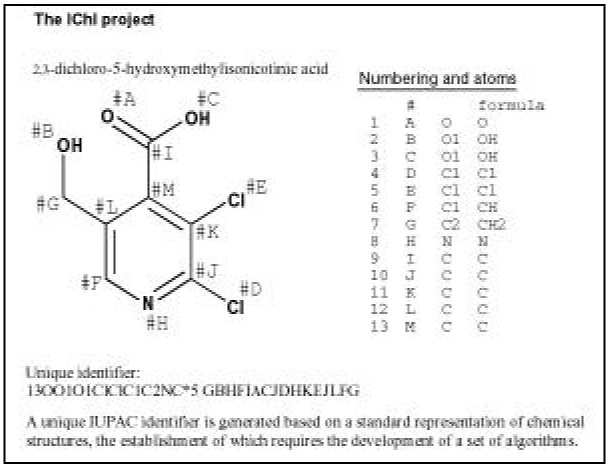
- Extension to all chemical compounds of procedures for identifying IUPAC-preferred names
- Organometallic nomenclature
- Computer-assisted cluster nomenclature
- Stereochemical nomenclature
- Fullerene nomenclature
- Dendritic and hyperbranched polymers
- Databases of synonyms for compounds in common use

How Will the New Division Operate?

A division committee has been assembled consisting of 12 members plus National Representatives, including people with extensive experience in developing conventional nomenclature recommendations and others with expert knowledge of computerized systems for designating chemical structures. The division has an advisory subcommittee of about 40 people, charged with advising the division committee on the needs of the community, and developing project proposals. This subcommittee contains many individuals with experience in nomenclature work, as well as chemical software developers, journal editors, and a range of other users of IUPAC recommendations. It is expected that these people will lead or otherwise participate in projects as well as provide advice to the division committee. Apart from meetings of task groups, most of the subcommittee's work will be carried out via electronic communication. A Web discussion board has been set up, to which drafts of new recommendations and comments on them are to be posted. Where possible, meetings of task groups will be organized to take place concurrently, to enable informal discussions between members of different groups. At suitable intervals (probably about every 5 years), we will convene a roundtable meeting with the user community to review results and define future requirements.

Of course, this way of working is quite new to IUPAC, and we shall need to adjust our procedures as we gain more experience. However, this scheme will allow better use of resources than previously, and will expedite the development of the standards that the community needs.

This new arrangement also accommodates the IUPAC/IUBMB Joint Commission on Biochemical Nomenclature, as a commission attached to the new division. This commission meets jointly with the Nomenclature Committee of IUBMB and the combined committee acts essentially as a single body. Its main responsibility is the upkeep and development of the Enzyme List, a very substantial and ongoing project.[6] It is also increasingly involved with standards for bioinformatics, needed to accommodate the explosion of information on biopolymers. In addition, JCBN has traditionally dealt with specialist biochemical nomenclature systems (e.g., carbohydrates, lipids, and polypeptides), and this is where a close link with the new Division of Chemical Nomenclature and Structure Representation is important. For nomenclature work, this commission has always operated through project task groups, something we envisage for future work managed by the new division.



The IChI project

2,3-dichloro-5-hydroxymethylisonicotinic acid

Numbering and atoms

	#		formula
1	A	O	O
2	B	O1	OH
3	C	O1	OH
4	D	C1	C1
5	E	C1	C1
6	F	C1	CH
7	G	C2	CH2
8	H	N	N
9	I	C	C
10	J	C	C
11	K	C	C
12	L	C	C
13	M	C	C

Unique identifier:
13OO1O1C1C1C1C2NC*5 GBHFIACJDHKEJLFG

A unique IUPAC identifier is generated based on a standard representation of chemical structures, the establishment of which requires the development of a set of algorithms.

<http://www.iupac.org/projects/2000/2000-025-1-800.html>

We should not lose sight of the fact that IUPAC can retain a credible role in nomenclature development only by paying close attention to the needs of the community and responding to them. We need to give wide publicity to the fact that IUPAC's project system now allows ideas for future work to be developed by anyone. My colleagues and I welcome project proposals[7] from any source, and are happy to discuss suggestions informally. Only if we have a clear view of what our "customers" want can we hope to make the best use of IUPAC's resources.

Division Committee

Alan D. McNaught, UK
Division President
Warren H. Powell, USA
Division Secretary
Michael Dennis, USA
Michael Hess, Germany
Herbert D. Kaesz, USA
G. Jeffery Leigh, UK
Gerard P. Moss, UK
William G. Town, UK
Antony Williams, USA
Stephen Heller, USA
Alexander J. Lawson, Germany
Bruce M. Novak, USA

National Representatives

Roberto de Barros Faria, Brazil
Jiasong He, China
Jean Marie François Toullec, France
Yohsuke Yamamoto, Japan
Osman Achmatowicz, Poland
Bernardo Jerosch Herold, Portugal

Alan McNaught is President of the IUPAC Division of Chemical Nomenclature and Structure Representation. He is General Manager of the Production Division of the Royal Society of Chemistry, Cambridge, UK.

References
[1] http://www.iupac.org/projects/1998/310_28_98.html
[2] http://www.iupac.org/news/archives/2000/NRT_Report.html
[3] http://www.iupac.org/organ/ad_hoc_cmt/ccins.html
[4] http://www.iupac.org/projects/2000/2000-025-1-050.html
[5] http://www.iupac.org/divisions/VIII/index.html
[6] http://www.chem.qmw.ac.uk/iubmb/enzyme/
[7] http://www.iupac.org/projects/form_guide.html

Nomenclature of Inorganic Chemistry

by Herbert D. Kaesz

The Commission on Nomenclature of Inorganic Chemistry (CNIC) met for the last time in Brisbane, Australia on 30 June to 2 July, 2001. Among those attending were three National Representatives, Profs. Risto Laitinen, Dan Meyerstein, and Lars Elding (standing in for Ebbe Norlander), Prof. Wim Koppenol (a former Commission member involved in an individual project) and two observers from the U.S. Delegation, Profs. Vince Pecararo and Bernadette Donovan-Merkert. The observers were well received and participated fully in the discussions.

Naming of New Elements

Revisions in the document "The Naming of New Elements," prepared for publication by W. Koppenol, were discussed and approved for forwarding to the Interdivisional Committee on Terminology, Nomenclature, and Symbols for further review. This document is now posted online for public review.

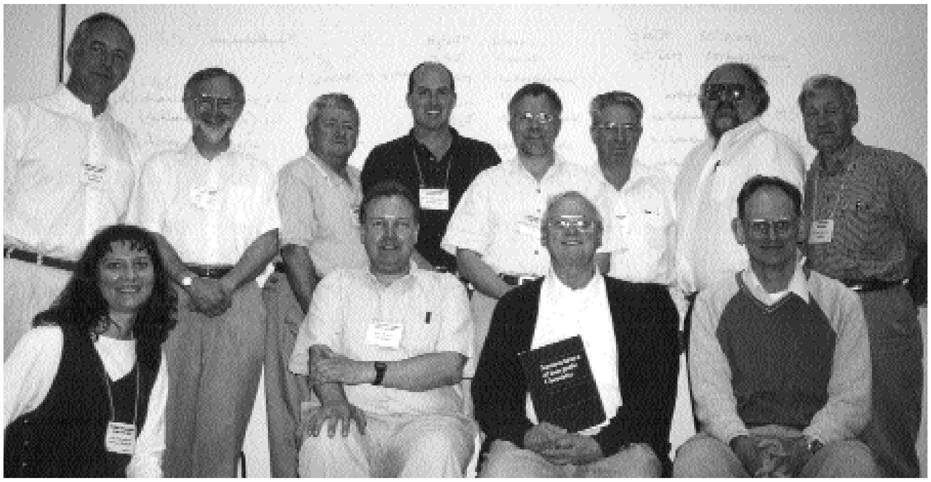
The *Red Book*

The Commission has been working on a revision of *Red Book I, Nomenclature of Inorganic Chemistry*, under project leader Dr. N. Connelly. This revision is planned to consist of eleven chapters, the first four of which were thoroughly reviewed before the meeting in Brisbane. Revised versions of six of the remaining chapters were examined in detail with completion targeted for mid 2002. In its revised version, the *Red Book I* will include the following chapters:

1. General Aims, Functions, and Methods of Chemical Nomenclature
2. Grammar
3. Elements, Atoms, and Groups of Atoms
4. Formulae
5. Compositional Nomenclature
6. Substitutive Nomenclature and Parent Hydride Names
7. Additive Nomenclature
8. Inorganic Acids and Derivatives
9. Coordination Compounds
10. Organometallic Compounds
11. Solids

New Projects

Other projects being considered by the current Commission include computer generation of names (Prof. Dress), a joint organometallic document including metalla-


CNIC Meeting, Brisbane, Australia, June/July 2001. Seated, from left to right: Bernadette Donovan-Merkert, Ture Damhus (Secretary), H.D. Kaesz (Chair), Wim Koppenol. Standing, left to right: Alan T. Hutton, Neil G. Connelly, James Casey, Richard M. Hartshorn, Risto Laitinen, Dan Meyerstein, Vince Pecaro, and Lars Elding. Photo courtesy W. Koppenol.

cycles and possibly stereochemistry (Prof. Hutton), and Preferred Names document for Inorganic compounds (Dr. Damhus).

Since January 2002, activities related to systematic nomenclature are being undertaken by the new IUPAC Division of Chemical Nomenclature and Structure Representation. (see this issue of *CI*, p. 12). In anticipation of that change, CNIC held a joint meeting with the *ad hoc* Committee on Chemical Identity and Nomenclature Systems, chaired by Alan McNaught, to discuss the future of nomenclature within IUPAC.

A second joint meeting of CNIC was with the Commission on Nomenclature of Organic Chemistry (CNOC) to discuss areas of overlap between inorganic and organic compounds in a Preferred-Names document presented by CNOC in draft form. There were three or four chapters with very strong overlap but not enough time available to carry out detailed discussions in Brisbane. Following that meeting a project to ensure minimum actual inconsistency in nomenclature recommendations, maximum alignment of approaches and principles, and appropriate cross-referencing between the areas covered by both the organic Preferred Names document and the inorganic *Red Book I* revision, was initiated. The interdisciplinary task group chaired by T. Damhus met in September 2001, with the additional participation of Neil G. Connelly and Alan McNaught. Major decisions about necessary revisions of one or the other document in order to achieve maximum alignment have been taken, and actual revisions are in progress. Only when the texts are in place, can the cross-referencing and appropriate footnotes be made to fine tune and fully align the two texts, so it is anticipated that this part of the project must take place concurrently with the review process in the Spring of 2002.

The Way Forward

Finally, CNIC heard a report from the Inorganic Division Officers. The Division has embraced the restructuring of the Union and has strived to implement the changes necessary following the decisions of the Council in Berlin of terminating the current Commissions. At that time however, the Division had two concerns with regard of the area of nomenclature. The first is to ensure that the needs of inorganic chemists are met by IUPAC nomenclature recommendations and that the current emphasis on preferred names does not result in the recommendations of names that will never see general use for inorganic compounds. The second is finding a mechanism to maintain IUPAC's considerable current expertise in inorganic nomenclature.

Close interaction between the new Division of Chemical Nomenclature and Structure Representation and area experts in the Inorganic Division will be one key to sustaining essential and successful projects in this area. Many of the active past members of CNIC have been invited to serve on the Advisory Committee to the new Division. Additionally, two members of the newly formed division, Dr. J. G. Leigh (a former chair of CNIC) and myself (immediate past chair of CNIC) stand ready to receive comments and hints on issues that might be of relevance to the community concerned with inorganic nomenclature.

Herbert D. Kaesz was a member of the Former CNIC from 1994 to 2001. He is currently a member of the Inorganic Chemistry Division Committee, the Division of Chemical Nomenclature and Structure Representation, and the Committee on Chemistry Education. He is a professor at the University of Caifornia at Los Angeles, California, USA.

http://www.iupac.org/reports/provisional/abstract01/koppenol_310302.html

More

The news section on the IUPAC Web site includes other news from IUPAC, inlcuding "A Report of the World Chemistry Leadership Meeting 9 July 2001, Brisbane, Australia."

http://www.iupac.org/news/

IUPAC Projects

SCOPE/IUPAC International Symposium on Endocrine Active Substances

The Scientific Committee on Problems of the Environment (SCOPE) and IUPAC are jointly organizing an International Project on "Environmental Implications of Endocrine Active Substances: Present State of the Art and Future Research Needs." The project started in April 2000 and is scheduled to be completed in March 2003. The SCOPE/IUPAC International Symposium on Endocrine Active Substances, to be held 17-21 November 2002 in Yokohama, Japan, will constitute a major milestone for the project. All of the project contributors (ca. 60 experts) will present papers dealing with the following topics:

- Molecular Mode of Action of Nuclear Receptors; Fundamentals for Understanding the Action of Endocrine Active Substances
- Environmental Fate and Metabolism of Endocrine Active Substances
- Effects of Endocrine Active Chemicals in Rodents and Humans, and Risk Assessments for Humans
- Effects of Endocrine Active Substances in Wildlife Species

In addition, six supplementary workshops will be held:

- Effectiveness of QSAR for prescreening of endocrine disruptor hazard
- Toxicogenomics as a rational approach to endocrine disruptor research
- The need for establishing integrated monitoring programs
- Simple, rapid assay for conventional definitive testings of endocrine disruptor hazard
- Precautionary principle/approach and weight of evidence in endocrine disruptor issues
- Risk management options for endocrine disruptors in national and international programs

See the symposium announcement in *CI*, Vol. 23, No. 5, p. 156, September 2001.

http://www.iupac.org/projects/2000/2000-016-1-600.html

Highlights from Pure and Applied Chemistry

Presenting recently published IUPAC technical reports and recommendations

Generic Source-Based Nomenclature for Polymers (IUPAC Recommendations 2001)

by E. Maréchal and E. S. Wilks
Pure and Applied Chemistry, Vol. 73, No. 9, pp. 1511-1519 (2001).

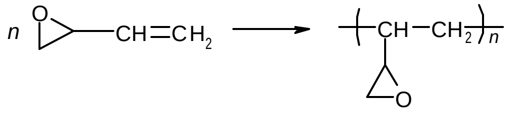
Present-day high-performance polymer materials are becoming increasingly difficult to name concisely with existing macromolecular nomenclature. Simple and practical names that refer to the monomer source (i.e., source-based nomenclature) are therefore highly desirable; thus, the rules that lead to such names need to be spelled out. That task was undertaken by an international group of experts of the former IUPAC Commission on Macromolecular Nomenclature. Their recent recommendations on generic source-based nomenclature for polymers describe an unambiguous naming system that is as rigorous as, but more practical than, structure-based nomenclature. This generic naming system complements the earlier source-based method, which in some cases leads to ambiguous names.

A generic source-based name comprises two parts:

1. polymer class (generic) name followed by a colon;

2. the actual or hypothetical monomer name(s) (source), always parenthesized in the case of a copolymer. (See figure for an example.)

In this document, five rules are presented and illustrated by 20 examples; the formula, the structure-based name, the source-based name, and the generic source-based name of the polymer are given for each example.



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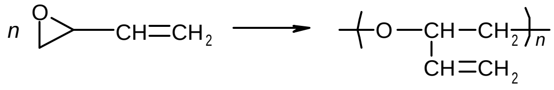


II

Structure-based names:
I. poly(1-oxiranylethylene)
II. poly[(oxy(1-vinylethylene)]

Source-based name:
I and II have the same source-based name:
poly(vinyloxirane).

Generic source-based names
I. polyalkylene:vinyloxirane
II. polyether:vinyloxirane

In some cases, only generic source-based nomenclature gives unambiguous names, for example, when a polymer has more than one name or when it is obtained through a series of intermediate structures. The rules concern mostly polymers with one or more types of functional groups or heterocyclic systems in the main chain, but to some extent they are applicable also to polymers with side-groups, carbon-chain polymers such as vinyl or diene polymers, spiro and cyclic polymers, and networks.

http://www.iupac.org/publications/
pac/2001/7309/7309x1511.html

Quantum Chemical B3LYP/cc-pvqz Computation of Ground-State Structures and Properties of Small Molecules with Atoms of $Z \leq 18$ (Hydrogen to Argon) (IUPAC Technical Report)

by Rudolf Janoschek
Pure and Applied Chemistry, Vol. 73, No. 9, pp. 1521-1553 (2001).

Since density functional theory achieved a remarkable breakthrough in computational chemistry, the important general question "How reliable are quantum chemical calculations for spectroscopic properties?" should be answered anew. In this project, the most successful density functionals, namely the Becke B3LYP functionals, and the correlation-consistent polarized valence quadruple zeta basis sets (cc-pvqz) are applied to small molecules. In particular, the complete set of experimentally known diatomic molecules formed by the atoms H to Ar (there are 214 systems) is uniformly calculated, and calculated spectroscopic properties are compared with experimental ones.

Computationally demanding molecules, such as open-shell systems, anions, or noble gas compounds, are included in this study. Investigated spectroscopic properties include spectroscopic ground state, equilibrium internuclear distance, harmonic vibrational wavenumber, anharmonicity, vibrational absolute absorption intensity, electric dipole moment, ionization energy, and dissociation energy. The same computational method has also been applied to the ground-state geometries of 56 polyatomic molecules up to the size of benzene. Special sections are dedicated to nuclear magnetic resonance chemical shifts and isotropic hyperfine coupling constants. Each set of systems for a chosen property is statistically analyzed, and the above important question "How reliable . . . ?" is mathematically answered by the mean absolute deviation between calculated and experimental data, as well as by the worst agreement. In addition to presentation of numerous quantum chemically calculated spectroscopic properties, a corresponding updated list of references for experimentally determined properties is presented.

http://www.iupac.org/publications/
pac/2001/7309/7309x1521.html

Standards in Isothermal Microcalorimetry (IUPAC Technical Report)

by Ingemar Wadsö and Robert N. Goldberg
Pure and Applied Chemistry, Vol. 73, No. 10, pp. 1625-1639 (2001).

Isothermal microcalorimetric techniques have been much improved during the past decades, and several types of instruments are commercially available. Application areas include, for example, ligand binding studies, dissolution and sorption measurements, estimation of the stability of chemical substances and technical products, and measurements of metabolic reactions in living cellular systems.

Most isothermal microcalorimeters are calibrated by the release of heat in an electrical heater positioned in the calorimetric vessel or in its close proximity. However, in some cases it is difficult to conduct electrical calibration experiments, which will closely mimic the heat flow pattern of the process or reaction under investigation. This can lead to a significant error in the calibration value and, in some cases, the use of some chemical calibration would therefore be preferable. Regardless of which calibration technique is used, it is often desirable to quantitatively control the overall performance of an instrument by use of a suitable test reaction. Simple and reliable test reactions are also very suitable for the training of experimenters. In order to allow a close comparison between results from chemical calibrations or test experiments and results from a calorimetric investigation, it is important to have many different chemical calibration and test reactions available.

In this report, guidelines are presented on the use of standardized chemical test and calibration reactions suitable for use in different areas of isothermal microcalorimetry. The focus is on reactions suitable for use under ambient conditions. Further, a standardized terminology in describing the characteristics of isothermal microcalorimeters is proposed. “Nanocalorimeters,” usually indicating calorimeters with a detection limit approaching the nanowatt range, are in this report not distinguished from “microcalorimeters.”

The Task Group responsible for the project was: I. Wadsö (Chairman), A. E. Beezer, R. N. Goldberg, G. Olofsson, K. Murphy, J. Rouquerol and J. Sipowska.

http://www.iupac.org/publications/pac/2001/7310/7310x1625.html

Critical Evaluation of Stability Constants of Phosphonic Acids (IUPAC Technical Report)

by Konstantin Popov, Hannu Rönkkömäki,
and Lauri H. J. Lajunen
Pure and Applied Chemistry, Vol. 73, No. 10, pp. 1641-1677 (2001).

Organophosphonate chelating compounds are widely used in a broad variety of applications.Their ability to prevent precipitation of calcium salts at substoichiometric concentrations (threshold effect) finds wide application in water treatment for scale inhibition. Phosphonates, particularly EDTPH and DTPPH, are used extensively in laundry detergents. These materials are also used as corrosion inhibitors, in industrial cleaning and in peroxy bleach stabilization. Uses of organophosphonates span applications in flame-resistant polymers, photographic processing, ore flotation (aminophosphonic surfactants), actinide separation processes, and analytical chemistry. Recently, organophosphonates have been identified as promising reagents for the creation of so-called “structurally tailored” materials and microporous materials, in catalysis, and in the electrochemical treatment of polluted soils.

The high biological activity of carboxyalkylphosphonates, aminoalkylphosphonates, and alkylenediphosphonates makes them useful agents as components of microfertilizers and pesticides in agriculture, as well as drugs and diagnostic reagents in biology and medicine. Annual industrial output of organophosphonates is in the thousands of tons.

The broad and intensive applications of organophosphonates require reliable data on the stability constants of the corresponding complexes in order to permit equilibrium modeling and prediction of the important technological, environmental, and pharmacokinetic equilibria. As phosphonates resist biodegradation, chemical speciation calculations based on numerical equilibrium data are of extreme importance for applications such as environmental science, waste management, agriculture, scale inhibition, magnetic resonance imaging, behavior of radiopharmaceuticals in blood plasma, and many others.

The data of interest are partly accumulated in some monographs, reviews, and compilations of stability constants. Recently, two computer databases have become commercially available. The IUPAC Stability Constants Database (SC-Database) is the more comprehensive. For organophosphonates, some data in the “critically evaluated compilations” are not consistent with later, more precise results. These are therefore rejected in the present work.

This study critically evaluated available experimental data on stability constants of proton and metal complexes for 10 phosphonic acids [methylphosphonic acid, 1-hydroxyethane-1,1-diylbisphosphonic acid, dichloromethylenebisphosphonic acid, amino-methanephosphonic acid, *N*-(phosphonomethyl)glycine, imino-*N*, *N*-bis(methylenephosphonic acid), *N*-methylamino-*N*, *N*-bis(methylenephosphonic acid), nitrilotris(methylenephosphonic acid), 1,2-diaminoethane-*N*,*N*,*N*´,*N*´-tetrakis-(methylenephosphonic acid), and diethylenetriamine-*N*,*N*,*N*´,*N*´´,*N*´´-pentakis-(methylenephosphonic acid)]. For the latter phosphonate, all the data are rejected, as well as protonation constants [HL]/[H][L] for three other ligands. Higher-quality data are selected and presented as “Recommended” and “Provisional.”

This review is generally based on the data published in the period 1965-1996, but some earlier and later publications are also included. The data collection embraced databases Chemical Abstracts, and the personal collections of the authors.

http://www.iupac.org/publications/pac/2001/7310/7310x1641.html

Provisional Recommendations

IUPAC Seeks Your Comments

In this section, we publish synopses of IUPAC's latest provisional recommendations on nomenclature and symbols. All comments on these recommendations are welcome and will be taken into consideration. The final revised versions are published in *Pure and Applied Chemistry*.

If you would like to comment on the provisional recommendations, please visit the IUPAC Web site at <http://www.iupac.org/reports/provisional/index.html>, where the full texts are available for downloading as draft Adobe PDF files. Alternatively, you can write to your nearest national/regional center to request a copy. The most recent list of national/regional centers is available on the Web site at the address above and last appeared in *CI*, Vol. 17, p. 141 (1997).

Quantities, Terminology, and Symbols in Photothermal and Related Spectroscopies

Photothermal spectroscopy is widely used in many fields such as physics, chemistry, biology, and engineering. In this article, various origins of the photothermal effects that give rise to photothermal signals and the terms related to photothermal spectroscopies are reviewed. Terminologies in grating spectroscopy, lens spectroscopy, light-induced acoustic spectroscopy, photothermal radiometry, photothermal calorimetry, photothermal interferometry, photothermal deflection, photothermal reflection change, and related methods are recommended. Symbols used in photothermal spectroscopy are summarized.

http://www.iupac.org/reports/provisional/abstract01/hirota_310702.html

Comments by 31 July 2002
To Prof. Noboru Hirota
Kyoto University
19-6, Otokoyama-Yoshii, Yawata-shi,
Kyoto-fu 614-8363, Japan
Tel.: +81 75 753 4023
Fax: +81 75 753 4000
E-mail: nhirota@ip.media.kyoto-u.ac.jp

The Naming of New Elements

A procedure is proposed to name new elements. After the discovery of a new element is established by a joint IUPAC-IUPAP (International Union of Pure and Applied Physics) Working Group, the discoverers are invited to propose a name and a symbol to the IUPAC Inorganic Chemistry Division. Elements can be named after a mythological concept, a mineral, a place or country, a property, or a scientist. After examination and acceptance by the Inorganic Chemistry Division, the proposal follows the accepted IUPAC procedure for recommendations, and is then submitted to the Council of IUPAC for approval.

http://www.iupac.org/reports/provisional/abstract01/koppenol_310302.html

Comments by 31 March 2002
To Prof. Dr. W. H. Koppenol
Laboratorium für Anorganische Chemie
Eidgenössische Technische Hochschule Hönggerberg, Universitätsstrasse 6
CH-8093 Zürich, Switzerland
Tel.: +41 1 632 2875
Fax: +41 1 632 1090
E-mail: koppenol@inorg.chem.ethz.ch

New Books and Publications

The Biogeochemistry of Iron in Seawater

David R. Turner and Keith A. Hunter
Series on Analytical and Physical Chemistry of Environmental Systems, Vol. 7
John Wiley & Sons, New York, 2001, pp. 396.
(ISBN 0-471-49068-7)

The proposal that a lack of iron can limit phytoplankton growth in the oceans was first put forward in the 1930s, but it was not until the 1980s that developments in clean sampling and analytical techniques had advanced sufficiently to allow accurate measurements of iron at trace levels. Intensive research carried out during the 1990s (known as the “Iron Age of Oceanography”) provided a wealth of new information on the biogeochemistry of iron in seawater. The field has now advanced to a stage where a critical analysis of progress to date can be of considerable benefit to the research community as a whole.

This book, written by acknowledged experts and reviewed by international specialists, provides the authoritative and comprehensive review of the subject area. A joint venture between the Scientific Committee for Ocean Research and IUPAC, it expertly addresses the current state of knowledge on the subject and covers chemical speciation, analytical techniques, and the transformation of iron.

The book includes evidence for iron limitation of primary production of high-nutrient, low-chlorophyll areas in the ocean and offers a wealth of new information. It is ideal for marine scientists, oceanographers, environmental analytical chemists scientists, and others studying the environmental impact of metals and their role in marine ecosystems.

http://www.iupac.org/publications/books/author/turner.html

Polymerization Processes and Polymer Materials, Volumes I and II

Z. Floranczyk, S. Penczek, S. Slomkowski (Eds.)
Macromolecular Symposia, Vol. 174 & 175.
Wiley-VCH, 2001, 434 pp. (Vol. I—ISBN 3-527-30336-7) and 428 pp. (Vol. II—ISBN 3-527-30337-5).

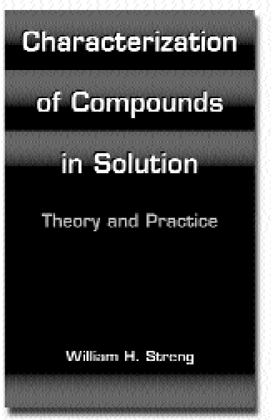
In 2000, over 1500 participants from 54 countries attended the World Polymer Congress—the 38th International Symposium on Macromolecules (sponsored by IUPAC), held 9-14 July at the Warsaw University of Technology. These books, Volumes 174 and 175 of the *Macromolecular Symposia*, contain 86 invited and plenary lectures from the Congress. The scientific program of the Congress—organized by the Department of Polymer Chemistry of the Centre of Molecular and Macromolecular Studies of the Polish Academy of Sciences in Lodz and the Chemistry Department of the Warsaw University of Technology—was divided into 16 Sections and covered such areas as synthesis, radical polymerization, ionic polymerization, polyolefins, branched and star-like macromolecules, biorelated and environmentally friendly polymers, and electrical, optical, and dielectric properties of polymers.

http://www.iupac.org/publications/macro/2001/174_preface.html

Characterization of Compounds in Solution: Theory and Practice

William H. Streng
Kluwer Academic/Plenum Publishers, New York, 2001.
(ISBN 3-306-46595-7)

The purpose of this book is to discuss concisely and comprehensively solution properties of compounds that are most important in the area of pharmaceutics. While there are many topics that can be included in a discussion on solution properties of compounds, the following are the most critical in the area of pharmaceutics: equilibrium constants, partition efficients, general solubility, solubility in protic solvents, and solution stability. The ambitious concept of this book is to bring together these topics in a logical and concise manner.



After an introductory chapter on compound characterization, the theoretical chapters of Streng’s book cover thermodynamics, kinetics, equilibrium constants, partition coefficient, solubility, solubility of weak acids and bases, solution stability, and instrumentation. Clearly, most of these chapters could easily fill a volume in itself, but the truly original idea of the book is the self-sufficient description of theory and practice used for characterizing compounds in solution. The remaining chapters cover procedures and examples for the practical investigation of equilibria, partitioning, solubility, and solution kinetics.

The strength of this book lies in the chapters on instrumentation and solution kinetics. Here the author draws from his scientific experience and convincingly shows how a general knowledge in physical chemistry is applied to obtain experimentally reliable information and theoretically sound interpretations.

The digressions in some of the introductory remarks of the individual chapters are doubtless a matter of taste. For example, the comparison of chemical kinetics with a road between two cities that are separated by a small or a tall mountain seems—from the reviewer's point of view—a bit too simplistic.

In addition, some misleading statements in the theoretical chapters should be eliminated in the next edition. For example, in one section a catalyst is described as "shifting the equilibrium to the right." However, catalysts increase the rate at which equilibrium is attained, but do not effect its position.

To summarize, it can be said that Streng's book covers compactly a wide variety of theoretical and practical aspects of characterizing compounds of pharmaceutical relevance using physicochemical methods. It will be most beneficial to readers who plan to set up their own experimental investigations to characterize compounds in solution.

Reviewed by Heinz Gamsjäger, Montanuniversität Leoben, Austria.

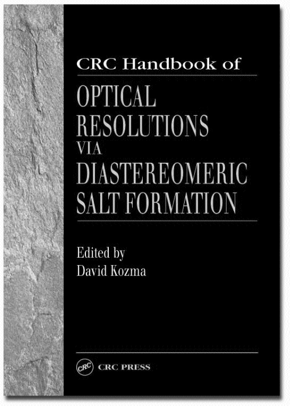
http://www.wkap.nl/prod/b/0-306-46595-7

CRC Handbook of Optical Resolutions via Diastereomeric Salt Formation

Dávid Kozma (Ed.)
CRC Press, September 2001, pp. 800.
(ISBN 0-8493-0019-3)

Optically active compounds are gaining ever-increasing importance in organic chemistry, both in the academic and the industrial arenas. The rational synthesis of the growing number of chiral chemicals, drugs, and natural products demands efficient methods for producing these compounds in an enantiomerically, highly pure form. Despite the available alternative techniques, optical resolution via diastereomeric salt formation remains the most widely used method of preparing pure enantiomers.

This is the first book to exclusively address this important organic chemical process. It provides fast, one-stop access to a wealth of information, including all of the available data on 100 resolving agents, a list of 500 optically active compounds available in bulk and a list of their suppliers, data on more than 3500 resolutions, and 4200 citations. With an abundance of analyzed examples, this single, authoritative reference provides all of the information necessary to perform, develop, and optimize optical resolutions via diastereomeric salt formation.



http://www.crcpress.com

New Books from the World Health Organization

Water Quality: Guidelines, Standards, and Health-Assessment of Risk and Risk Management for Water-Related Infectious Disease

L. Fewtrell amd J. Bartram (Eds.)
World Health Organization, Geneva, Switzerland, 2001.
(ISBN 92-4-154533-X)

Evaluation of Certain Food Additives and Contaminants: Fifty-Fifth Report of the Joint FAO/WHO Expert Committee on Food Additives

WHO Technical Report Series, No. 901. World Health Organization, Geneva, Switzerland, 2001.
(ISBN 9-241-20901-1)

WHO Model Prescribing Information: Drugs Uses in Bacterial Infections

World Health Organization, Geneva, Switzerland, 2001,
(ISBN 9-241-40107-9)

Current Challenges in Pharmaco-vigilance: Pragmatic Approaches-Report of CIOMS Working Group V

Council for International Organizations of Medical Sciences, Geneva, Switzerland, 2001.
(ISBN 9-290-36074-7)

http://www.who.int/dsa/justpub/justpub.htm

New Books from the American Oil Chemists' Society Press

Proceedings of the World Conference on Oilseed Processing and Utilization

Richard Wilson (Ed.)
American Oil Chemists' Society Press, Champaign, IL, USA, 2001. (ISBN 1-893-99720-0)

Soy Protein Products: Characteristics, Nutritional Aspects, and Utilization (Revised and Expanded)

Joseph G. Endres (Ed.)
American Oil Chemists' Society, Champaign, IL, USA, 2001. (ISBN 1-893-99727-8)

http://www.aocs.org

Reports from Conferences

Medicinal Chemistry

by Ernõ Pungor

A Hungarian-German-Italian-Polish Joint Meeting on Medicinal Chemistry was held in Budapest, Hungary, 2-6 September 2001. The conference was organized by the Organic and Medicinal Chemistry Division of the Hungarian Chemical Society and the Medicinal Chemistry Divisions of the Chemical Societies of Germany, Italy, and Poland, with the contribution of the Medicinal Chemical and Pharmaceutical Technological Committee of the Hungarian Academy of Sciences and the 100-year-old Gedeon Richter Ltd. Prof. Péter Mátyus was the chairman of the meeting, and Dr. János Wölfling was the secretary.

The meeting followed two previous joint meetings held in Taormina, Italy (1999) and Jelenia Góra, Poland (2000). This third meeting was organized by the Organic and Medicinal Chemistry Division of the Hungarian Chemical Society and the Medicinal Chemistry Divisions of the Chemical Societies of Germany, Italy and Poland, with the contribution of the Medicinal Chemistry and Pharmaceutical Technological Committee of Hungarian academy of Sciences and the Gedeon Richter Ltd, and was sponsored by IUPAC.

The medicinal chemistry is very complex. It contains many areas of chemistry, molecular biology, and material sciences as well as computer science. It plays a central role in drug design, discovery and development. This meeting focused in particular on certain challenging fields in current medicinal chemistry, such as CNS, cardiovascular and metabolic diseases, and new methods of drug research. More than 270 registered participants attended the conference (mainly from the four organizing countries, but scientists from more than 20 countries altogether) and 17 plenary lectures, 9 short lectures and 164 posters from academic and industrial areas were presented and this resulted in a high-level scientific program.

The Hungarian-German-Italian-Polish Joint Meeting on Medicinal Chemistry was a successful meeting about the co-operation of these countries. It strengthened the developing of new pharmaceutical products.

Ernõ Pungor is the Chairman of Hungarian National Committee for IUPAC.

http://www.iupac.org/publications/
pac/2001/7309/index.html

Analytical Sciences

by David S. Moore

The International Congress on Analytical Sciences 2001 was held 6-10 August at Waseda University in Tokyo, Japan. It was an extreme honor for me to be able to represent the IUPAC at this wonderfully-organized and executed congress. The congress is organized every ten years and is a huge undertaking—26 symposia, 5 plenary lectures, 281 invited talks, 250 other oral presentations and nearly 450 posters. It is truly international in scope and attendance—with nearly a thousand participants from 39 countries. If that isn't enough, this time the Congress was held jointly with Asianalysis VI—the Sixth Asian Conference on Analytical Sciences—and a Symposium on Traditional Chinese Medicine! Clearly the organizers of ICAS 2001—chaired by Tsuguo Sawada (Univ. of Tokyo), along with his Vice-Chairs: N. Nakamura (Sci. Univ. of Tokyo), Y. Umezawa (Univ. of Tokyo—member of the IUPAC Analytical Chemistry Division Committee), and K. Matsumoto (Waseda Univ.—member of the IUPAC Analytical Chemistry Division Committee) and the other 29 members of the Organizing Committee and 17 members of the International Advisory Board (chaired by H. Akaiwa, Gunma, Japan)—and the organizers of Asianalysis VI—chaired by T. Hobo (Tokyo Metropolitan Univ.) and the other 10 members of the Organizing Committee and 17 members of the International Advisory Board (chaired by B. Huang, Xiamen, China)—had to work together efficiently and smoothly. The excellent conferences they produced provide strong evidence that they more than succeeded in their task.

The symposia at ICAS 2001 covered all the fields of analytical chemistry that it seems possible to think of. From analytical atomic spectrometry and applied laser spectroscopy to nano-technology, separation science, and sensors of all kinds, the symposia and posters painted a broad canvas of the present state of the art in analytical science, and also suggested future directions and dreamed about future capabilities. What else could one want in such a conference? The only problem was selecting which of the many relevant and varied symposia to attend. I found myself wishing cloning was already a reality, or that I had accomplices with whom to share the task!

The International Advisory Board suggested to the ICAS organizers that the field of Analytical Science was developing rapidly enough to warrant thinking about increasing the frequency of this conference from once per decade to twice. The general consensus was that, while this increase would mean a doubling of their work load, the payoff to the international analytical science community would be worth the price. Regardless of their decision, the international analytical science community anxiously awaits the next ICAS, and we at IUPAC hope to be again involved.

The plenary lectures by Drs. A. Manz, S. Terabe, M. Takagi, G. M. Hieftje, and Y. R. Shen as well as two selected invited talks by Drs. E. Yeung and T. Sawada are now published in the October 2001 issue of *Pure and Applied Chemistry*. The Conference editor, Dr. Yoshio Umezawa insured that the papers were like the lectures, well balanced in terms of chemical and physical methods of analysis, and all were seminal.

David S. Moore is President of the IUPAC Analytical Chemistry Division.

http://www.iupac.org/publications/pac/2001/7310/index.html

Conference Announcements

designates IUPAC sponsorship

CAS/IUPAC Conference on Chemical Identifiers and XML for Chemistry

1 July 2002, Columbus, Ohio, USA

This conference will bring together experts to survey current activities in the research and development of chemical substance representations and identifiers, including both nomenclature and computer-based structural descriptions, and of chemical markup language. It will be held 1 July 2002 at the Pfahl Executive Education and Conference Center and The Blackwell Hotel at Ohio State University, Columbus, Ohio, USA.

The conference is designed for researchers and developers working in the areas of chemical identifiers and chemical markup language and chemical information specialists, database producers, and others who have an interest in or utilize chemical substance information.

The conference will cover the following topics:

- From chemical name to structure: finding a needle in the haystack
- Nomenclature practice and post-Postman factors
- The chemical semantic web: a common infrastructure for chemistry
- The vision of a chemical semantic web
- The IUPAC Chemical Identifier
- CAS chemical identifier systems
- Unifying chemical nomenclature standards—the roundabout of names and structures
- Computer-based naming service for very large chemical databases

Contact: Dr. Alan McNaught
Royal Society of Chemistry
RSC Publishing
Thomas Graham House
Science Park, Milton Road
Cambridge, CB4 0WF, UK
Tel.: +44 1223 432119
Fax: +44 1223 420247
E-mail: adm@rsc.org

http://www.iupac.org/symposia/conferences/CIandXML_jul02/index.html

Central European Conference on "Chemistry Towards Biology"

8-12 September 2002, Portoroz, Slovenia

Biology and chemistry represent a large multidisciplinary environment within which biochemists and chemists cooperate on theoretical and practical grounds with a view to gain detailed descriptions of biomolecular systems. This first-time conference, to be held 8-12 September 2002 in Portoroz, Slovenia, has its origins in a long-term cooperation among scientists who met at several joint crystallographic conferences during the seventies and eighties and discussed topics pertaining to inorganic and structural chemistry. The aim of the conference is to provide an opportunity to promote discoveries within this large context that can further aid in the development of new advances in biotechnology and serve in the evaluation and predictions for further studies. Topics will include high-resolution crystallography of macromolecules, advanced spectroscopic methods as well as computational simulations.

Contact: Prof. V. Kaucic, National Institute of Chemistry, Hajdrihova 19, SI-1000, Ljubljana, Slovenia.
Tel.: +386 1 47 60 256
Fax: +386 1 42 59 244
E-mail: kaucic@ki.si

http://www.portoroz2002.ki.si

The Ninth International Conference on Flow Analysis
10-14 February 2003, Geelong, Victoria, Australia

The International Conference on Flow Analysis has been held on a triennial basis since 1979. It is is the premier meeting in the field of flow analysis and draws participants from a wide cross section of disciplines within chemistry. This conference aims to draw together members of the international flow analysis community for the purposes of information exchange in the area of flow analysis (incorporating flow injection analysis, sequential injection analysis, segmented continuous flow analysis, and variants of these techniques). The program includes the theoretical and practical aspects of flow analysis in areas such as environmental, clinical, food and beverage, industrial and biotechnological process monitoring. IUPAC has given its imprimatur to at least the last three of these meetings. The conference will be held 10-14 February 2003 in Geelong, Victoria, Australia.

Contact: Associate Professor Ian McKelvie
School of Chemistry
PO Box 23
Monash University
Victoria, 3800 Australia
Tel.:+61 3 9905 4558
Fax: +61 3 99054196
E-mail: ian.mckelvie@sci.monash.edu.au

http://www.deakin.edu.au/flowanalysis9/

Conference Announcements in Brief

Raw Materials
26-29 May 2002
International Association for Cereal Science and Technology (ICC) Conference 2002, Budapest, Hungary.
Prof. András Salgó
Tel.: +36 1 463 1255
Fax: +36 1 463 3855
E-mail: ICC2002@mail.bme.hu
<http://www.ch.bme.hu/ICC2002>

Antiprotozoal Chemotherapy
23-26 June 2002
5th COST C9 Congress, London, UK
Dr. Simon L Croft
Tel: +44 0 20 7927 2345
Fax: +44 0 20 7323 5687
E-mail: COSTB9Congress@lshtm.ac.uk
<http://www.lshtm.ac.uk/cost/b9congress/>

Stable Isotopes
7-9 July 2002
2nd French Meeting on Stable Isotopes, Nantes, France.
Chantal Iannarelli
Tel.: +33 0 1 47 71 90 04
Fax: +33 0 1 47 71 90 05
E-mail: c2s@club-internet.fr
<www.http://www.congre-scientifiques.com /ISOTOPES/>

Bioorganometallic Chemistry
18-20 July 2002
1st International Symposium on Bioorganometallic Chemistry, Paris, France.
Chantal Iannarelli
Tel.: +33 0 1 47 71 90 04
Fax: +33 0 1 47 71 90 05
E-mail: c2s@club-internet.fr
<http://www.congres-scientifiques.com/ISBOMCO2/>

Organosilicon Chemistry
25-30 August 2002
13th International Symposium on Organosilicon Chemistry, Guanajuanto, Mexico.
Prof. Jorge Cervantes
Tel.: +52 473 7326885, ext. 8111 and 8113
Fax: +52 473 7351903
E-mail: jauregi@quijote.ugto.mx
<http://www.ugto.mx/Eventos/ISOSXIII/index.html>

Luminescence Phenomena
25-30 August 2002
The International Conference on Luminescence and Optical Spectroscopy of Condensed Matter (ICL'02), Jerusalem, Israel.
Prof. Shammai Speiser
Tel.: +972 4 829 3735
Fax: +972 4 823 3735
<http://www.technion.ac.il/technion/chemistry/ICL/>

Food Science
4-6 September 2002
6th International Conference on Applications of Magnetic Resonance in Food Science, Paris, France.
Chantal Iannarelli
Tel.: +33 0 1 47 71 90 04
Fax: +33 0 1 47 71 90 05
E-mail: c2s@club-internet.fr
<http://congres-scientifiques.com/MRFOOD/>

Scientific and Technical Data
29 September-3 October 2002
18th International CODATA Conference on Frontiers of Scientific and Technical Data, Montreal, Canada.
Dr. Gordon Wood
Tel.: +1 613 993 4165
Fax: +1 613 952 8246

E-mail: gordon.wood@nrc.ca
<http://www.codata.org>

Clinical Chemistry
20-25 October 2002
18th International Congress of Clinical Chemistry and Laboratory Medicine (18th ICCC 2002 Kyoto) Kyoto, Japan.
Secretariat of the 18th ICCC 2002 Kyoto
Tel: +81 6 6873 2301
Fax: +81 6 6873 2300
E-mail: iccckyoto@bcasj.or.jp
<http://edpex104.bcasj.or.jp/iccc2002/>

Preserving Data
5-7 November 2002
Ensuring Long-term Preservation and Adding Value to Scientific and Technical Data, Toulouse, France.
Joëlle Guinle
Tel.: +33 0 5 61 27 40 18
Fax: +33 0 5 61 28 29 39
E-mail: joelle.guinle@cnes.fr
<www.http://www.cnes.fr/pvdst/>

High-Temperature Materials
19–23 May 2003
11th International Conference on High Temperature Materials Chemistry, Tokyo, Japan.
Prof. Michio Yamawaki
Tel.: +81 3 5841 7422
Fax: +81 3 5841 8633
E-mail: yamawaki@q.t.u-tokyo.ac.jp
<yamawaki@q.t.u-tokyo.ac.jp>

Plutonium and Other Actinide Elements
6-10 July 2003
Plutonium Futures—The Science 2003, Albuquerque, New Mexico, USA.
Plutonium Futures—The Science
Tel.: +1 505 667-7753
Fax: +1 505 667 6569
E-mail: puconf2003@lanl.gov
<http://www.lanl.gov/pu2003>

Calendar of IUPAC Sponsored Conferences

Visit http://www.iupac.org for complete information and further links

NEW *designates a new conference since the last issue*

2002

Heterocycles
6–8 March 2002
3rd Florida Heterocyclic Conference, Gainesville, Florida, USA.
Prof. Alan R. Katritzky, Department of Chemistry, University of Florida, P.O. Box 11720, Gainesville, Florida 32611, USA
Tel.: +1 352 392 0554
Fax: +1 352 392 9199
E-mail: katritzky@chem.ufl.edu

Macromolecules
25–28 March 2002
5th Annual UNESCO School and South African IUPAC Conference on Macromolecules and Materials Science, Stellenbosch, South Africa.
Prof. R. D. Sanderson, UNESCO Associated Centre for Macromolecules and Materials, Institute for Polymer Science, University of Stellenbosch, Private Bag X1, Matieland 7602, South Africa
Tel.: +27 21 808 3172
Fax: +27 21 808 4967
E-mail: rds@maties.sun.ac.za

p-Electron Systems
30 May–4 June 2002
5th International Symposium on Functional p–Electron Systems (Fπ5), Ulm/Neu-Ulm, Germany.
Prof. Dr. Peter Bäuerle, Abteilung Organische Chemie II, Universität Ulm, Albert-Einstein-Allee 11, 89081 Ulm, Germany
Tel.: +49 731 502 2850
Fax: +49 731 502 2840
E-mail: peter.baeuerle@chemie.uni-ulm.de

Polymer Systems
3–7 June 2002
4th International Symposium on Molecular Order and Mobility in Polymer Systems, St. Petersburg, Russia.
Prof. T. M. Birshtein, Institute of Macromolecular Compounds, Russian Academy of Sciences, Bolshoi pr. 31, St. Petersburg 199004, Russia
Tel.: +7 812 328 85 42
Fax: +7 812 328 68 69
E-mail: birshtein@imc.macro.ru

Nuclear Analytical Methods
16–21 June 2002
7th International Conference on Nuclear Analytical Methods in the Life Sciences, Antalya, Turkey.
Prof. Namik K. Aras, Bahcesehir University, 34900 Istanbul, Turkey
Tel.: +90 212 669 6523
Fax: +90 212 669 4398

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. Constantinos 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

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 06 49912783
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

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, 17 th 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

Flow Analysis
NEW
10-14 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

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

39th IUPAC Congress
10–15 August 2003
39th IUPAC Congress and 86th Conference of The Canadian Society for Chemistry: Chemistry at the Interfaces, Ottawa, Ontario, Canada.
National Research Council Canada (NRC), Conference Services Office, Building M-19, Montreal Road, Ottawa, Ontario, Canada K1A 0R6
Tel.: +1 613 993 0414
Fax: +1 613 993 7250
E-mail: iupac2003@nrc.ca

How to Apply for IUPAC Sponsorship
To apply for IUPAC sponsorship, conference organizers should complete an Advance Information Questionnaire (AIQ). The AIQ form is available at http://www.iupac.org or by request at the IUPAC Secretariat, and should be returned between 2 years and 12 months before the conference. Further information on granting sponsorship is included in the AIQ and available online.

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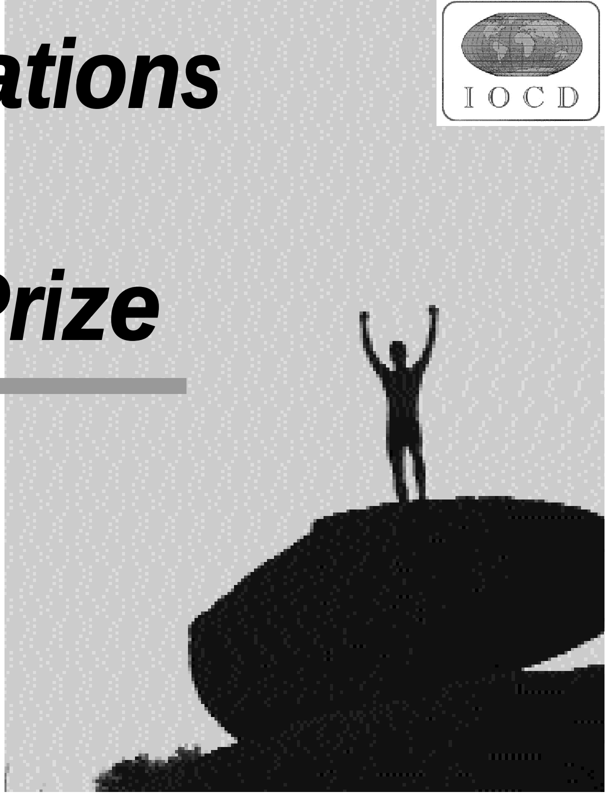
It is a condition of sponsorship that organizers of meetings under the auspices of IUPAC, in considering the locations of such meetings, should take all possible steps to ensure the freedom of all bona fide chemists from throughout the world to attend irrespective of race, religion, or political philosophy.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

Call for Nominations for the Pierre Crabbé-IOCD Prize



Submission Deadline
31 March 2002

The International Organization for Chemical Sciences in Development (IOCD), on the occasion of its 20th anniversary, is pleased to announce the initiation of the Pierre Crabbé-IOCD Prize. Pierre Crabbé was a distinguished Belgian scientist who conceived and, in 1981, founded IOCD as an international organization for helping scientists in developing countries. He served as its director until his untimely death in 1987. IOCD has continued to pursue its mission of collaborating with scientists in developing countries in major ways.

The Pierre Crabbé-IOCD Prize will be awarded in 2002 to the person who the Prize Committee finds has made the most significant contribution during the past two years to the encouragement of better science and education in a developing country. The Prize will consist of a medal and a $10,000 (USD) cash award.

You may nominate one or more candidates for the Pierre Crabbé-IOCD Prize. The nominee may be from any country, with special attention being given to those from developing countries.

Your nomination, not longer than one typed page, should consist of the following:

1. a short description (no more than 150 words) of the work of the candidate that supports the nomination;
2. a curriculum vitae of no more than 10 lines in length;
3. a statement of the impact of the work.

Nominations should be submitted no later than 31 March 2002 to:

Executive Director, IOCD
P.O. Box 8156
Falls Church, Virginia 22041 USA

For more information about IOCD, please e-mail: iocd@igc.org or look on the Web at <http://www.iocd.org>.

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The International Union of Pure and Applied Chemistry (IUPAC), formed in 1919, is a voluntary non-governmental, nonprofit association of organizations, each of which represents the chemists of a member country. Its objectives are as follows:

- to promote continuing cooperation among the chemists of the member countries
- to study topics of international importance to pure and applied chemistry which need standardization or codification
- to cooperate with other international organizations that deal with topics of a chemical nature
- to contribute to the advancement and understanding of pure and applied chemistry in all its aspects

The membership of IUPAC currently comprises 44 national organizations.

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Union of Yugoslav Chemical Societies **(Yugoslavia)**

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