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Who Doesn't Like Quotes?

Not one day passes by without receiving a friendly e-mail that ends with a quote, and I like that. It is a simple statement that says a lot about the sender. When one communicates in person, that statement is in our speech, our appearance, but when we quickly write a memo/e-mail, a quote at the end can simply be a "nice touch."

"Facts do not cease to exist because they are ignored," (Aldous Huxley) is one of my favorites. I have kept this within sight for many years, and find it relevant in my work everyday. It gives me the will to question what I do not understand.

In his recent special topic article published in *Pure and Applied Chemistry* and featured in this issue, Professor Paul Erhardt reminds us of a saying of mathematician David Hilbert that dates from 1900: "Who of us would not be glad to lift the veil behind which the future lies hidden; to cast a glance at the next advances of our science and at the secrets of its development during future centuries?" With these words providing a preview, Professor Erhardt gives us a glance into the future of medicinal chemistry. This exciting field, which is continuously redefining itself, is presented here with critical insight that highlights new and emerging concepts. "Cast a glance" and read more on page 4.

Fabienne Meyers <fabienne@iupac.org>

Treasurer's Column

Balancing Sources and Uses

As in the past (see *CI*, September 2001), I would like to discuss the financial situation of the Union and make some comments on the role of the Union's finances in furthering its activities. The financial situation of the Union is good, our reserves are strong, and we have suffered minimally from the recent decline in the stock market due to the conservative approach taken by the Finance Committee in managing our investments. This allows us to continue to do the work for which the Union exists. The management of our finances is part of the strategic planning of the Union, matching our resources to our needs. If our activities are focused on the strategic goals, I believe the recognition of the value of IUPAC will increase substantially.

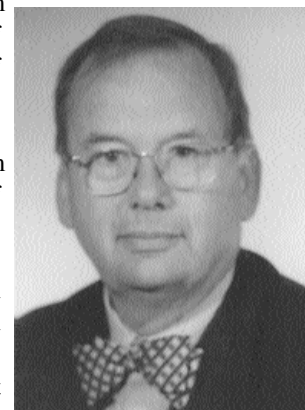
What is the Current Financial Position of IUPAC?

A complete review of our financial position as well as the audited statement for 2001 can be found on the IUPAC Web site at www.iupac.org/news/archives/2002/treasurer-01.html.

Who Provides the Funds?—Sources

The financial resources of the Union come from three major sources: National Subscriptions paid by the National Adhering Organizations; income from publications, mainly *Pure and Applied Chemistry*; and investment income. The Finance Committee manages the reserves of the Union to preserve capital, not to maximize income. The main purpose of the Reserve Fund is to cushion the effect of changes in revenue or expenses from biennium to biennium. The Committee on Printed

and Electronic Publications oversees the publication activities of the Union and is faced with maintaining the income to the Union from publications in the face of the declining number of subscribers to our journal, *Pure and Applied Chemistry*. This is a problem faced by all publishers of scientific journals.

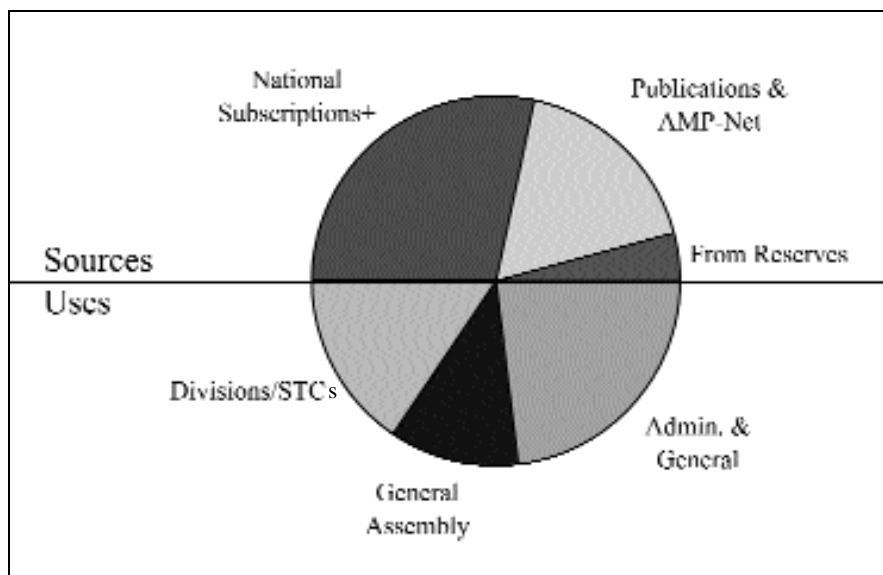


Christoph F. Buxtorf
IUPAC Treasurer

The pie chart shows the sources of the funds used by IUPAC on the top and the uses of the funds on the bottom. IUPAC spent more than it received in revenue in the biennium 2000–2001 and therefore used reserves to meet its needs. The wedge labeled National Subscriptions includes all income other than that from publications or reserves, but is almost entirely from National Subscriptions. The wedge labeled Publications and AMP (Affiliate Membership Program) is the net of income from the sale of the Union's journal, books, and magazine and that from the AMP, less the expenses associated with those activities. This item is almost entirely income from subscriptions to our journal, *Pure and Applied Chemistry*.

Where Does the Money Go?—Uses

The Union's expenses can be put into three broad categories. The first is the allocation to Divisions and Standing Committees (STCs), including the Project Committee. The second is the cost of the General Assembly. The third is the cost of the support services provided by the Secretariat and the cost of other items such as the IUPAC Prize, ICSU dues, and support of conferences in developing countries. The support services of the Secretariat include management of the project system, disbursing funds, program support to the Divisions, and maintenance of the Web site. During the current and future biennia, the cost of the General Assembly will be much small-



Sources and uses of IUPAC funds, 2000-2001 biennium.

er, with those funds being diverted to the first sector in support of projects.

The level of National Subscriptions is set by the IUPAC Council and is influenced both by a desire to fund the necessary work of the Union and the difficulty some National Adhering Organizations have in paying their National Subscriptions, especially the smaller, less affluent NAOs. However, a number of the larger countries also have difficulty in funding their National Subscriptions. This concern led to the formation of a Working Party on National Subscriptions by the Council at Brisbane.

From discussions at Brisbane and in the meeting of the Working Party, it appeared that in addition to the financial impact, other issues were buried in the problems around National Subscriptions. The Working Party started their activities very quickly and closed with a meeting in February 2002, making several proposals to the Executive Committee and further to the Bureau. These will be discussed by the Bureau and recommendations made at the next Council meeting, Ottawa 2003. I have greatly appreciated the fine cooperation and open discussions of the Working Party.

What Are the Challenges Ahead?

The future of IUPAC is dependent on our financial resources. The problems as outlined above show that there are some clouds ahead and we must make special efforts to assure our funding. We have heard some critical comments by different groups—in and outside of IUPAC.

We take those seriously and will keep an open dialog. One issue that became clear in our discussions is the

lack of recognition of our work in the view of some of our partners and customers, NAOs, the chemical industry, and governments. In most countries, government and industry pay the National Subscription. It is extremely important that our customers perceive the value of IUPAC's work.

It is extremely important that our customers perceive the value of IUPAC's work.

Please actively convince IUPAC "Partners and Customers" in your country and in your industry that IUPAC's contribution to "Advancing Worldwide Chemistry" is to the benefit of Mankind. When this message is appreciated, financial support for IUPAC will follow. Only on a strong income base can we provide activities that are in line with the IUPAC strategic plan.

The work of the treasurer was only possible with the great help of the executive director and the Finance Committee. We are always open to good thoughts and inputs.

Dr. Christoph F. Buxtorf is the current treasurer of IUPAC. He is retired from Novartis Crop Protection where he was head of the Production and Technology Division and a member of the Executive Committee.

Advancing Worldwide Chemistry IUPAC Biennial Report, 2000-2001

This report, organized by the goals of the IUPAC Strategic Plan, summarizes the many accomplishments of IUPAC's members working as part of Task Groups, Committees, and Commissions in the last biennium, 2000-2001.

All of those who contributed to the work of IUPAC over the past biennium can feel proud of their accomplishments as described in this report. Please accept my thanks and those of the Officers for your contributions to this record of accomplishment.

I would like to encourage those of you who are not currently active in IUPAC to use this report as a source of ideas for new projects. The work described in the report demonstrates what an IUPAC project is and where there is room for further work.

A complimentary copy of this report is enclosed with this issue of *Chemistry International*. It is also available on the IUPAC Web site, and if extra copies are needed, please send your request to the IUPAC Secretariat at <secretariat@iupac.org>.

John W. Jost
IUPAC Executive Director

 www.iupac.org/news/archives/2002/report.html

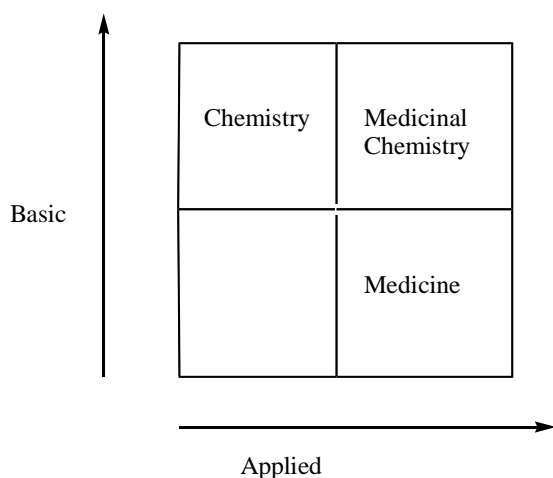
Medicinal Chemistry in the New Millennium

The entry into a new millennium has been accompanied by unrelenting growth in the rate of scientific discovery, and this is no better exemplified than in the field of medicinal chemistry. This subject has flourished under the influence of major advances in the component disciplines that make it distinctive, but continues to be confronted by new opportunities to explore and refine the predictive potential of drug design in response to the quest for greater selectivity and subtlety to meet new challenges to human health. A special topic article in *Pure and Applied Chemistry* appears in this context very timely. The author, Paul W. Erhardt, has undertaken the mammoth task of addressing this complex and rapidly evolving field of endeavor, and offers his distinctive interpretation and vision of challenges and opportunities. The following has been extracted from the article abstract and introduction that appeared in *Pure and Applied Chemistry*, Vol. 74, No. 5, pp. 703-785 (2002).

A Glance Into the Future

by Paul W. Erhardt

The future of medicinal chemistry as both a pure and an applied science has been considered relative to trends that are already having a significant impact upon drug discovery and development. Such trends include pursuing therapeutic efficacy, addressing 3-D structure within database settings, assuring absorption, directing distribution, controlling metabolism, optimizing elimination, and avoiding toxicity. As the exploration of these topics proceeds by deploying combinatorial chemistry coupled to high-throughput screening, medicinal chemistry will play a key role in interpreting the underlying structure-activity relationships. This will cause the overall process of drug discovery and development to be knowledge generating. As fundamental knowledge accumulates across all of these areas, virtual approach-

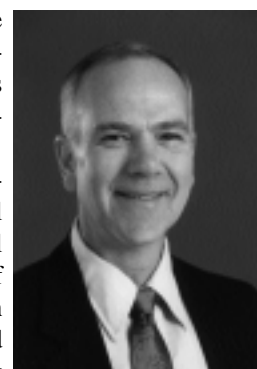


Non-linear Relationship of Medicinal Chemistry to Basic and Applied Research. Adapted from a figure provided by F.A. Cotton (*Chem. Eng. News* Dec. 4, p. 5, 2000) as part of his summary and commentary about a book entitled "Pasteur's Quadrant" (D.E. Stokes, Brooking Press, Washington, DC, 1997).

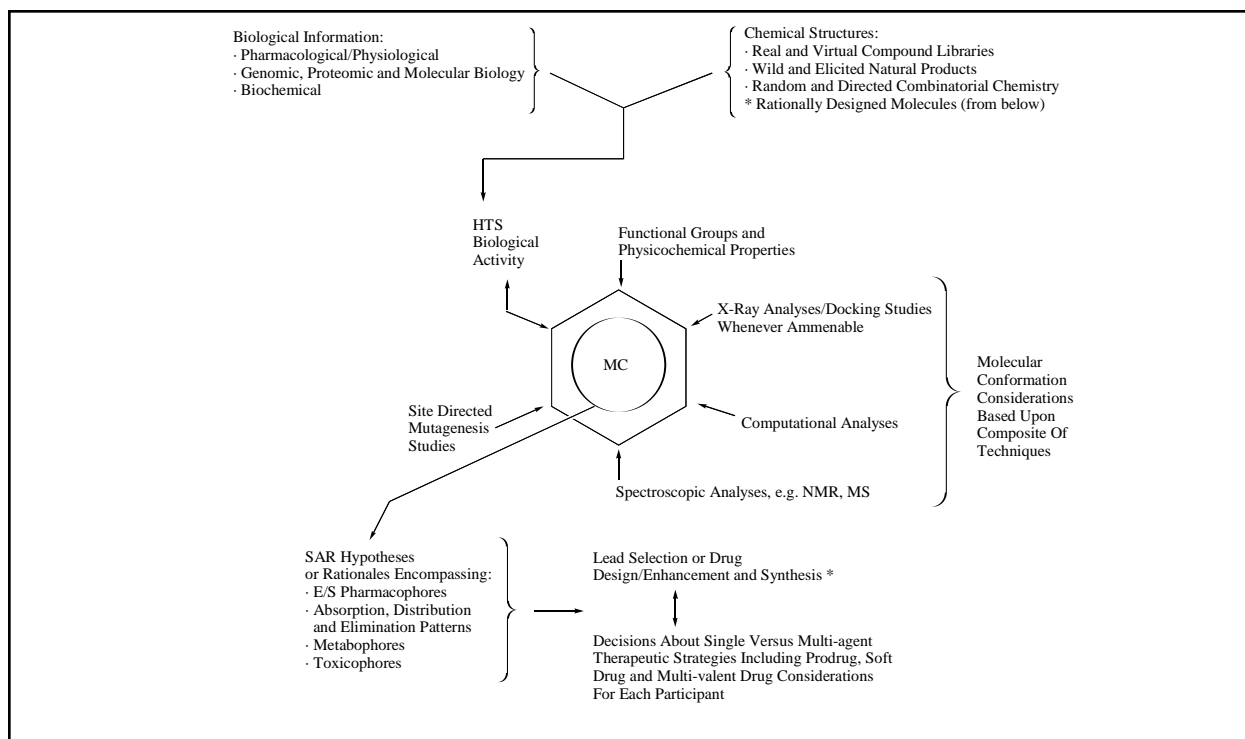
es will eventually become firmly anchored to experimental and theoretical databases having validated clinical predictability.

Given the highly interdisciplinary nature of medicinal chemistry and its potential applications across a myriad of future life-science research activities, the review presented in *Pure and Applied Chemistry* is necessarily limited only to those possibilities that stand out upon taking a broad purview of the field's most prominent trends. From this vantage point, however, at least a glance is cast toward some of the more exciting opportunities for the future of medicinal chemistry. The document includes nine sections. Each section's overview presented below lists what topics are and are not covered and indicates the reasoning behind these choices. It also describes the consistent tone that was sought while attempting to elucidate the numerous technologies that necessarily become encompassed by the variously highlighted activities.

While initially contemplating how medicinal chemistry might continue to evolve as both a basic and applied science, it became apparent that it would be useful to first consider where medicinal chemistry has been and how it has come to be what it is today. Thus, toward quickly establishing a context from which the future might be better appreciated, and perhaps even seen to already be repeating itself amongst a new set of players and technologies. **Section 2—Practice of Medicinal Chemistry** provides a short discourse about medicinal chemistry's emergence as a formalized discipline, its early developments, and its present status by considering how medicinal chemistry has been practiced across jumps of about 25-year increments. This section does



Paul W. Erhardt



Practice of Medicinal Chemistry (MC) in the New Millennium

(reproduced from **Section 3—Evolving Drug Discovery and Development Process**)

The most striking differences from the long-standing practice of MC are: (i) Data reduction of huge amounts of rapidly derived high-throughput screening (HTS) biological results; (ii) Greater emphasis upon multi-technique chemical structure considerations; and most importantly, (iii) The simultaneous attention given to all of the ADMET-related parameters along with efficacy and efficacy-related selectivity during lead compound selection and further design or enhancement coupled with an expanding knowledge base that offers the possibility for achieving synergistic benefits by taking advantage of various combinations of multi-agent, prodrug, soft drug and/or multi-valent drug strategies.

not include a chronological list of medicinal chemistry's many contributions, nor does it highlight the many accomplishments of its noted investigators. Both of the latter can be found elsewhere as part of more traditional, historical treatments.

Medicinal chemistry's near and longer-term futures are considered in **Section 3—Evolving Drug Discovery and Development Process** relative to several of today's trends that are already having a major impact upon the drug discovery process. A working definition for medicinal chemistry is recited at the opening of this section so that medicinal chemistry's immediate and future roles can be more clearly ascertained. Section 3 also sets the stage to later consider where several drug development topics may be headed in the near and longer term.

Discussions about gene therapy, vaccines, and biotech-derived therapeutic agents have not been included in **Section 4—Pursuing Efficacy**, which addresses medicinal chemistry's continued pursuit of efficacy. The aforementioned topics primarily reside within the domains of other disciplines. Readers are encouraged, however, to consult other reviews offered for these areas in order to appreciate how their advances are sure to have a dramatic impact upon future life-science research and its interface with medicinal chemistry. Alternatively, because assessing molecular conformation is such an

integral part of practicing medicinal chemistry, several aspects of this key topic are considered within **Section 5—Assessing and Handling Molecular Conformation**. In particular, the handling of chemical structures within database settings (e.g., chemoinformatics) is discussed in detail.

Several drug development topics are regarded as critical factors that will have a pivotal influence upon medicinal chemistry's continuing evolution in the future. Each of these topics is briefly addressed within **Section 6—ADMET Considerations**. These key topics include assuring absorption; directing distribution; controlling metabolism; assisting elimination; and, avoiding toxicity (i.e., the traditional absorption, distribution, metabolism, elimination, and toxicity [ADMET] studies that previously have been undertaken by pharmaceutical companies during the secondary stages of preclinical drug development). As an important extension of the ADMET discussions, nutraceuticals considered in parallel with pharmacological synergy are also addressed in this section.

Issues pertaining to medicinal chemistry's future roles in pharmaceutical intellectual property (IP) and to trends associated with process chemistry, are raised within **Section 7—Process Chemistry Considerations**. With today's highly publicized emphasis upon

genomics and proteomics, at least an abbreviated discourse about process chemistry is included so that this fundamental aspect of medicinal chemistry's link with synthetic chemistry remains appreciated. Thus, the unmet need for large-scale, stereoselective synthetic methodologies is briefly discussed.

As fundamental knowledge accumulates across all of these areas, virtual approaches will eventually become firmly anchored to experimental and theoretical databases having validated clinical predictability.

While it is beyond the scope of this review to discuss the impact that progress in each of several analytical methods is likely to have upon medicinal chemistry, X-ray diffraction has been selected to provide a representative discussion within **Section 8—Analytical Chemistry/X-ray Diffraction**. As is often acknowledged by researchers from various disciplines, "science moves forward according to what it can measure." Presently, there appear to be numerous promising advances among various analytical techniques that can be used to study drug-receptor interactions. For example, readers are encouraged to seek other reviews in order to appreciate the potential impact that anticipated developments in nuclear magnetic resonance (NMR inclusive of LC-NMR and high-flowthrough techniques), mass spectrometry (MS inclusive of LC-MS and LC-MS/MS), microcalorimetry, and surface plasmon resonance may have upon medicinal chemistry.

Section 9—Summary serves as an overall summary for the document. In addition it discusses some areas for concern, including training of medicinal chemists, inventorship, and the interplay of patent trends and future research within the context of IP.

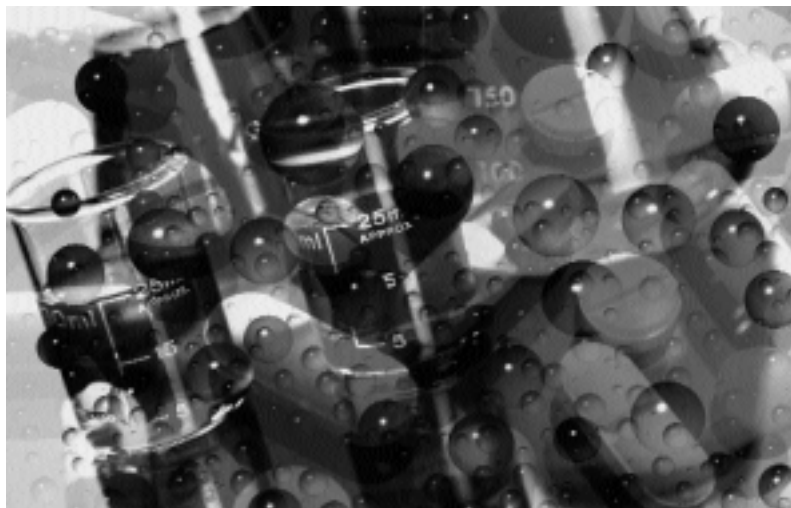
The document's running dialogue has been developed from future possibilities suggested by the current medicinal chemistry and drug discovery literature, as well as from general observations afforded while consulting with both the private and public sectors. Descriptions of specific research projects have been interspersed throughout so that real case examples, along with their chemical structures, could be explicitly conveyed. A concerted effort has been made to keep

hype to a minimum. Alternatively, jargon has been used whenever it was thought that such terms portray the mind-sets that were important for a given period, or because a particular term or phrase appears to be taking on an enduring significance. Some of the more technical of these terms are listed in a table in **Section 1—Introduction**, along with a short definition in each case. Since several acronyms have been used for repeating phrases, an alphabetical listing of all acronyms and their definitions is provided to assist readers as they move deeper into the document.

The potential impact of some of the recent trends in process chemistry, and in analytical chemistry using X-ray diffraction as an exemplary method, are additionally highlighted before reiterating the article's major points in Section 9. From this purview, the summary also considers the education of future medicinal chemists, notes potential issues related to the future of pharmaceutical-related IP, and concludes by alluding to a brewing paradox between enhanced knowledge and enhanced molecular diversity relative to the future discovery of new drugs.

Numerous references to secondary scientific/primary news journals have been cited because these journals are doing an excellent job of both reporting the most recent trends and forecasting the potential future. In several cases, a single citation has been used to list many of the informational Web sites that can often be found for a given topic.

Topics are considered into the future only for about 75 years, with the first 25 being regarded as near term, and the next 50 being regarded as long term. The speculation that has necessarily been interjected throughout the review was done with the thought that one of the goals for this type of article is to prompt the broadest contemplation possible about the future directions that medicinal chemistry might take. Finally, the review considers medicinal chemistry as both a distinct, pure science discipline and, equally important, as a key interdisciplinary, applied-science collaborator seeking to mingle with what should certainly prove to be an



extremely dynamic and exciting environment within the life sciences arena of the new millennium.

About the Author

Dr. Paul W. Erhardt received a Ph.D. in medicinal chemistry from the University of Minnesota in 1974 and undertook postdoctoral studies in the area of bioanalytical chemistry and drug metabolism at the University of Texas at Austin. His early career involved bench-level research as a synthetic medicinal chemist within the pharmaceutical industry. He was with American Critical Care in Chicago for about 10 years as a research scientist, senior research scientist, and as a group leader. During this period he was directly responsible for the chemical design, synthesis and entire chemical-related pre-clinical/Phase I development of esmolol, a drug presently marketed as Brevibloc.® He then joined Berlex Laboratories in New Jersey as a Section Head where over the course of 10 years he became the assistant director of medicinal chemistry in charge of drug discovery and, finally, the assistant director across all pharmaceutical research and development activities. When the research operation of Berlex was merged with the biotechnology operations of two new corporate purchases located on the West coast, he became the medicinal chemist representative on a key task force that evaluated external technologies for the purpose of maintaining the company's drug development pipeline. During this period he became a Certified U.S. Patent Agent in order to better deal with

the patent issues that often accompany external technology and its in-licensing. He also led the development of a unified technology 'beschluss' (decision making) document which harmonized the optimal use of R&D resources across the Berlex/SAG corporate triad (Europe, U.S., and Japan) relative to the progression of all internal and in-licensed technologies from concept to market. With a lingering desire to be closer to the day-to-day experimental practice of bench-level medicinal chemistry, he returned to academia about seven years ago when he joined the University of Toledo College of Pharmacy as a tenured professor and director of the Center for Drug Design and Development. During this latest period he was awarded the College's Outstanding Faculty Award, and has stepped-in for one year as an acting assistant dean so as to directly participate in the College's formal academic accreditation process. Erhardt has also become active in IUPAC where he has edited a book about using drug metabolism considerations during drug design and development and where he has recently been voted president elect for the IUPAC Division of Chemistry and Human Health. His present research focuses on medicinal chemistry considerations pertaining to oncology, soft drug technologies, ADMET-related SAR and synergy, and chiral auxiliary synthetic reagents amenable to drug-related process chemistry.



www.iupac.org/publications/pac/2002/7405/7405x0703.html

The Special Topics Project

by James Bull

The Special Topics project aims to broaden the scope of *Pure and Applied Chemistry* coverage through publication of reviews on new and emerging concepts in chemical sciences. The project takes the form of journal issues devoted entirely to specific topics arising from IUPAC initiatives, as well as feature articles that highlight the state of the art and future prospects in topical subdisciplines of the subject. The latter feature offers scope for individuals to present authoritative and critical reviews in a way that will inspire and challenge the readership, and even attract debate. Although feature articles have not hitherto enjoyed sufficient support to ensure their regular appearance in *Pure and Applied Chemistry*, as the Special Topics editor, I welcome inquiries and expressions of interest in the belief that such articles offer a highly visible forum through which to publicize and popularize the rapidly evolving face of chemistry and to identify IUPAC more closely with themes of growing international importance.

A Reminder and Invitation

Feature articles in *Pure and Applied Chemistry* can comprise the publishable output of any legitimate activity of IUPAC, and reflect any aspect of current and future directed chemical sciences. In reality, this merely extends the scope of current publication policy, from the traditional, reactive role, to a more flexible and dynamic approach, in which IUPAC members and interest groups can propose and undertake projects leading to publication of feature articles. A proposal for a special issue should first be submitted to me, outlining the intended scope and coverage of a theme, together with a draft proposal on prospective authorship, and a target date for submission of the manuscript. Following assessment and approval of the concept, a procedure will be set up for submission and evaluation of the manuscript and the author(s) will be assured that the manuscript will be processed and published expeditiously.

James R. Bull <bull@science.uct.ac.za> is a professor at the University of Cape Town in South Africa. He has been IUPAC Special Topics editor since 1999.

Medicinal Chemistry in IUPAC

Accomplishments During the Past Decade and Relationships With Industry

by *Robin Ganellin*

Medicinal chemistry is a key discipline vitally important to the pharmaceutical industry. Medicinal chemists are involved in new drug discovery and solving the problem of designing molecules to optimize their biological properties. In the past decade the Medicinal Chemistry Section of IUPAC has been very active, meeting twice yearly and providing a forum for the exchange of knowledge and views among medicinal chemists from different countries who are in academia and the pharmaceutical industry. This cross fertilization of ideas has been stimulating and invaluable to the chemists involved and has without doubt benefited the wider community of medicinal chemists. For the industrially advanced countries these meetings have provided useful information sources and improved understanding of the subject. For the less industrialized countries they have helped further the establishment of medicinal chemistry in their respective societies.



Robin Ganellin

The tangible output of the Medicinal Chemistry Section is seen in the publication of books and articles, the organization of international meetings and educational schools, the presentation of lectures, and in the formation of the Asian Federation of Medicinal Chemistry (AFMC), as detailed below.

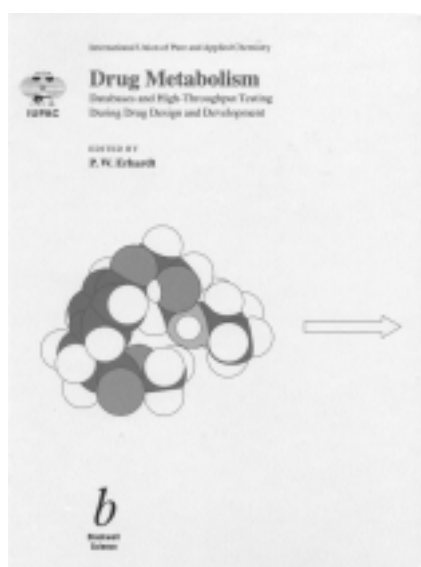
Books

Three important books have been published by the Medicinal Chemistry Section. *Medicinal Chemistry for the 21st Century*,¹ published in 1992, forms part of the IUPAC series "Chemistry for the 21st Century Monographs" and contains 24 chapters by eminent scientists from industry and academia. It is organized into four parts: new lead discovery, protein structure-function relationships, pharmacophore studies, and bioavail-

ability manipulations. It contains many thought-provoking suggestions about the future of drug discovery.

More recently, *Drug Metabolism: Databases and High Throughput Testing During Drug Design and Development* was published.² It deals with the issue of predicting the likely metabolic transformations of candidate drugs, a critical problem for pharmaceutical companies engaged in the development of new medicines. Knowledge of likely metabolism is valuable for prediction of the likely half-life of drug duration and for assessing potential side effects that may have adverse toxicological consequences. What then is predictable from structure-mechanism relationships? Past experience has not been well publicized so that databases of compilations of experimental information or predictive modelling would be very useful. Current models are, however, of limited applicability and this book identifies their potential uses and limitations. The book describes how a joint project with the International Union of Pharmacology, IUPHAR, is being conducted that aims to establish a human metabolism database that can be accessed around the world for specific applications that directly affect human welfare. The availability of such a searchable database would be potentially very valuable in the design and development of new therapeutic substances. The book also provides some case studies by various practitioners from the pharmaceutical industry.

The Section has also scored a real hit by producing this year the *IUPAC Handbook of Pharmaceutically Acceptable Salts*.³ Because many drug substances are acids or bases it is convenient to convert them into salts to improve stability and increase water solubility. Of course the counter ion must be suitable and non-toxic



and must not interfere with the desired biological action of the drug. This aspect of drug presentation is of fundamental importance for drug development and yet there is very little helpful literature for guidance. Preparation of the optimal pharmaceutically acceptable salt form of a new drug substance is a problem frequently faced by medicinal chemists who could greatly benefit from a convenient, comprehensive, and authoritative source of information concerning the full range of possibilities including the more unusual salts. This book reviews the literature and generates a critical compilation of information in this subject area. It is definitive and will doubtless be the source book for the future.

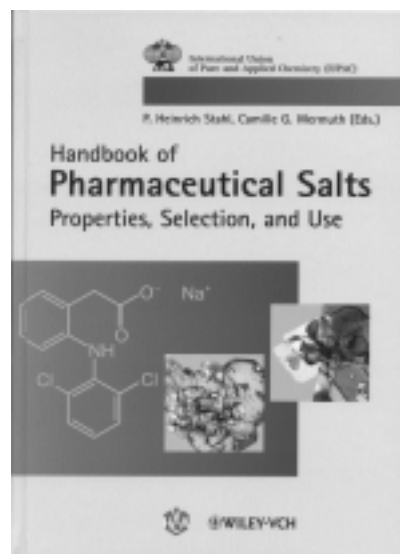
Glossaries

A "Glossary of Terms Used in Medicinal Chemistry" was compiled with the aim of providing concise definitions to those for whom the usage and meaning may not always be clear.^{4a} This is probably especially helpful to chemists whose native language is not English. The glossary was published in the *Annual Report on Medicinal Chemistry*,^{4b} which is distributed by the American Chemical Society to over 10 000 medicinal chemists, and also made available on the Web.^{4c}

Computational drug design is a continuously developing field which is now a very important component in the discipline of medicinal chemistry. At the same time, many medicinal chemists lack significant formal training in the field and may not have a clear understanding of the terminology used. Furthermore, there is the possibility that in different countries certain terms may not have the same meaning, a fact that gives added value to the establishment of a standard international definition. This led to production and publication of a "Glossary of Terms Used in Computational Drug Design."⁵

Combinatorial chemistry—involving the rapid synthetic assembly of structural building blocks in various possible combinations to produce large libraries of compounds for drug screening purposes—is a rapidly expanding field of medicinal chemistry. It is also generating a new vocabulary to describe the various operations and components. To assist medicinal chemists in their understanding of this field and to help with the acceptance of a universally understood language, a "Glossary of Combinatorial Chemistry Terms"⁶ was published in *Pure and Applied Chemistry* and subsequently, in the *Journal of Combinatorial Chemistry*. This ensures its use within the American Chemical Society as a standard glossary of terms. Further work is focused on producing an opinion document on the legal implications of patenting virtual libraries. This is a very important issue which has profound implications for research and development in the pharmaceutical industry.

Other glossaries of terms are being prepared, including a Glossary of Drug Metabolism Terms, Glossary of Terms in Pharmaceutical Process Chemistry, and Glossary of Terms in Pharmaceutical Technology.



A recent project has been approved to publish as a book, a compilation of the glossaries pertinent to chemistry and drug development that have been published in *Pure and Applied Chemistry* during the past decade, i.e., since 1992. See the Web site at <www.iupac.org/projects/2002/2002-001-1-700.html>.

Training of Medicinal Chemists

Medicinal chemists are critical in the design, discovery, and synthesis of new chemical entities in the pharmaceutical industry. Without them there would be no successful research for new medicines. The path for chemists to become medicinal chemists is, however, often indirect and training is commonly "on the job." As a contribution to the discussion about suitable formal training, the Medicinal Chemistry Section has published between 1993 and 2001 a series of papers on this subject.⁷⁻¹³ The series is based on the information received in answers to questionnaires sent to leading pharmaceutical research companies and universities that teach medicinal chemistry in Europe, Japan, and the USA. The results have also been presented at international symposia in the Netherlands (1993), Italy (1994), and Egypt (1998). A syllabus for a short course on medicinal chemistry has also been published,¹⁴ and courses have been initiated in some Latin American countries.

Guidelines for Natural Product Collaborations

Scientists in many countries throughout the world are interested in collaborating with companies for the study and evaluation of natural products as potential sources or leads to new medicinal agents. At the same time, there is concern—particularly from scientists in developing countries who typically have had little experience in this field—regarding how to proceed in such matters and how to handle related intellectual property issues. The collaboration between pharmaceutical research companies in the developed countries and natural products scientists in developing countries is often hindered

by suspicion on the part of the latter that they are not being treated fairly. This can lead to protracted negotiations, which may well founder because of the lack of understanding among all concerned parties. To facilitate such collaborations, the Medicinal Chemistry Section prepared a document of guidelines, which was published in 1996 as IUPAC Recommendations entitled "Preservation and utilization of natural biodiversity in context of the search for economically valuable medicinal biota."¹⁵ This article is independent from the Manila Declaration and Melaka Accord and describes general topics and potential issues to be considered in a collaboration on natural products. The Section also produced two other documents on the subject: a technical report¹⁶ intended to help with drawing up contracts and an article titled "Medicinal Chemistry in the Development of Societies."¹⁷

Formation of the Asian Federation of Medicinal Chemistry

Under the leadership of Dr. Naofumi Koga, the Section facilitated the formation of the Asian Federation of Medicinal Chemistry (AFMC). An inaugural meeting was held at the Pharmaceutical Society of Japan's Nagai Memorial Hall on 11 May 1992. The members include nine societies from four countries: Australia (1), China (2), Japan (4) and Korea (2). The AFMC has been very active in sponsoring symposia between countries (e.g., The Fourth Korea-Japan Joint Symposium on Drug Design and Development, April 1994 in Tokushima, Japan and The First Australia-Japan Symposium on Drug Design and Development, May 1994, Coolum, Australia). The first AFMC Symposium on Medicinal Chemistry was held in Tokyo, September 1995 (AIMECS 95); subsequent meetings have been held in Seoul, Korea (1997), Beijing, China (1999), and Brisbane, Australia (2001). The next meetings will be in Kyoto in 2003 (AIMECS 03). The proceedings of the first meeting were published in a book.¹⁸

Future Representation of Medicinal Chemistry in IUPAC

With the restructuring of the divisions in IUPAC, the Medicinal Chemistry Section was combined in 1996 with the Division of Clinical Chemistry to form Division VII, Chemistry and Human Health. The medicinal chemistry interest is now represented by a Subcommittee on Drug Discovery and Development. It is anticipated that it will continue to support the activities of medicinal chemists in the future and contribute to the technical success of the pharmaceutical industry. New members to the subcommittee are always welcome.

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www.iupac.org/divisions/VII

Candid Chemistry

by István Hargittai

Interviews with eminent scientists often provide for excellent oral history, a more engaging way to learn about science. As science has become increasingly impersonal, interviews allow readers to become personally acquainted with great scientists. Also, they provide a forum for these scientists to profess their opinions on various issues. Current chemical literature is often so terse and journal space is at such a premium that it is often impossible for authors to describe their unsuccessful attempts on the way to their discoveries. However, in an unhurried conversation, scientists are willing to reminisce about their failures as well as their successes. With this article, I want to share some of the experiences that I have gathered while conducting interviews.

There is a plethora of questions that one may ask of great scientists. In addition to asking them about their family background, education, and their most important achievements in science, many other questions, such as the following come up: What turned them to science? What was the determining factor in their success? Did they recognize the importance of their discovery right away? Was it easy to publish their groundbreaking findings? And so on. I have found most scientists communicative with a few exceptions. In most cases, once we immerse ourselves into the conversation, I have to ask few questions to get a lot of information. In some other cases, a little prodding is needed. These are in-depth interviews, sometimes going on for hours.

A scientist is willing to reveal more about his inner self to an understanding colleague than to an aggressive investigating reporter.

My technique of interviewing is the following. I contact the scientist informing him (or her) that I will be in his neighborhood because of a conference or some other reason and would like to record a conversation with him. If we can arrange a meeting, we record a conversation. I live in Budapest, so this is almost always connected with a trip. Before the interview, I try to do as much homework as possible in my preparation for the interview. Usually, the more I know in advance, the more new information I can get during the encounter. However, for the sake of my future readers, I must try not to boast about my knowledge. To me the best interviewer is almost invisible. I would like to stress that no two interviews and no two sets of questions are ever the same. There are exceptional cases, when there is no possibility for any preparation.

In 1994, while I was attending an American Chemical Society meeting in Anaheim, California, I came across Glenn Seaborg, who was taking a leisurely walk alone. I introduced myself and asked him for an interview. The only available time was right then. Fortunately, my camera and miniature Dictaphone were with me, so we found a relatively quiet corner and recorded a conversation. The interview was brief but good, thanks to his gracious, cooperative nature. I later followed up with some additional questions in writing. I was lucky to have interviewed Seaborg when I did, because there was no other opportunity for me to meet with him before he passed away a few years later.

Upon my return home I prepare the transcript of the conversation, edit it slightly, and send the material to the interviewee for checking and changing. We repeat this process until the interviewee feels comfortable with the text. I consider the original recording merely a framework for the interview, which takes its final shape at a more leisurely pace. It may be argued that by doing so, some of the original spontaneity is lost. Also, when I feel during the conversation that a topic seems uncomfortable for the interviewee, I rather drop it than try to force getting more information. My experience is that it would not work anyway. A scientist is willing to reveal



István Hargittai (left) with Nobel Prize Laureates Arthur Kornberg (‘59 Physiology and Medicine) and James Watson (‘62 Physiology and Medicine)

more about his inner self to an understanding colleague than to an aggressive investigating reporter. A famous American chemist wrote me after I had sent him the edited transcript of our conversation that, having read several of my previous interviews, he had decided to be on his guard and be reserved. When he received the transcripts, he was astonished that he had told me about things that he had not thought about for a long time and never disclosed, even to his wife. After that remark I would have expected him to delete substantial parts of the interview before publication, but he hardly touched the text.

I would like to sample here some of the answers to the example questions I mentioned above. What turned today's great chemists to chemistry? The most frequent answer is either Paul de Kruif's book *Microbe Hunters* or a chemistry set. It is interesting that de Kruif's book is about pioneers of science, but not so much about chemists. On the other hand, a chemistry set has been the original source of interest not only for many future chemists but for many future physicists and biologists as well. De Kruif's book first appeared in 1926 and has remained in print ever since. Its popularity has faded though. I suspect that nowadays the computer, let alone television, is a great competitor for books among youngsters (we are talking about early teenagers) and, besides, *Microbe Hunters* may be somewhat too romantic for the modern young adult. Chemistry sets may have also lost some of their luster. Today they are less popular than they used to be and part of the reason may be safety precautions that have excluded some of the most spectacular experiments from their repertoire.

To the question about the determining factor in their success, most great scientists name one or two mentors. The determining period of their lives as scientists is their graduate studies in most cases. The venue where they happen to do their graduate work or where they start their independent research career is also a determining factor.



Glenn Seaborg ('51 Nobel Laureate in Chemistry)

The mentor effect may come as a result of a tight interaction with one's thesis supervisor, but it may also be just a casual remark by someone whose impact may then last for a whole research career. My favorite example is Frank Westheimer's story. Westheimer went to pursue his graduate studies at Harvard University because he wanted to work with James

B. Conant, who, in the meantime, had become the president of Harvard. Thus, Westheimer had another supervisor, a rather indifferent one. When he finished and was about to leave, Conant called him into his office and asked him about his plans. Westheimer told Conant what he was planning to do as his research project.

*What turned today's great chemists to chemistry? The most frequent answer is either Paul de Kruif's book *Microbe Hunters* or a chemistry set.*

Conant's reaction was devastating for Westheimer: "If you are successful with that project, it will be a footnote to a footnote in the history of chemistry." At that point Westheimer realized that he was supposed to do important things. For his long and successful career, Westheimer measured everything against Conant's words. Conant, in his turn, had a great career as a public servant. They met one more time when Conant had retired and Westheimer was a professor at Harvard. He was working in his office when someone knocked on his door. It was Conant. He looked at Westheimer and asked, "Do you remember me?" At this point in the interview, Westheimer became so moved that we could not continue for some time, but it was also a good finishing point for the conversation. Whenever I re-read this interview or tell others about it I can't help being deeply moved as well.

There are many examples of the importance of the venue for the start of research careers. I found Sidney Altman's description of his postdoctoral stint in the late 1960s at the Laboratory of Molecular Biology (LMB) in Cambridge, United Kingdom, especially interesting. Altman was a co-recipient with Thomas Cech of the chemistry Nobel Prize in 1989 "for their discovery of catalytic properties of RNA." He felt in Cambridge as he thinks young physicists must have felt in Copenhagen in the 1920s at the dawn of modern physics. Altman narrates how everyone went to tea at the LMB, according to the English custom, twice a day, and the "gods" of molecular biology were there. They were accessible in fact, eager to discuss things with everyone else in the lab. The scientists included Francis Crick, Sydney Brenner, Frederick Sanger, César Milstein, Max Perutz, Hugh Huxley, and Aaron Klug. It was a very formative atmosphere indeed.

The question about whether a discoverer recognizes the importance of his discovery right away is less trivial than it sounds. It does happen sometimes that the recognition comes much later after some other people had

done additional work in the field. The story of buckminsterfullerene provides a conspicuous example. Eiji Osawa in Japan proposed the C_{60} molecule of the truncated icosahedral shape 15 years before its discovery. However, he did not recognize its importance and restricted himself to publish about it in the Japanese language only, although he published his other works almost exclusively in English. A few years later two Russian authors, Gal'pern and the late Bochvar reported this structure from their quantum chemical computations. Although their Russian-language article had been translated into English, nobody had noticed it until after the actual discovery in 1985 by Kroto, Curl, Smalley, and their students. The original idea of the truncated icosahedral shape came from a colleague of Bochvar and Gal'pern, Ivan Stankevich, but they failed to include him among the authors because they, and Stankevich too, thought that this piece of work was of no particular interest. Stankevich used to play soccer and the shape of the soccer ball gave him the idea. The interviews with Osawa and with Gal'pern and Stankevich, along with those with the Nobel laureates Curl, Kroto, and Smalley, reflect a lot of human drama.

I have gradually warmed up to asking famous scientists whether it was easy to publish their groundbreaking findings. Originally, I thought that the best journals would be eager to publish Nobel Prize-level discoveries.



Levi-Montalcini
(*86 Nobel Laureate in
Physiology and Medicine)

However, the experience is different, although seldom can one read about it. For some, even for Nobel laureates, it is an uncomfortable topic to narrate about rejections by stern editors of studies that later would merit the highest recognition. Yet it is instructive to observe that perhaps mediocre papers have the easiest way onto the printed page.

Very poor papers get filtered out, of course. However, real groundbreaking papers often have their hurdles because of their pioneering character.

These are but a small sample of questions and the answers. There is great diversity among the fates and personalities of great scientists just as among the rest of us. It sounds commonplace, but the most succinct way to characterize great careers is for the right person to be there in the right place at the right time. In addition to being gifted though, many of the greatest scientists worked very hard to be there just when it was the right time and to move around until they "happened to be" in the right place.

Recently, Alan MacDiarmid of the University of Pennsylvania and co-recipient of the chemistry Nobel Prize in 2000 summed up his philosophy in the guise of a Chinese proverb: "I am a very lucky person and the harder I work the luckier I seem to be."

So far, two volumes of my Candid Science series have appeared, *Candid Science: Conversations with Famous Chemists* (2000) and *Candid Science II: Conversations with Famous*



Reiko Kuroda
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Biomedical Scientists (2002). The third volume is now coming out, *Candid Science III: More Conversations with Famous Chemists*. Each volume contains 36 interviews, and more than half are Nobel Laureates. The Candid Science series published by Imperial College Press London is open ended, and one more volume has been contracted (*Candid Science IV: Conversations with Famous Physicists*). Beyond that, I already have material for yet another volume. I have been doing this interviewing mostly during the past half a dozen years.

It was the interaction with Linus Pauling that initiated this project in 1993. However, my very first interview with a famous scientist was 1965 with Nikolai Semenov (1896-1986), the Russian Nobel laureate of 1956. I was asked to do this interview by the science section of Radio Budapest. Semenov came to Budapest to receive an honorary doctorate from the University of Technology. The interview was not only broadcast on radio, later it was also printed in the *Radio and Television Yearbook*, a volume of the best programs. Recently, I purchased a copy of the original tape from the Archives of Radio Budapest

It sounds commonplace, but the most succinct way to characterize great careers is for the right person to be there in the right place at the right time.

and, after more than 35 years, I still found it interesting. I was lucky that Semenov was as experienced in such matters as he was gracious. I was as inexperienced as one

could be, but had the self-assurance of an ignorant beginner. The Radio supplied me with a tape recorder of the size of a trunk and a technician who operated it. One of the interesting features of the interview was that I asked Semenov to prognosticate about science from the perspective of the mid-1960s, and he did. From today's perspective, he did not say anything extraordinary, but this is what makes his prognostication so valid. I was happy to include Semenov in my first interviews volume.

For six years (1995-2000) I published most of my interviews in *The Chemical Intelligencer*, a now defunct magazine. I have now an interview in each issue of the magazine *Chemical Heritage* published by the Chemical Heritage Foundation. These interviews have

been my second university education and I am happy to share all that I have learned from them with everyone.

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Photos: I. Hargittai.

 www.tki.aak.bme.hu/hargittai/hargittai.htm

Pesticide Residues

IUPAC Representative's Report on the 34th Codex Committee Session

The Codex Committee on Pesticide Residues (CCPR) convened at The Hague this past May to continue its mission of promulgating recommendations on international standards for maximum residue level (MRL) of pesticides on internationally traded agricultural commodities. In this report, Kenneth Racke, the IUPAC representative on Codex, offers a brief summary and major highlights of the past meeting. The CCPR serves as a forum for discussion and decisions regarding aspects of MRL process risk management. Actual technical recommendations regarding MRLs and the acceptable daily intake (ADI) and acute reference dose (ARfD) toxicological endpoints arise from the annual Joint Meeting on Pesticide Residues (JMPR) of the Food and Agricultural Organization of the United Nations/World Health Organization (FAO/WHO). MRLs recommended by CCPR are subject to formal approval by the biennial Codex Alimentarius Commission (CAC) as Codex MRLs.

by **Kenneth D. Racke**

Big Group, Small Steps

Two-hundred-fifty delegates representing 51 countries and 15 international organizations attended but, as is typical, achieved few definitive outcomes or concrete decisions. The CCPR enthusiastically debates particular topics and position papers, appoints working groups to prepare new or revised position papers for future discussion, and refers technical matters to the JMPR for learned consideration. Eventually, the CCPR recommends finalized policies and MRLs that have proceeded through an eight-step process to formal adoption by the CAC.

In addition to the frequent interventions of national delegations, opinions aplenty were forthcoming from the manufacturers' representative, CropLife International, and the self-appointed committee conscience, Consumers International. With CropLife International anxious to see reasonable and pragmatic progress in promulgation of MRLs and Consumers International most concerned that the precautionary

principle be observed with every action, these delegations found little common ground.

Referrals from CAC and JMPR

Acting on an early agenda item, the committee initiated a comprehensive review of the standard-setting and technical-evaluation processes employed by all Codex-sponsored bodies, including that of CCPR and JMPR. An independent panel of experts' report will be available for discussion at the July 2003 CAC meeting and could yield recommendations for process changes or further study. Included in the ongoing review will be an overall consideration of harmonized approaches across all Codex bodies toward food standards establishment and the associated risk analysis and management.

Several general considerations from the 2001 JMPR were briefly discussed. Among them, the WHO will be developing a guidance document on ARfD establishment. A pilot program for sharing chemical reviews from national regulatory authorities with the JMPR will be advanced later. The JMPR also noted impending availability of a new guidance document, "FAO Plant

Production and Protection Paper 170,” on the submission and evaluation of pesticide residue data for MRL estimation.

Protection of Infants and Children

The Consumers International delegation requested that CCPR give further consideration to special MRLs for processed commodities such as infant formula and cereals. Back in 2000, the CCPR debated the need for default MRLs for those commodities and concluded that no such initiative was warranted since children were already well protected by the current MRL-setting process. The CCPR had recommended that food preparation methods be generally practiced that best minimize pesticide residue carryover. The CCPR recommendation to the Codex Committee on Nutrition and Foods for Special Dietary Uses for adoption of such language had been debated and supported. So, the committee decided that reconsideration was fruitless and inimical to progress in MRL setting.

Acute Dietary Intake Assessment

For the past couple of years, JMPR has undertaken to establish ARfDs and conduct acute dietary intake (ADI) assessments on a commodity-by-commodity basis using a simple, deterministic calculation. Short-term intake calculations are resulting in a significant number of cautions being raised which are blocking advancements of MRLs for approximately half of the pesticides examined. This stands in opposition to long-term dietary intake assessment, which infrequently is observed to exceed the ADI. The WHO's Dr. Jerry Moy shared example calculations for the organophosphorus (OP) insecticide disulfoton and highlighted his reliance

for large-portion size estimates on the data matrix he has constructed to reflect the highest intake for each commodity at the 97.5 percentile reported from any single country. He reported that the delegation from South Africa had just supplied data which would increase the highest maize grain intake by some 25-fold. Based on that new data, the committee agreed with Dr. Moy's suggestion that all past short-term intake assessments for maize be recalculated.

A discussion of probabilistic ADI assessment followed, based on the paper prepared by the USA in cooperation with the Netherlands, Australia, CropLife International, and Consumers International. The paper highlighted the probabilistic assessment methodology employed by the U.S. Environmental Protection Agency and—while emphasizing the refined nature of such an approach in providing the most accurate reflection of the likelihood of any particular exposure across all crop commodities—also reflected its data-intensive nature. The majority of delegations were pessimistic about the utility of such an approach in light of the scarcity of data distributions at the international level on large-portion size consumption and limited JMPR technical resources. Germany also indicated that significant policy decisions would also be required, citing the selection of reference level as a particularly thorny issue. Based on the interest but lack of firm support, the committee referred the matter to JMPR for a technical opinion and will await the outcome of the general evaluation of risk assessment approaches planned as part of the ongoing CAC review process.

Regarding refinement of the currently employed methodology for acute dietary intake assessment, the committee noted a nearly completed IUPAC project (see



The Codex Committee on Pesticide Residues considers international standards for maximum residue levels of pesticides on internationally traded agricultural commodities, such as oranges.

www.iupac.org/projects/1999/1999-009-1-600.html), agreed to consider advancements in acute dietary assessment calculations, and appointed the Netherlands to work with IUPAC and several other delegations to bring specific discussions forward for the 2003 CCPR meeting.

Cumulative Dietary Intake Assessment

At earlier CCPR meetings, the committee expressed an intention to take into consideration the cumulative intake of dietary pesticides that share a common toxicity mechanism. The USA delegation presented a paper outlining the current approach being pioneered by the U.S. EPA with the OP class of insecticides. The USA delegation noted the preliminary nature of methods for such an assessment, but projected finalization of a first example by mid-2002. A few delegations noted the importance and desirability of including such considerations at the international level, but there were considerable reservations expressed for such an approach based on the complexity and data-rich nature of such methodology. Several delegations also noted the prerequisite of developing a probabilistic methodology before such cumulative intake assessments could be considered. The committee agreed that, given the immature nature of cumulative assessment approaches at even the national level, it was too early for CCPR to undertake any actions related to cumulative dietary intake assessment.

Criteria for Prioritization

The criteria employed by CCPR in prioritizing new chemical evaluations and periodic reevaluations of existing chemicals were debated based on a paper pre-

sented by the Australian delegation. The need for prioritization is driven by JMPR overcapacity in handling a significant backlog of technical evaluation requests. As a general principle, the committee agreed to maintain a 50:50 ratio between new and existing chemical evaluations. With the assumption that candidate products must give rise to residues in food commodities moving in international trade and which may give rise to public health concerns and/or impediments to trade, CCPR agreed once again that when establishing priorities, preference be given to those chemicals:

- the intake and/or toxicity profile of which indicate a high level of public concern
- that are new and safer and have the potential to replace existing chemicals that present a public health concern on which national reviews are available
- that may be responsible for actual or potential losses owing to trade disruption

The USA delegation, Consumer's International, and a few other delegations supported making the "safer" or "reduced risk" pesticide prioritization criterion broader in scope than just "public health" to include descriptions such as "reduced environmental impact," "safer for applicators," and "replacement of ozone depleter." The committee agreed that such factors could be taken into account in prioritization, but that they were secondary to public health considerations and likely already being taken into account when nominating "reduced risk" pesticides for CCPR prioritization.

Tentative JMPR Schedule

The Australian delegation also presented the report of the Ad Hoc Working Group on the Establishment of Codex Priority Lists of Pesticides. The committee accepted the report with several modifications related to agenda items that came up during the CCPR meeting. Of particular interest were the new chemical toxicological (T) and residue chemistry (R) evaluations scheduled for future JMPR meetings:

- 2002 JMPR: esfenvalerate (T,R), flutolanil (T,R), imidacloprid (R)
- 2003 JMPR: cyprodinil (T,R), famoxadone (T,R), methoxyfenozide (T,R), pyraclostrobin (T,R)
- 2004 JMPR: fludioxinil (T,R), zeta-/alpha-cypermethrin (T,R), trifloxystrobin (T,R)
- 2005 JMPR: dimethenamid-P (T,R), fenhexamid (T,R), indoxacarb (T,R), novaluron (T,R)

Accelerating the Codex MRL Process

A report focused on the Codex MRL process refinement and acceleration provoked considerable discussion. Unfortunately, the committee agreed on few practical steps and a move toward acceleration appears likely to



proceed at an agonizingly slow pace. The bulk of the discussion centered around a paper introduced by the USA delegation that focused on options for solving the “window of vulnerability” in trade resulting from the extensive time required to establish Codex MRLs. The process from new compound nomination for MRLs to promulgation of those MRLs may take four or more years. The paper highlighted eight practical suggestions, which ranged from simple, no-cost administrative changes such as holding the JMPR three months earlier so that first CCPR discussion can occur the next year, to extensive and costly program overhauls such as replacing the volunteer JMPR with a full-time technical evaluation staff. Projected process savings ranged from one to six years.

One idea that attracted much discussion was the establishment of “interim Codex MRLs” based on early adoption of the JMPR evaluations or reference to national evaluations and MRLs. Although a number of delegations supported serious consideration of such options, others were concerned about the need for caution and additional procedural safeguards. The only points of consensus emerging included the preparation of yet another paper for further discussion at the 2003 CCPR meeting and for CCPR to review MRL proposals at Step 3 the year following the JMPR meeting instead of automatically postponing by another year.

MRLs for Minor Crops

A paper prepared by the Spice Trade Association and introduced by the South Africa delegation, which highlighted the problem of MRLs for dried spices, also prompted discussion. Many of these products come from small farms in developing countries lacking adequate description of good agricultural practice in the use of pesticides and supervised field residue trials. Given the generally limited dietary intake of such commodities, it was proposed to base Codex MRLs and extraneous maximum residue limits (EMRLs) on available monitoring data as long as several criteria were met, including per capita consumption <0.5% of regional diets, substantial trade involvement, and availability of ongoing residue monitoring data from the producing country. The committee agreed to ask JMPR to establish guidance on monitoring data submission and also to have South Africa prepare a paper for discussion at the 2003 CCPR providing a definition and listing of candidate spices. The committee noted that current considerations be restricted to spices and not include tea, fresh herbs, or tropical fruits—all minor crops with similar MRL problems to spices. Future discussion on these leftover points is anticipated, and a recently initiated IUPAC project dealing with international chemistry and regulatory aspects for minor crops should also provide additional guidance (see www.iupac.org/projects/2001/2001-039-1-600.html).

OPs and Carbamates

Some of the more acutely toxic OP and carbamate insecticides were the subject of CCPR discussions and actions. Due to implementation of the periodic reevaluation process and acute dietary intake assessment, a number of Codex MRLs for these insecticides are being put on hold or being revoked based on inadequate numbers of residue trials, especially for minor crops, and short-term intake concerns. Most or all MRLs are being revoked for bendiocarb, fenitrothion, fenthion, mebarbam, mevinphos, monocrotophos, parathion, and phosphamidon. A significant number of MRLs are being stalled or revoked for aldicarb, carbofuran, diazinon, dimethoate, methamidaphos, methomyl, parathion-methyl, phosalone, and phosmet.

EMRLs

In addition to MRLs based on approved uses, CCPR has also established EMRLs for compounds no longer used, but for which inadvertent contamination of food commodities may occur. There are a number of EMRLs for DDT (21), and the 1996 JMPR had recommended revised values for mammal meat and poultry products based on available monitoring data and projected frequency of noncompliance rates for commodity shipments. The CAC had considered decreased EMRLs for meat during 2001 based on a CCPR proposal, but could not reach consensus. The committee agreed to indefinitely shelve the revised meat MRL proposal for DDT, but would in the future determine availability of new monitoring data to support future discussions. However, a proposed poultry meat MRL advanced to Step 5 for future consideration. The 1996 JMPR had concluded no dietary intake concerns would result from the existing or revised EMRLs. Although the Canada delegation indicated that a national intake assessment had flagged short-term intake concerns for children, the Netherlands delegation reported that short-term dietary intake was estimated at 14% of the ARfD for children based on a recent assessment. Canada tends to adopt additional uncertainty factors based on endocrine-disruption concerns.

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 www.codexalimentarius.net/ccpr34/pr02_01e.html

IUPAC News

Young Chemists to the 39th IUPAC Congress, Ottawa, August 2003

The 39th IUPAC Congress and 86th Conference of the Canadian Society for Chemistry will be held 10-15 August 2003 at the Ottawa Congress Centre in Ottawa, Ontario, Canada. The theme of the Congress is "Chemistry at the Interfaces."

To encourage young chemists to participate in this unique congress, the organizers have established two different programs, both offering travel assistance. The first program is especially targeted to young scientists from developing and economically disadvantaged countries; the second is open to chemists from any country. For each program respectively, about 30 and 20 awards of up to USD 1500 will be made available to qualified candidates as a contribution to the costs of their travel to attend the Congress and to meet Congress registration fees.

Applications from candidates under age 40 are welcomed. Scientists from academia, government, or industry may submit applications directly to the address below. Those accepted will be expected to submit an abstract of a poster or paper to be presented at the Congress. Such abstracts will be subject to adjudication as will all other submissions for presentation at the meeting. There is no specific application form, but applicants are required to provide:

- a letter of application
- a brief curriculum vitae
- a confirmation of their current status and affiliation
- a publication list
- a letter of support from the appropriate department head, dean, or laboratory supervisor

Estimates of the economy airfare to and from the Congress should also be provided.

The deadline for receipt of applications is **30 November 2002**. Applications should be sent to:

Dr. Hamid Jorjani
National Research Council of Canada
Building M 58, Montreal Road
Ottawa, Ontario K1A 0R6, Canada
E-mail: <Hamid.Jorjani@nrc.ca>



www.nrc.ca/confserv/iupac2003
www.iupac.org/symposia/conferences/ga03

Chemical Education International

A couple of years ago, the International Newsletter on Chemical Education (INCE) was transformed into an electronic medium, designed as its paper parent to be accessible to the majority of the worldwide community of teaching chemists. Now known as *Chemical Education International* (CEI), the newsletter of the Committee on Chemistry Education (CCE) only appears on the Internet and offers a variety of articles, including the following:

1. Reports on activities of CCE and its members, such as projects
2. News and reports on events held or supported by IUPAC and related organizations, such as ICCE, CHEMRAWN, etc.
3. News and reports written or communicated by a CCE member on chemical education in member countries of international interest
4. General articles on chemical education written or recommended by a CCE member that meet the international interest of readers, such as "Interview with Nobel Laureate," facts and figures, opinions, and essays

As the work of CCE transcends the subdisciplines of chemistry and international borders, the current Committee continues to be interested in, and supportive of, a variety of devices—conferences, reports, newsletters, etc.—for the dissemination of its efforts and the efforts of others interested in chemical education. While modernizing the creation, production, and distribution of the CCE newsletter by making it a online publication, the Committee still does recognize that a cohort of teaching chemists exist in areas of the world that currently are not served by the Internet. Incidentally, these areas were also difficult to reach with the original printed INCE; however, it is hoped that access to the Internet will continue to expand, making this new electronic newsletter more widely accessible.

The intended readership includes mostly school-teachers and professors interested in chemical education, and, most recently, students. A series of interviews with Nobel laureates in chemistry is specially targeted at this new group of readers. The recently released third interview in that series is with professor Shirakawa. Interviews with professors Rowland and Kroto appeared in previous issues. Other articles in the current issue include a review by A. F. M. Fahmy and J. J. Lagowski

http://www.chem-ed.org/publications/cei/index.html

Chemical Education International

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Published by Committee on Chemistry Education (CCE), International Union of Pure and Applied Chemistry

In the latest Newsletter > Vol 2

To the youth of the World who aspire to a career in chemistry

Message from Nobel Laureates to Young People



For the benefit of those who aspire to a career in chemistry, each issue contains a short interview with a Nobel Laureate in chemistry. In this issue, we

of the "Systemic Approach to Teaching and Learning Chemistry in Egypt" and a report by Y. Takeuchi on the status of science education in Japan.

The chief editor, Masato M. Ito, intends to use, as before, the voluntary efforts of CCE members who should have easy access to national information and who could benefit from a broader and international dissemination. Ito also invites relevant opinions and essays from all sources. E-mail: <itomasa@t.soka.ac.jp>



www.iupac.org/publications/cei

The "Orange Book" Online

Conceived a couple of years ago, the Web edition of the IUPAC Compendium of Analytical Nomenclature—the "Orange Book"—has now been completed. Its purpose is to ease access to and extend the influence of the extensive information contained in its recommendations. The work involved extensive proofreading of the electronic files and editing them to correspond in detail to the printed version, or to the earlier *Pure and Applied Chemistry* publications when there were conflicts. This work involved all members of the Analytical Chemistry Division Committee and others.

The Officers of the Analytical Chemistry Division during 2000-2002 (F. Ingman, D. S. Moore, K. Powell, and R. Lobinski) are extremely grateful for the help provided by the ACD Committee members and the staff of the Secretariat, and to C. Townsend for hyperlinking the index.

The home page for the Web edition is in frames, with the left-hand frame serving as a shorthand table of contents. Clicking on a chapter loads its table of contents into the main frame. The sections of each chapter are linked to Adobe PDF files of that particular section.

These can then be searched and/or printed, as desired. The margins were chosen so that they would print on either US Letter or A4 paper. The Index is presented as alphabetical sections, and each term is hyperlinked to the pdf file of the appropriate section of the book. Some book sections are quite long, so that a simple search on the term after downloading the pdf should quickly yield the appropriate location.



www.iupac.org/publications/analytical_compendium

IUPAC—Empfehlungen

The German National Adhering Organization, the Deutscher Zentralausschuss für Chemie, through one of its component Societies, the Gesellschaft Deutscher Chemiker, has arranged for the translation and publication of selected IUPAC Reports and Recommendations in the journal *Angewandte Chemie*.

According to *Angewandte Chemie*, publishing translations of IUPAC Recommendations and Technical Reports is a way to promote the use of chemical professional language in German. Properly defined terms and clear nomenclature form the basis of the understanding among scientists in a discipline and are essential for the exchange among scientific and professional language and general language. All translations are examined, corrected, and authorized by an acknowledged expert, the "Obmann."

The following translations have been published to date:

- Glossary of Terms Used in Combinatorial Chemistry, *Pure Appl. Chem.* **71**, 2349-2365 (1999); Expert Prof. Dr. S. Bräse, translator B. Neuß; *Angew. Chem.* **114**, 893-906 (2002).
- Guidelines for Presentations of Methodological Choices in the Publication of Computational Results. A. Ab Initio Electronic Structure Calculations, *Pure Appl. Chem.* **70**, 1015-1018 (1998); Expert and Translator, Prof. Dr. R. Janoschek; *Angew. Chem.* **114**, 1497-1499 (2002).
- Nomenclature of Organometallic Compounds of the Transition Elements, *Pure Appl. Chem.* **71**, 1557-1585 (1999); Expert and translator Prof. Dr. A. Salzer; *Angew. Chem.* **114**, 2043-2058 (2002).

Suggestions for themes and experts are welcomed. For more information, please contact Elisabeth Weber <angewandte@wiley-vch.de> or visit the journal Web site.



www.angewandte.com

IUPAC Projects

Chemical Actinometry

The project intends to update a document published in *Pure and Applied Chemistry* **61**, 187-210 (1989) on Chemical Actinometry. The purpose is to extend the coverage to the solid state, expand the gas phase systems and cover in more detail the near-UV radiation region, in view of the renewed interest on research in this area, due to environmental reasons. Thus, the updated document should provide a complete collection of chemical actinometers, i.e., of appropriate substances for the absolute measurement of the number of photons in a light beam exciting a sample. These measurements are required for the quantitative determination of efficiencies of photoinduced reactions. A list of recommended procedures for the most commonly used actinometers is also provided, as well as a critical discussion regarding the pros and cons of the use of chemical actinometers vs. electronic devices. Actinometers are also included for the use in biological media.

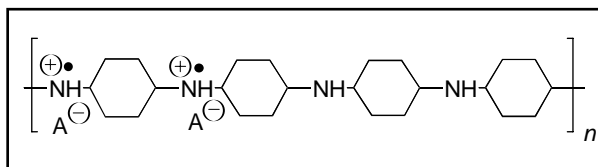
The document should be ready this summer for discussion at the IUPAC Subcommittee on Photochemistry which will meet in Budapest at the end of July on the occasion of the IUPAC Symposium on Photochemistry. A preliminary version of the document will be published in the Web sites of the three multinational photochemical associations, i.e., the Inter-American Photochemical Society (I-APS), the European Photochemical Society (EPS), and the Asia Photochemical Society (APS). Comments are welcome to this preliminary version.

Silvia E. Braslavsky <braslavskys@mpi-muelheim.mpg.de>

 www.iupac.org/projects/2002/2002-008-1-300.html

Conducting Polymer Colloids and Nanofilms

Conducting polymers, polyaniline being a typical example, are the object of numerous studies because of their scientific challenge and potential applications. These proposed uses range from micro-electronics, sensors, electronic noses, electromagnetic shielding, and military camouflage, to intelligent materials and anti-corrosion protection. The results of an IUPAC project on the preparation of polyaniline have been recently reported in *Pure and Applied Chemistry* **74**, 857-867 (2002); see page 26.



Polyaniline (PANI) exists in a variety of forms that differ in chemical and physical properties; the most common green protonated emeraldine has conductivity on a semiconductor level of the order of 1-10 S cm⁻¹, many orders of magnitude higher than that of common polymers (<10⁻⁹ S cm⁻¹) but lower than that of typical metals (>10⁴ S cm⁻¹).

While the synthesis of many conducting polymers is easy, their poor processibility presents a serious obstacle to application. A new IUPAC project (#2002-019-1-400) addresses this problem by studying two types of processible forms, polyaniline colloids and in-situ-polymerized polyaniline nanofilms. The colloids are produced during the oxidation of aniline with ammonium peroxydisulfate in acidic aqueous medium in the presence of a suitable polymeric stabilizer; polyaniline films grow under reaction conditions of this kind on virtually any surface or interface. The nanofilms are of particular interest because of the brush-like ordering of polymer chains in them.

Continued on page 21

Information for Task Group Chairmen

The project-based structure of IUPAC makes Task Groups a key mode for implementation of the IUPAC mandate to enhance and improve communication worldwide among scientists in the chemical sciences. The Task Group chairman, in turn, is responsible for the implementation of the project and, subject to approval by the Division Committee, for the appointment of the Task Group Members. He/she also decides how the budget will be spent and reports periodically to the monitoring body as to progress toward the stated goals. A new, comprehensive online document is now available on the IUPAC Web site that will help chairmen navigate their Task Groups through issues of accountability, budgeting, outcomes, dissemination of findings, and evaluations. The document describes in detail what is expected in terms of publications and workshops and it tells how to compile a Standard Measures Report and a Final Status Report. The report is available in either HTML or Adobe Acrobat PDF at the address below.

 www.iupac.org/projects/TGC-info.html

Members of the task-group from six countries will follow the same preparative protocol in various laboratories, and the properties of the resulting materials will be compared at the international level. For the colloidal forms, the particle size and polydispersity determined by dynamic light scattering will be the main criterion. The films will be characterized with respect to their thickness, assessed by optical absorption measurements after calibration. The results of the project will contribute to the development of reproducible procedures

for forming conducting polymers. Various macroscopic and microscopic substrates coated with conducting-polymer overlayer can find uses in analytical chemistry, separation science, the catalysis of organic reactions, conducting composite materials and in the development of micro-electronics.

Jaroslav Stejskal <stejskal@imc.cas.cz>

 www.iupac.org/projects/2002/2002-019-1-400.html

Highlights from Pure and Applied Chemistry

Presenting recently published IUPAC technical reports and recommendations

Information Essential for Characterizing a Flow-Based Analytical System (IUPAC Technical Report)

by Elias A.G. Zagatto, Jacobus F. van Staden, Nelson Maniasso, Raluca I. Stefan, and Graham D. Marshall
Pure and Applied Chemistry, Vol. 74, No. 4, pp. 585-592 (2002)

Terminology related to classification and definition of analytical methods based on flowing media, as well as terms describing the flow-based analytical procedure or system and its components have been presented in previous publications, including *Pure and Applied Chemistry* and the "Orange Book," 3rd edition. However, a literature survey reveals that a number of such analytical procedures and/or related instrumentation are only partially described. As a proper description of any methodology is essential, it is important to complement the earlier recommendations by taking into account the recent progress in flow analysis. The objective of this report is to provide guidelines for characterizing a flow analyzer and/or related flow-based methods, emphasizing the minimum but adequate information that should be included in scientific or technical reports. Aspects more related to chromatographic procedures are not considered.

According to the report, for a complete description of a flow system, the following elements should be considered and described: flow pattern (technique), stream parameters, sample introduction (with possibility of reagent introduction), manifold, sample processing, and detection. The report also describes the following important performance parameters of a flow-based procedure: sampling rate, analytical characteristics, robustness, and portability.

This report should benefit practitioners and developers by permitting normalized proposals to be presented in the field of flow analysis. The authors intend to use this report to prepare a checklist that will lead to a protocol for reporting results and systems in flow analysis,

which would result in the development of systems that are more consistently designed.

 www.iupac.org/publications/pac/2002/7404/7404x0585.html

Sulfate-Sensing Electrodes. The Lead-Amalgam/Lead-Sulfate Electrode (IUPAC Technical Report)

by Patrizia R. Mussini and Torquato Mussini
Pure and Applied Chemistry, Vol. 74, No. 4, pp. 593-600 (2002)

It has long been recognized that sensitive and reproducible sulfate-reversible electrodes (e.g., the Pb|PbSO₄ or Hg|Hg₂SO₄ electrode) are not as readily available as chloride-reversible electrodes (e.g., a widespread Hg|Hg₂Cl₂ or Ag|AgCl electrode). In this context, two major features are evident: the activity solubility products of PbSO₄ and Hg₂SO₄ are larger than those of Hg₂Cl₂ and AgCl by several orders of magnitude, and in the case of the Pb|PbSO₄ electrode, the preparative and operational procedure had not been assessed satisfactorily until recently, so that the electrode in both Pb|PbSO₄ and Pb(Hg)|PbSO₄ forms proved difficult to use and/or was unsatisfactorily reproducible.

In this report a new, simplified design and a convenient preparation procedure for the Pb(Hg)|PbSO₄|SO₄²⁻ electrode is proposed. This procedure ensures preparation of stable amalgams and reproducible electrode potentials, which make this electrode useful and attractive for both thermodynamic investigations and electro-analytical applications. For these purposes, the electrode prepared according to the proposed procedure has been exhaustively characterized both thermodynamically and as a sulfate-sensing electrode, in different sulfate solutions, including H₂SO₄.

The report also proposes a practical standardization procedure. The Pb(Hg)|PbSO₄|SO₄²⁻ electrode can be

structured with a built-in concentrated Li_2SO_4 salt bridge for use as a sulfate-based reference electrode. Li_2SO_4 also has favorable properties as a salt bridge in some mixed aqueous-organic solvents, e.g., acetonitrile-water mixtures, and its combination with the lead-amalgam|lead-sulfate electrode in such solvents is an interesting perspective, for which further accumulation of data is awaited. This electrode can be operated as a reference electrode alternative to the conventional calomel or $\text{Ag}|\text{AgCl}$ reference electrodes in electroanalytical practice.



www.iupac.org/publications/pac/2002/7404/7404x0593.html

Future Requirements In the Characterization of Continuous Fiber Reinforced Polymeric Composites (IUPAC Technical Report)

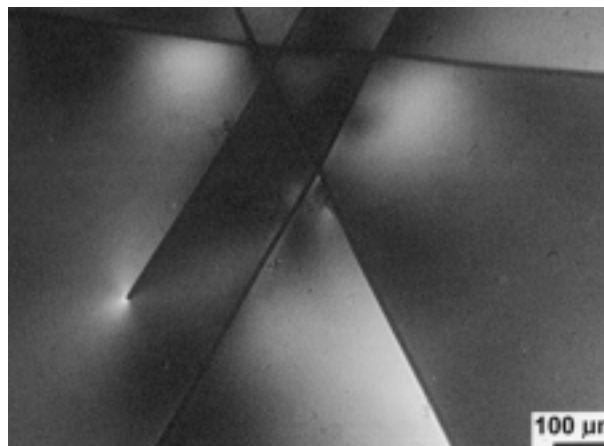
by D. R. Moore and A. Cervenka

Pure and Applied Chemistry, Vol. 74, No. 4, pp. 601-628 (2002)

There has been enormous activity in the field of continuous fiber reinforced polymeric composites research, particularly in the period between 1980 and the present. Although there has also been a decline in this activity in the last few years, nevertheless, there is likely to be future expansion for these materials in a range of areas, most of which will be motivated by a specific property per unit weight. Consequently, characterization of composites is likely to remain a key issue.

Much of the historic activity on characterization has been associated with processing, properties, and structure. In addition, there remains plenty yet to explore. A number of the scientists associated with the historic activities are active on the IUPAC Working Party on Structure and Properties of Commercial Polymers, under the chairmanship of Martin Laun. Therefore, this group has considered what activities might be required in the future in order to better characterize continuous fiber reinforced composites and in addition to contemplate some current and future issues.

This report examines the characterization of continuous fiber reinforced composites in terms of processing, properties, and structure. The historic background of five processing and five property topics are then reviewed with the aim of identifying current issues and requirements for the future. The topics covered in the processing section are polymeric matrix, impregnation, interfacial effects, residual stresses, and pre-preg tack. In the mechanical properties section the topics include choice of standard, recycling and re-usability, durability, environmental strength, and toughness. The paper provides a 10-point plan for future requirements.



An example of a complicated stress field illustrated by a photoelastic image of an assembly of long carbon fibers embedded in Araldite epoxy matrix.

In common with this IUPAC Working Party's activities, the contributions for this work come from a wide international group of scientists from both industry and academia and include C. B. Bucknall (UK), R. S. Bailey (UK), B. Pukansky (Hungary), A. Galeski (Poland), D. R. Moore (UK), L. Glas (Belgium), W. Alstadt (Germany), B. Gunesin (Turkey), A. Cervenka (Holland), and J. G. Williams (UK).



www.iupac.org/publications/pac/2002/7404/7404x0601.html

Nomenclature for the C_{60} - I_h and C_{70} - $D_{5h(6)}$ Fullerenes (IUPAC Recommendations 2002)

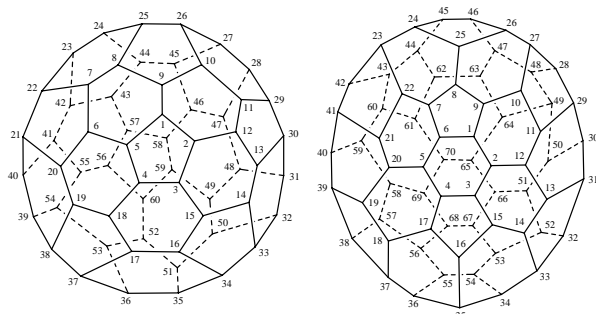
by W. H. Powell, F. Cozzi, G. P. Moss, C. Thilgen, R. J.-R. Hwu, and A. Yerin

Pure and Applied Chemistry, Vol. 74, No. 4, pp. 629-695 (2002)

Fullerenes are a new allotrope of carbon characterized by a closed-cage structure consisting of an even number of three-coordinate carbon atoms devoid of hydrogen atoms. This class was originally limited to closed-cage structures with 12 isolated five-membered rings, the rest being six-membered rings.

Although it was recognized that existing organic ring nomenclature could be used for these structures, the resulting names would be extremely unwieldy and inconvenient for use. Incorrect von Baeyer ring names have been published. At the same time it was also recognized that established organic nomenclature principles could be used, or adapted, to provide a consistent nomenclature for this unique class of compounds based on the class name fullerene. However, it was necessary to develop an entirely new method for uniquely numbering closed-cage systems.

This paper describes IUPAC recommendations for naming and uniquely numbering the two most common fullerenes with isolated pentagons, the icosahedral C_{60} fullerene and a D_{5h} - C_{70} fullerene.



$(C_{60}-I_h)[5,6]$ fullerene

$(C_{70}-D_{5h(6)})[5,6]$ fullerene

It also describes recommendations for adapting organic nomenclature principles for naming fullerenes with nonclosed-cage structures, heterofullerenes, derivatives formed by substitution of hydrofullerenes, and the fusion of organic rings or ring systems to the fullerene cage. Finally, the paper suggests methods for describing structures consisting of two or more fullerene units and for denoting configurations of chiral fullerenes and their derivatives.

 www.iupac.org/publications/pac/2002/7404/7404x0629.html

Molecular Basis of Biodiversity, Conservation, and Sustained Innovative Utilization (IUPAC Technical Report)

by A. E. Fischli, U. K. Pandit, and D. StC. Black
Pure and Applied Chemistry, Vol. 74, No. 4, pp. 697-702 (2002)

Biodiversity is a complex issue requiring global, coordinated attention from various branches of natural and social sciences, but especially from physical and life sciences. One salient aspect of biodiversity is chemical in origin. The unique and diverse molecular libraries provided by the planetary flora, fauna, and microorganisms have been a source of immense practical value to mankind.

Different parts of the globe have varying endemic biological resources, so international cooperation is required to ensure that the benefits of global bioresources can be distributed fairly and equitably. Today, the same regions rich in bioresources may not be in an ideal position to extract the maximum benefit from those assets. The necessity for mutually advantageous global cooperation in the utilization of bioresources is obvious.

Innovative utilization of bioresources links society, governments, academia, and industry. They are the main stakeholders in both preservation and utilization of bioresources, investing in and at the same time benefiting from the products and services originating from those assets. Because molecular systems or information at the molecular level are used higher up in the value chain, the chemical community is called upon to contribute to the discussion of the various scientific, economic, and ethical issues that are associated with this sort of international cooperation. To this end, IUPAC can and must play a crucial role in developing suitable recommendations, which can also be submitted to the International Council for Science.

In this report, recommendations are presented for international cooperation between academia and industry on molecular biodiversity. The following recommendations are based on discussions in workshops/meetings held in Amsterdam (the Netherlands), Belo Horizonte (Brazil), Bangkok (Thailand), Kunming (China), and Antalya (Turkey) involving national and international representatives of relevant organizations.

Recommendations

Recommendations for Global Cooperation on Sustainable Prospecting for Molecular Systems and Information at the Molecular Level derived from Natural Resources are as follows.

Preamble

- Dedicated to the conservation of biomolecular resources for future generations
- Recognizing the vital role of science worldwide in education, research, and innovation
- Recognizing the important ecological roles played by local and regional biodiversity
- Recognizing the contributions which the molecular diversity of natural products from the biome have made to the health and welfare of humankind
- Recognizing the need of avoidance of environmental pollution and ecological destruction arising from over-exploitation of biological resources
- Affirming their commitment to cooperate fairly and equitably with stakeholders for the benefit of humankind and the sustainable use of diversity at both the molecular and organism level
- Recognizing the sovereign rights of states over their own natural resources and the authority of national governments to determine access to biological and genetic resources, subject to national legislation
- Acknowledging the interests of other stakeholders from the country or from abroad, including indigenous and local communities and farmers, in natural resources and existing knowledge

- Determined to honor the spirit of international, regional, national, and subnational laws and policies concerning biological and molecular diversity as well as intellectual property rights
- Committed to ensure fair and equitable sharing of benefits arising from the sustainable utilization of natural resources
- Dedicated to the fostering of research, and the accumulation and dissemination of all knowledge, especially at the molecular level
- Dedicated to the enhancement of the scientific and technological expertise and resources of developing countries

IUPAC subscribes to the following views:

Authorization of Cooperation

Following an agreement to cooperate, all material exchange, early steps in innovation and commercial cooperation must be conducted under the auspices of relevant authorities.

All countries should facilitate the rapid and efficient formulation of contracts between interacting partners based upon their legal requirements.

Interests of Cooperating Partners

Academic interaction is directed at generating fundamental scientific knowledge in the first instance. It has to be recognized that such basic knowledge can become the subject of translation into products and services with the potential to bring about economic benefits.

There is a genuine interest of all partners in the translation of scientific knowledge into commercially viable products and services and in the fair sharing of ensuing benefits.

All of the cooperating partners are interested in fast and simple mechanisms regulating the common activities, and in avoiding a slow and complex process.

The bioaffluent countries are interested in enhancing their technical training, in improving their facilities as well as in safeguarding sustainable management of their natural resources and harnessing biodiversity for economic development.

Partners from high-technology regions are motivated by the search for novel molecular structures and the underlying biomolecular chemistry made available by the partnership.

All partners should appreciate each other's genuine interests and work in a spirit of mutual understanding, common accountability, and trust.

Authorities in bioaffluent countries are expected to invest in infrastructure and mechanisms for innovation facilitating the emergence of small- and medium-sized R&D enterprises (SMEs), as they constitute the main business partners for globally active companies.

Bioaffluent countries are expected to offer the biota within their jurisdiction for scientific investigation.

They are also expected to contribute traditional information on empirical correlations between biocomponents and their potentially exploitable functions.

At all times of the collaboration, bioaffluent countries remain the owners of material from biota and of contributed information, but are obliged to enter into benefit-sharing agreements with their partners prior to commercialization.

High-technology partners are expected to provide modern technical expertise for the isolation, identification, evaluation, and eventual generation of molecular libraries of biocomponents judged to be of value. In many cases, they contribute their share of financial commitment as well, from both private and public sources.

High-technology partners are expected to provide for transfer of appropriate technology to parties in bioaffluent countries.

Bioaffluent countries are expected to contribute technical manpower and field labor to the project.

All cooperating parties are expected to contribute appropriately to the financial investments supporting the project.

Obligations

The terms of any contract constitute the basis of the formal obligations for all parties.

The partners should insure free flow of scientific information where possible. They should collaborate in any publication of scientific results, after due protection of economic interests of any partner and guided by the clauses of eventual patent laws.

Benefit sharing

Collaborating partners are expected to share fairly and equitably the benefits arising from the utilization of bioresources.



www.iupac.org/publications/pac/2002/7404/7404x0697.html

Naming of New Elements (IUPAC Recommendations 2002)

by W. H. Koppenol

Pure and Applied Chemistry, Vol. 74, No. 5, pp. 787-791 (2002)

The recent debate on the naming of the transfermium elements has centered on two issues: (1) priority of discovery and (2) the right of discoverers to suggest names. This paper proposes a procedure to name new elements that clarifies these issues. After the discovery of a new element is established by a joint IUPAC-IUPAP 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 and is then submitted to the IUPAC Council for approval.

www.iupac.org/publications/pac/2002/7405/7405x0787.html

“Heavy Metals”—A Meaningless Term? (IUPAC Technical Report)

by J. H. Duffus

Pure and Applied Chemistry, Vol. 74, No. 5, pp. 793-807 (2002)

Over the past two decades, the term “heavy metals” has been widely used. It is often used as a group name for metals and semimetals (metalloids) that have been associated with contamination and potential toxicity or ecotoxicity. At the same time, legal regulations often specify a list of “heavy metals” to which they apply. Such lists differ from one set of regulations to another and the term is sometimes used without even specifying which “heavy metals” are covered. However, there is no authoritative definition to be found in the relevant literature. There is a tendency, unsupported by the facts, to assume that all so-called “heavy metals” and their compounds have highly toxic or ecotoxic properties. This has no basis in chemical or toxicological data. Thus, the term “heavy metals” is both meaningless and misleading. Even the term “metal” is commonly misused in both toxicological literature and in legislation to mean the pure metal and all the chemical species in which it may exist. This usage implies that the pure metal and all its compounds have the same physicochemical, biological, and toxicological properties, which is untrue. In order to avoid the use of the term “heavy metal,” a new classification based on the periodic table is needed. Such a classification should reflect our understanding of the chemical basis of toxicity and allow toxic effects to be predicted.

www.iupac.org/publications/pac/2002/7405/7405x0793.html

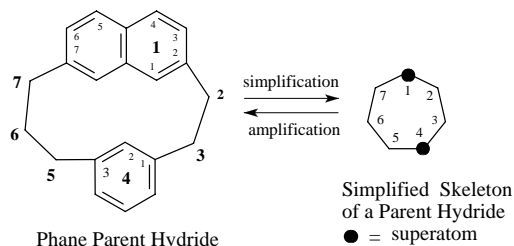
Phane Nomenclature. Part II. Modification of the Degree of Hydrogenation and Substitution Derivatives of Phane Parent Hydrides (IUPAC Recommendations 2002)

by H. A. Favre, D. Hellwinkel, W. H. Powell, H. A. Smith, Jr., and S. S.-C. Tsay

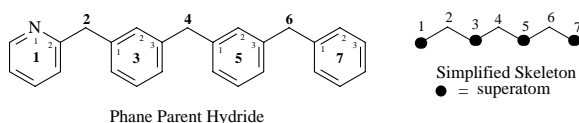
Pure and Applied Chemistry, Vol. 74, No. 5, pp. 809-834 (2002)

Phane nomenclature is a new method for building names for organic structures by assembling names that describe component parts of a complex structure. It is based on the idea that a relatively simple skeleton for a parent hydride structure can be modified by an operation called “amplification,” a process that replaces one or more special atoms (superatoms) of the simplified skeleton by multiatomic structure(s).

Examples:



Simplified skeletal name: cycloheptaphane
Phane parent hydride name:
1(2,7)-naphthalena-4(1,3)-benzenacycloheptaphane



Simplified skeletal name: heptaphane
Phane parent hydride name:
1(2)-pyridina-3,5(1,3),7(1)-tribenzeneheptaphane

The multiatomic structure is a fully saturated or mancude ring or ring system. A mancude ring or ring system contains the maximum number of noncumulative double bonds. In the amplification operation, each superatom is replaced by an amplificant denoted by an “amplification prefix” attached to a stem called a “simplified skeletal name.” The latter ends with the term “phane” and is formed according to the principles for deriving names of saturated hydrocarbons. Accordingly, all of the atoms implied by the skeletal name, except for those replaced by amplification prefixes are, by convention, saturated carbon atoms. An amplification prefix is derived from the name of the corresponding cyclic parent hydride by the addition of the terminal letter “a” with elision of a terminal vowel of the parent hydride name, if present. Phane prefixes thus resemble the prefixes, such as “oxa,” “aza,” etc., that indicate replacement of a single atom, usually a carbon atom, by a different atom.

The locants in front of the parentheses in the phane parent hydride name identify the positions of the superatoms in the simplified skeleton that are replaced by the ring structure specified by the amplification prefix immediately following. By the same token, they also identify the positions of the rings and ring systems in the phane parent hydride. These locants are determined by

the inherent numbering of the simplified skeleton and the seniority of the rings and ring systems in the phane parent hydride. The locants within the parentheses specify the atoms of the ring structure specified by the amplification prefixes that are linked to the adjacent normal atoms of the simplified parent skeleton.

In addition to the basic principles, rules and conventions of Phane Nomenclature, Part I [*Pure Appl. Chem.* 70(8), 1513-1545 (1998)] contains the fundamental methodology for numbering phane parent hydrides and the application of skeletal replacement (“a”) nomenclature for naming heterophane parent hydrides.

Part II of Phane Nomenclature describes derivatives of phane systems formed by substitutive nomenclature. The following nomenclatural features are described: indicated and added hydrogen, order of seniority for numbering, substituents expressed as suffixes, substituents cited as prefixes, phane parent hydrides modified by addition or subtraction of hydrogen atoms, and polyfunctional derivatives.



www.iupac.org/publications/pac/2002/7405/7405x0809.html

Harmonized Guidelines for Single-Laboratory Validation of Methods of Analysis (IUPAC Technical Report)

by M. Thompson, S. L. R. Ellison, and R. Wood
Pure and Applied Chemistry, Vol. 74, No. 5, pp. 835-855 (2002)

Method validation is one of the measures universally recognized as a necessary part of a comprehensive system of quality assurance in analytical chemistry. In the past, ISO, IUPAC, and AOAC International have cooperated to produce agreed protocols or guidelines on the “design, conduct and interpretation of method performance studies,” on the “Proficiency testing of (chemical) analytical laboratories,” on “internal quality control in analytical chemistry laboratories,” and on “the use of recovery information in analytical measurement.” The Working Group that produced these protocols/guidelines has now been mandated by IUPAC to prepare guidelines on the single-laboratory validation of methods of analysis. These guidelines provide minimum recommendations on procedures that should be employed to ensure adequate validation of analytical methods. A draft of the guidelines has been discussed at an International Symposium on the Harmonization of Quality Assurance Systems in Chemical Laboratory, the proceedings from which have been published by the UK Royal Society of Chemistry.



www.iupac.org/publications/pac/2002/7405/7405x0835.html

Polyaniline. Preparation of a Conducting Polymer (IUPAC Technical Report)

by J. Stejskal and R. G. Gilbert
Pure and Applied Chemistry, Vol. 74, No. 5, pp. 857-867 (2002)

Eight persons from five institutions in different countries carried out polymerizations of aniline following the same preparation protocol. In a “standard” procedure, aniline hydrochloride was oxidized with ammonium peroxydisulfate in aqueous medium at ambient temperature. The yield of polyaniline was higher than 90% in all cases. The electrical conductivity of polyaniline hydrochloride thus prepared was $4.4 \pm 1.7 \text{ S cm}^{-1}$ (average of 59 samples), measured at room temperature. A product with defined electrical properties could be obtained in various laboratories by following the same synthetic procedure. The influence of reduced reaction temperature and increased acidity of the polymerization medium on polyaniline conductivity were also addressed. The conductivity changes occurring during the storage of polyaniline were monitored. The density of polyaniline hydrochloride was 1.329 g cm^{-3} . The average conductivity of corresponding polyaniline bases was $1.4 \times 10^8 \text{ S cm}^{-1}$, the density being 1.245 g cm^{-1} . Additional changes in the conductivity take place during storage. Aging is more pronounced in powders than in compressed samples. As far as aging effects are concerned, their assessment is relative. The observed reduction in the conductivity by ~10% after more than one-year storage is large but, compared with the low conductivity of corresponding polyaniline (PANI) base, such a change is negligible. For most applications, an acceptable level of conductivity may be maintained throughout the expected lifetime.



www.iupac.org/publications/pac/2002/7405/7405x0869.html

Studies on Biodegradable Poly[hexano-6-lactone] Fibers. Part 3. Enzymatic Degradation in Vitro (IUPAC Technical Report)

by T. Hayashi, K. Nakayama, M. Mochizuki, and T. Masuda
Pure and Applied Chemistry, Vol. 74, No. 5, pp. 869-880 (2002)

This report describes how poly(hexano-6-lactone) (PCL) fibers were enzymatically degraded by a hydrolyase in vitro. The extent of degradation of PCL fibers was examined by weight loss, mechanical properties loss such as tensile strength and ultimate elongation decreases, and visual observations by scanning electron

microscopy. The in vitro degradation of PCL fibers was carried out using a lipoprotein lipase (Lipase-PS) as a hydrolase. The kinetic study on the weight loss of PCL fiber accompanying the enzymatic degradation suggested that the degradation of PCL fibers gradually takes place from the surface, not bulk degradation. The rate of degradation was found to depend on draw ratio and crystallinity of the PCL fibers. The strength loss of PCL fibers in the course of degradation took place faster than the weight loss of PCL fibers. Sonic velocity measure-

ments as well as dynamic mechanical properties of PCL fibers were also examined as a function of weight loss of sample fibers with Lipase-PS treatments. It was shown that sonic velocity and value of loss tangent δ changed steeply for undrawn PCL fiber in the first step with enzymatic digestion.

 www.iupac.org/publications/pac/2002/7405/7405x0869.html

New Books and Publications

Free-Radical Polymerization: Kinetics and Mechanism

M. Buback and A. L. German, editors
Macromolecular Symposium, Vol. 182, pp. 1-303, 2002.
Wiley-VCH, 2002, ISBN 3-527-30472-x

Nowadays, many polymerization processes of commercial interest are based on the free-radical principle. The free-radical process is often preferred over other methods of preparation as it is rather robust and less sensitive to trace amounts of impurities. However, until the late 1980s the prevailing opinion was that free-radical polymerization was a mature technique, unable to afford polymers with well-defined structures, and lacking the ability to yield narrow molecular weight distributions and block copolymers.

In 1985, a small group of chemists discussed the possibility of holding a meeting devoted to radical polymerization. Chemists Ken O'Driscoll and Saverio Russo organized such a conference (SML-87) in Santa Margherita Ligure, Italy, in May 1987. It was a great success, demonstrating that there was indeed a renaissance in the radical polymerization field, and it catalyzed an even stronger resurgence immediately afterwards.

In May 1996 the second conference (SML-96) of the same title was held, again in Santa Margherita Ligure, and again arranged by O'Driscoll and Russo. The IUPAC-Sponsored "International Symposium on Free-Radical Polymerization: Kinetics and Mechanism" (SML'01), held in June 2001 in Ciocco, Tuscany, was the third conference in the series, and continued the tradition of holding these meetings in Italy.

SML'01 was attended by 235 scientists from 25 countries, with a good balance between attendees from industry and academia. It is also noteworthy that quite a large number of Ph.D. students, mostly from European countries, attended and actively participated in the scientific program.

During the five-day program, 23 invited main lectures, 11 contributed papers, and 135 posters were presented. Most of the main lectures and some of the short lectures are in this issue of *Macromolecular Symposia*.

The symposium comprised six major themes:

- Fundamentals of Free-Radical Polymerization
- Free-Radical Polymerization in Supercritical Fluids
- Polymer Characterization
- Polymer Reaction Engineering
- Controlled Radical Polymerization
- Polymerization in Heterogeneous Systems


In looking back, it is striking that not a single paper at SML-87 dealt with "living radicals" (in the current sense of the term), Atom Transfer Radical Polymerization or Reversible Addition Fragmentation Chain. At the second meeting, SML-96, these topics were addressed in only a small number of papers. But at SML'01, they dominated large sections of the program.

Through this series of three conferences, important lines of development become clearly visible:

- Our knowledge of the basic kinetics and mechanisms of free-radical polymerization has increased tremendously over the past years, due to the advent of new powerful experimental techniques like pulsed laser polymerization and advanced mass spectrometry.
- The explanations of anomalies in traditional radical polymerization kinetics have been couched in terms that have tended partially to shift from termination towards propagation.
- The overwhelming progress in the area of "Controlled (or Living) Radical Polymerization" (CRP), has created a more definable link between polymerization conditions and polymer (micro) structure.
- Hand in hand with the rapid developments in the chemistry of CRP and in the understanding of its kinetics and mechanisms, increasing attention is

being given to emulsion systems, which will facilitate the commercialization of CRP.

The above advances now offer the opportunity to introduce high degrees of control over physical and chemical properties through the manipulation of molecular weight, polydispersity, intramolecular chemical composition distribution, glass transition temperature, branching and branching distribution, particle morphology in heterogeneous systems, and the incorporation of functional groups. Improved control over the resultant properties will lead to more efficient polymer production and new polymer products.

 www.iupac.org/publications/macro/2002/182_preface.html


C₂₊ Nitroalkanes With Water or Organic Solvents: Binary and Multicomponent Systems

Valerii P. Sazonov, David G. Shaw, Kenneth N. Marsh, Nikolai V. Sazonov, Nikolai I. Lisov, and Mariya F. Chernysheva

IUPAC-NIST Solubility Data Series. 77.

Journal of Physical and Chemical Reference Data, Vol. 31, No. 1, pp. 1-121, 2002.

The mutual solubilities and liquid-liquid equilibria of binary and multicomponent systems composed of C₂₊ nitroalkanes with solvents are reviewed. The solvents (mainly in liquid phase) include water, inorganic compounds and a variety of organic compounds such as hydrocarbons, halogenated hydrocarbons, alcohols, acids, esters, and nitrogen compounds. A total 81 binary, 21 ternary, 2 quaternary, and 1 five component systems whose properties were described in the chemical literature through 1998 are compiled. For 14 systems sufficient data were available to allow critical evaluation. All data are expressed as mass and mole fractions as well as the originally reported units. Similar reviews of gas, liquid and solid solubilities for other systems have been within the Solubility Data Series.

 www.iupac.org/publications/sds/2002/77_abstract.html

Advanced Organic Chemistry Part A: Structure and Mechanisms Part B: Reactions and Synthesis

Francis A. Carey and Richard J. Sundberg
Kluwer Academic/Plenum Publishers, 4th edition, (Part A: 823 pages), (Part B: 965 pages)2001.

A fourth edition, of Carey and Sundberg's two-volume treatise of organic chemistry is now available. Much has happened in chemistry as well as in the field of scientific textbook publishing since the third edition appeared some 12 years ago, so publication of a revised version of this almost classical text is not surprising.

The book covers are both colorful and modern, hinting that a profound revision of the books has been carried out, but this appears not to be the case. On the contrary, the completely black-and-white text looks very similar to its first edition: many of the figures are in fact identical to those used 25 years ago, the style of presentation is almost unchanged, and the division of topics between the two volumes has barely changed. Thus, part A still covers fundamental topics related to the structure of organic molecules (bonding theory, stereochemistry, and conformation) as well as reaction mechanisms in organic chemistry, whereas part B still has the subtitle "Reactions and Synthesis" and gives an overview of the main reactions used in organic synthesis. Furthermore, the material in part A is presented in chapters and sub-chapters, which in essence have been kept unchanged since the very first edition.

The previous paragraph may leave the impression that the new editions of the books are both outdated and dull, but that is not the case (if you don't insist on colorful illustrations to keep the concentration). Although a significant fraction of the material has not been revised at all, the texts appear clear and lucid and serve the material very well. A few figures still give a poor impression, particularly in Part A (for instance on pages 3, 34, 41, and 149), but also in Part B (e.g., pages 200 and 201), and some are still unnecessarily large (for instance on pages 39, 44, and 45 in Part A). It is also noteworthy that there are very few outright mistakes (two rare exceptions are found on p. 100 in Part A and in the table on p. 217 in Part B). And last, but not least, the problems at the end of each chapter have been increased in number and extended in scope and are excellent exercises for those wishing to test their understanding and apply the material presented in each chapter.

Reading of Part A discloses over and over again that most chapters have been updated in a balanced manner with respect to both material and key references. (An exception is chapter 13, which gives a rather shallow presentation of bits and pieces of photochemistry.) One characteristic feature of the book is clearly visible: Advances made in computational chemistry during the last couple of decades have been applied and used pedagogically to analyze structural and mechanistic problems, particularly in discussions of strained molecules and more or less unstable intermediates. But the theoretical treatment is kept at a reasonable level from an organic chemist's point of view; the theoretical discussions therefore serve the purpose and add clarity to the text. As a result, the perspective and style in Carey and Sundberg's presentation of structural and mechanistic

organic chemistry appear different from those found in other comparable textbooks (e.g., J. March, *Advanced Organic Chemistry*, and T. H. Lowry and K. S. Richardson, *Mechanism and Theory in Organic Chemistry*). This is particularly beneficial for the clarity of some of the topics dealt with, and Part A is therefore highly recommended as a thorough graduate-level introduction to structural and mechanistic aspects of organic chemistry.

Part B gives an extensive presentation of a broad selection of organic reactions of synthetic importance, organized by reaction type. Structurally, the book is similar to W. Carruthers' book *Some Modern Methods of Organic Chemistry*, but one significant difference is Carey and Sundberg's much more comprehensive coverage of organometallic reagents and intermediates. Similarities and differences between a variety of reagents are discussed systematically and related to metal properties, particularly the metals' ability to form complexes with substrates and ligands. As a result, the discussion becomes rather mechanistic, and this gives a profound understanding at the molecular level of stereocontrol, which is so important in modern synthetic organic chemistry. Only one chapter, which amounts to 10 percent of the book, is devoted to synthetic planning and retrosynthetic analysis, which is the modern vehicle used to present organic synthesis (for instance in S. Warren, *Designing Organic Synthesis—A Programmed Introduction to the Synthron Approach*, and E. J. Corey and X.-M. Cheng, *The Logic of Chemical Synthesis*). However, intelligent retrosynthesis requires solid reagent knowledge, and to acquire such knowledge, reading of "Advanced Organic Chemistry, Part B: Reactions and Synthesis" is highly recommended.

Reviewed by Leiv K. Sydnes, University of Bergen, Norway.

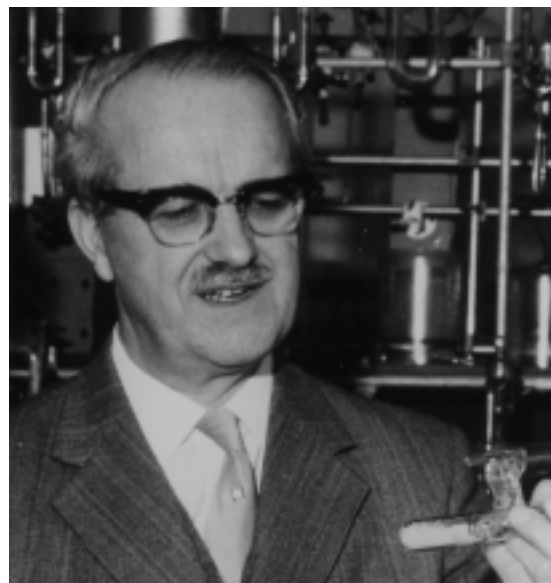


www.wkap.nl/prod/b/0-306-46243-5
www.wkap.nl/prod/b/0-306-46245-1

Modern Coordination Chemistry—The Legacy of Joseph Chatt

G. J. Leigh and N. Winterton, editors
Royal Society of Chemistry, Cambridge, United Kingdom, pp. xviii + 386, 2002.
(ISBN 0-85404-469-8)

The scientific work of Joseph Chatt played a significant role in shaping the field of coordination chemistry as we know it today. The volume under review is an outgrowth of discussions held at the 34th International Coordination Conference (ICCC 34) in Edinburgh, Scotland in July 2000 commemorating Chatt's contributions, while also celebrating the Golden Jubilee of the first meeting of this body organized by Chatt at the ICI



Joseph Chatt

Laboratories at the Frythe, Welwyn (near London). The present work is intended to provide a historical perspective of the scientific achievements of J. Chatt and to show how his contributions have led to current research in the field. These goals have been admirably achieved.

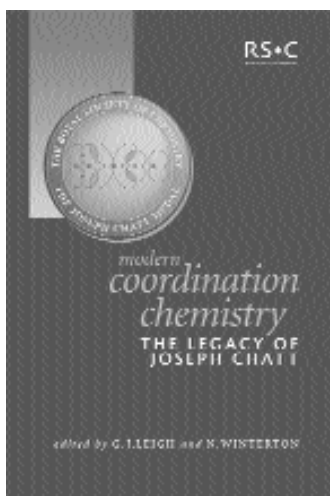
The volume is headed by a section containing personal reminiscences of five close co-workers: G. J. Leigh, R. G. Wilkins, G. A. Gamlen, D. M. Adams, and L. A. Duncanson. Reminiscences of other contributors are also dispersed throughout the subsequent chapters. The next seven sections feature chapters by active contributors organized around the broad range of interests of Joseph Chatt, namely hydrido and dihydrogen complexes, the chemistry of phosphines, transition metal complexes of olefins and other unsaturated hydrocarbons, chemistry related to dinitrogen complexes, biological nitrogen fixation, and patterns in stability and reactivity. One example worth mentioning here is the chapter by G. Frenking titled "The Dewar-Chatt-Duncanson Bonding Model of Transition Metal-Olefin Complexes Examined by Modern Quantum Chemical Methods."

In this review I would like to call attention to two original papers that have become classics in the field of hydridometal complexes. The first of these is "A Volatile Chlorohydride of Platinum" by J. Chatt, L. A. Duncanson, and B. L. Shaw, *Proc. Chem. Soc.* (1957) 343 announcing the synthesis of the new hydrido complex $\text{Pt}(\text{H})\text{Cl}(\text{PEt}_3)_2$. The substitution reactions of this and related complexes were subjected to kinetic studies by F. Basolo and his soon to be famous graduate student H. B. Gray. The non- π bonding hydrido ligand was found to confer a high kinetic trans effect lending support to the polarizability theory promulgated by the Russian school. A summary of this work including an amusing anecdote about a friendly competition between B. L. Shaw and H. B. Gray are recounted in the chapter

by F. Basolo titled "Mechanisms of Platinum Reactions."

A second contribution that had enormous impact is "The Tautomerism of Arene and Ditertiary Phosphine Complexes of Ruthenium(0), and the Preparation of New Types of Hydrido-complexes of Ruthenium (II)," by J. Chatt and J. M. Davidson, *J. Chem. Soc.* (1965) 843-855. This paper established for the first time a reversible oxidative addition of aryl C-H bonds at a low valent metal center as also the remarkable intra-molecular oxidative C-H addition of a methyl group on the chelated diphosphine ligand, 1,2-bis(dimethylphosphino)ethane, *dmpc*. A continuation of this chemistry is presented in a chapter by S. Sabo-Etienne and B. Chaudret and also in a contribution by M. A. Bennett and J. R. Harper.

For readers interested in IUPAC affairs, it is appropriate to note here that J. Chatt served as secretary of the



Commission on the Nomenclature of Inorganic Chemistry (CNIC) from 1959-1963 and continued on as a member through 1971.

This volume makes a unique contribution to the history of coordination chemistry and to the record of contemporary developments in this multifaceted field. I recommend the volume as a necessary addition to institutional libraries and also for the personal book collections of chemists who are active in the practice and in the teaching of transition metal chemistry.

Reviewed by H. D. Kaesz, Department of Chemistry and Biochemistry, University of California, Los Angeles, USA.

 www.rsc.org/is/books/mccdesc.html

Reports from Conferences

Biodiversity

by *Torbjörn Norin*

Biodiversity is an important international topic and the biological implications of biodiversity have been extensively discussed from both scientific and political points of view. However, biodiversity ultimately rests on chemodiversity and, consequently, studies in the field of natural products chemistry offer a deeper understanding of the chemistry of life processes and of complex biological and ecological interactions in Nature. Biomolecular aspects of biodiversity have therefore become an important topic. The scientific challenges and opportunities in the field as well as the possibilities for sustainable utilization of our rich natural resources are enormous. However, they need dedicated attention in order not to threaten future development and welfare.

A few years ago IUPAC's Division of Organic and Biomolecular Chemistry initiated activities in the field of biodiversity. The past president of the Division, Professor Upendra Pandit, took the lead. A series of successful conferences was initiated: the first in Thailand and the second in Brazil. The 3rd IUPAC International Conference on Biodiversity (ICOB-3) was held 3-8 November 2001 in Antalya, Turkey, which was appropriate as it is a country that abounds in biodiversity. Furthermore, Turkey's rich history and diversified cultural heritage provided an extra dimension to the atmosphere of the conference.

The period of the meeting followed, unfortunately, hard on the heels of the tragic events of September 11 in the United States. This presented the organizers with special problems in view of the cancellation of attendance by a number of participants, including several speakers. In some cases the participants could not receive permission to travel from their home countries. However, despite these adverse circumstances, the chairperson of the conference, Professor Bilge Sener of Gazi University, Ankara, through her enormous effort and constructive inventiveness, managed to organize a highly successful scientific event.

The conference listed about 196 participants from 40 countries. The program consisted of five days of exciting interdisciplinary science. Biomolecular aspects of biodiversity and innovative utilization of natural resources were discussed from very diverse points of view—ranging from their botanical, zoological, taxonomic, and genomic expressions to their biomolecular, structural, mechanistic, and functional aspects. There were 11 plenary lectures that covered a range of subjects, including the following:

- Professor William S. Bowers (USA) provided us with exciting information about chemical communication in the insect world and on insect/plant interactions.
- Professor Magid Abou-Gharbia (USA) presented some successful discoveries of new drugs based on natural products.

- Professor S. Qasim Mehdi (Pakistan) gave an account of a current study of the human genome diversity. He presented population studies of protein polymorphism and human leucocyte antigens supported by mitochondrial DNA, autosomal microsatellite diversity, and single nucleotide polymorphism.
- Professor K. Hüsni Can Baser (Turkey) described the fascinating chemodiversity of herbs and other plants producing essential oils, some of which are of commercial significance.
- Professor Neriman Özhatay (Turkey) presented an interesting lecture on the diversity of bulbous monocots, with special reference to the chromosome numbers.
- Professor Brian J. Huntley (South Africa) highlighted botanical aspects of biodiversity, preservation, and sustainable use of natural resources with focus on the flora of South Africa.
- Dr. Jag Mohan Khanna (India) presented a critical review with pro's and con's on the development of new drugs derived from natural products.
- Professor Atta-ur-Rahman, despite duties as the Minister of Science and Technology in Pakistan, was able to attend the conference and deliver a lecture on his successful research in natural product chemistry with the aim to develop new drugs and other useful chemicals.
- Professor Ya-Ping Zhang (China) provided information about the importance of genetic variation for the survival and conservation of species.
- Dr. Priscila de Almeida Leone (Australia) presented a brilliant overview of recent work carried out at AstraZeneca R&D Griffith University, Brisbane, on Australian plants and marine organisms.
- Professor Günay Sariyar (Turkey) presented the final lecture on infraspecific variation of alkaloid content in Papaver species and its chemotaxonomic implications.

In addition to these plenary lectures, there were 30 session lectures and two poster sessions. The almost 60 posters were on display during the whole conference. This arrangement provided excellent opportunities for informal contacts, especially with the young Turkish scientists. One session was devoted to a panel discussion on the means for international cooperation on molecular diversity. A draft report from the IUPAC project on Molecular Basis of Biodiversity; Conservation and Sustained Innovative Utilisation was also discussed (see report page 23).

The social arrangements included a beautiful and memorable ballet performance at the opening ceremony, a lavish get-together mixer, and a relaxed, joyful, and excellent banquet dinner. A conference tour to the old Roman city of Demre was also part of the program.

We thank Professor Bilge Sener for providing us with this opportunity to discuss exciting results and the significant progress in the emerging field of molecular biodiversity. We now look forward to the 4th conference in this series, which will be combined with the 24th IUPAC Symposium on the Chemistry of Natural Products in New Delhi, India 2004.

Torbjörn Norin is past president of the Division of Organic and Biomolecular Chemistry. He is a professor at the Royal Institute of Technology, in Stockholm, Sweden.



www.iupac.org/publications/pac/2002/7404

Macromolecules and Materials Science

by Robert G. Gilbert

The 5th Annual UNESCO school and IUPAC Conference on Macromolecules and Materials Science, held 23-28 March 2002 in Stellenbosch, South Africa, continues a series that has established an excellent reputation in Africa and beyond. The 2002 meeting was attended by about 151 delegates from 17 countries located in Africa, Europe, North America, East Asia, and Oceania.

The school instructed students on the basics of polymer chemistry, physics, and technology and introduced them to some of the latest techniques, such as controlled-radical polymerization. Excellent learning opportunities were provided to young African researchers.

Plenary lectures at the conference provided powerful insights into new polymer technologies, including advances made at SASOL (the South African petrochemical giant). Topics of the plenary lectures included the following: new materials by polymerization of olefins and styrene by metallocene catalysts (W. Kaminsky, Hamburg); green technology, preparation of moisture-proof polymer coatings that leave paper recy-



The participants of the 5th Annual South African UNESCO School/IUPAC Conference on Macromolecules and Materials Science.

clable (R. Sanderson, Stellenbosch); molecular chirality-influencing material properties in subtle ways (B. Novak, North Carolina); and solid state NMR characterization of nanocomposites (L. Matthias, Southern Mississippi).

The conference organizers, professors Ronald Sanderson (Stellenbosch), Bert Klumperman (Eindhoven), Harold Pasch (Darmstadt), and Albert van Reenen (Stellenbosch) are to be congratulated for a program that was outstanding in both breadth and depth.

Professor Robert G. Gilbert is past president of IUPAC Macromolecular Division and is a member of the IUPAC Bureau. He is a professor at the University of Sydney, Australia.



[www.sun.ac.za/unesco/Conferences/
Homepage.htm](http://www.sun.ac.za/unesco/Conferences/Homepage.htm)

Nuclear Analytical Techniques in the Life Sciences

by *Jeroen J. M. de Goeij*

The 7th International Conference on Nuclear Analytical Techniques in the Life Sciences (NAMLS-7), cosponsored by IUPAC, was held 16-21 June 2002 in Antalya, Turkey. The preparations and entire organization were handled by Dr. Namik K. Aras (University of Bahcesehir, Istanbul, Turkey), with the help of Dr. R.M. Parr (formerly of IAEA, Vienna, Austria). About 170 participants from 39 countries, attended the conference. The conference was held in an excellent on-shore hotel with a beautiful panorama. There were no parallel sessions, thereby enabling participants to follow all oral presentations. The program contained sufficient free time and some social and tourist activities, which stimulated the participants in having informal individual and group discussions.

After an introductory session, ten technical sessions followed on a rather wide range of topics: (i) speciation of trace elements in biological materials; (ii) osteoporosis and other bone-related studies; (iii) zinc in human nutrition and biological samples; (iv-vi) reference materials and quality assurance; (vii) selenium in human nutrition and biological samples, (viii-ix) nuclear analytical techniques in environmental studies; (xi-xii) biomonitoring of environmental pollution based on studies of trace elements in lichens, mosses, and other biomonitors; and (xiii) development of methods. One session (x) displayed all posters. In total, 71 oral presentations, including many invited ones, and 119 posters were given. After a peer review, accepted manuscripts will be published in a regular volume of the *Journal of Radioanalytical and Nuclear Chemistry*. Dr. A. Chatt

(Dalhousie University, Halifax, Nova Scotia, Canada) will act as the conference editor.

It was clearly demonstrated that nuclear analytical techniques (NATs)—sometimes together with complementary isotope tracer techniques—are still important, in spite of the development of many other analytical techniques. They may provide interesting additional information, and sometimes even unique information that cannot be obtained otherwise. Following are a few examples: radioactive selenium in the elucidation of the composition and function of selenoproteins, radioactive and stable zinc isotopes in assessing zinc status and utilization of dietary zinc, NATs for the determination of “difficult” elements, for certification of reference materials, and/or for testing other analytical techniques, including speciation.

At the start of the conference, the 2002 Hevesy Medal Award—the premier international award of excellence in radioanalytical and nuclear chemistry—was presented to Dr. Enrico Sabbioni (Joint Research Centre, European Commission, Ispra, Italy). This was in recognition of his excellence through outstanding, sustained career achievements in the field, particularly applications to nuclear analytical chemistry. In his acceptance speech Dr. Sabbioni highlighted advanced research on metal metabolism and toxicity and the irreplaceable role of radioanalytical techniques therein.

The chairman of the NAMLS international committee, Dr. Rolf Zeisler (NIST, Gaithersburg, Maryland, USA) stepped down from this position after many years of service. Dr. Jan Kucera (Nuclear Physics Institute, Rez, Czech Republic) was chosen as his successor. Dr. R.M. Parr was reelected as committee secretary. The next NAMLS con-



(L to R) Prof. Tibor Braun, chief editor of the *Journal of Radioanalytical and Nuclear Chemistry*, donor of Hevesy Medal; Prof. Namik Aras, Chairman, Local Organizing Committee, NAMLS-7; Prof. A. Chatt, president of the International Committee on Activation Analysis Modern Trends in Activation Analysis (ICAA/MTAA); Prof. Enrico Sabbioni, 2002 Hevesy Medal Awardee; and Prof. Robert Jervis, chairman, 2002 Hevesy Medal Selection Panel.

ference will take place in 2005 in a Latin-American country. Information on the conference—as well on previous ones—may be found at the Web address below.

Jeroen J. M. de Goeij is a professor of radiochemistry at Delft University of Technology and at Eindhoven University of Technology, both in the Netherlands.



www.members.aon.at/naml/index.html

Prohibiting Chemical Weapons

by *Edwin D. Becker*

Bergen, Norway, was the site of an IUPAC Workshop on “Impact of Scientific Developments on the Chemical Weapons Convention.” The Workshop, held 30 June to 3 July 2002, brought together 80 participants from 33 countries—scientific leaders in chemical synthesis, analysis, and industrial processing, along with experts in chemical weapons.

The Chemical Weapons Convention, which has been ratified by 145 countries (“States Parties”), went into effect in 1997. It prohibits the use of chemical weapons, provides a schedule for the destruction of existing stockpiles of chemical weapons, and mandates international inspections to verify weapons destruction and to preclude the production of new chemical weapons. The operation of the treaty during its first six years will be examined at a Review Conference to be held by the States Parties beginning 28 April 2003.

The IUPAC Workshop was designed to highlight advances in synthetic methods and in chemical processing technology that could pose additional challenges to inspectors in verifying compliance with the treaty and to identify new analytical methods that might facilitate inspections. A report from IUPAC to the Organization for Prohibition of Chemical Weapons (OPCW) is being prepared. This report will provide scientific input into the political decisions to be made at the Review Conference. As part of the dissemination effort, the report will be sent to IUPAC’s National Adhering Organizations, Associate NAOs, national chemical societies, and the National Authorities of the 145 States Parties. It also will be posted on the IUPAC Web site.

The workshop was held in very pleasant and extremely well-appointed facilities at the University of Bergen. All local arrangements were handled superbly by Dr. Leiv K. Sydnes, professor of chemistry at the



The organizing committee (from left): Alan Hayes, UK; Pieter Steyn, RSA; George Parshall, USA; Douglas J. Raber, USA; Leiv K. Sydnes, Norway; Ted Becker, USA; Detlef Männig, Germany; and Chris Murphy, USA.

Photo credit: L.O. Orjaseter, *Norwegian Chemical Journal*

University, and current IUPAC vice president. IUPAC President Pieter S. Steyn and Dr. John Gee, acting Director of OPCW, addressed the opening session. Background on OPCW and reviews of scientific advances were presented in 21 lectures. Three working sessions permitted the participants to examine major issues in small groups, and a concluding session, chaired by IUPAC Past President Alan Hayes, summarized the findings and provided substantive material for the IUPAC report. Articles based on the lectures will be published in *Pure and Applied Chemistry* early in 2003.

The Workshop was conducted as part of IUPAC Project No. 2001-057-1-020, with financial support from the MacArthur Foundation, Ploughshares Fund, U.S. National Academies, NATO, Ministry of Foreign Affairs of Norway, Amersham Health AS, University of Bergen, Royal Society (London), and the International Council of Chemical Associations.

Edwin D. Becker is secretary general of IUPAC. He has been instrumental in organizing the Chemical Weapons Workshop.



[www.iupac.org/projects/2001/
2001-057-1-020.html](http://www.iupac.org/projects/2001/2001-057-1-020.html)

Conference Announcements



designates IUPAC sponsorship

Rejuvenating the Learning and Teaching of Chemistry 30 November–4 December 2002, Melbourne, Australia

The Royal Australian Chemical Institute's Division of Chemical Education is holding its national conference during 30 November to 4 December 2002 in Melbourne, Australia. The theme of the conference is "Rejuvenating the Learning and Teaching of Chemistry."

The conference will be of interest to both high school and university teachers, and includes a dedicated day for high school teachers (and student teachers) concentrating on "new developments in chemistry" (co-sponsored by the Chemistry Education Association). Other presentations and workshops which will be of interest to high school teachers are spread throughout the program.

The Division is planning a prize for the best lecture or poster presentation by a student or high school teacher. Note that November/December is spring/summer in Australia.

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www.deakin.edu.au/chem_ed_2002

4th Florida Heterocyclic Conference 10–12 March 2003, Gainesville, Florida, USA



The first three Florida Heterocyclic Conferences in March 2000, 2001, and 2002 brought together the academic and industrial communities with an abundance of information on heterocyclic chemistry. These conferences reflected the current interest in the subject, particularly from the industrial chemical community, where pharmaceuticals, agrochemicals, and colorants usually contain at least one heterocyclic ring.

This, the fourth conference, continues in the tradition of its highly successful predecessors. On the first day (10 March), Professors Dan Comins and Alan Katritzky will give a six-hour lecture course on heterocyclic chemistry. This will be an opportunity for chemists who are not familiar with all aspects of heterocyclic chemistry to gain an insight into the fundamental concepts underlying the subject.

A poster session combined with a buffet supper will follow on the evening of 10 March. On the second and third days, experts from academia and industry have been invited to present results from their latest research.

Organic and medicinal chemists of Ph.D. or MSc level, especially industrial chemists from the pharmaceutical, biotech, agrochemical, colorants, flavors, and fragrances industries are encouraged to attend.

Contact: Alan R. Katritzky, Department of Chemistry, University of Florida, P.O. Box 117200, Gainesville, Florida, USA 32611-7200
Tel.: +1 352 392 0554
Fax: +1 352 392 9199
E-mail: katritzky@chem.ufl.edu



www.arkat-usa.org/ark/conferences/FLOHET/conference.htm

12th IUPAC International Symposium on Organo-Metallic Chemistry (OMCOS-12) 6–10 July 2003, Toronto, Canada



This symposium continues a long and distinguished series of IUPAC-sponsored symposia in an important interdisciplinary area of organometallic chemistry and catalysis. OMCOS-12 will seek to bring together researchers from around the world in academia and industry to share the latest results in chemistry involving carbon-metal bonds and their utility in organic synthesis. The area of catalysis, organometallic reagents, synthesis using catalysts and reagents, and materials science have been selected as primary themes. The symposium will explore the impact of new reagents and catalytic processes on pharmaceuticals, agrochemicals, and materials science, as well as provide scientists with a fundamental understanding of chemical reactivity.

Contact: Mark Lautens, Department of Chemistry, University of Toronto, Toronto, ON M5S 3H6, Canada
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E-mail: mlautens@chem.utoronto.ca
or omcos@chem.utoronto.ca



www.chem.utoronto.ca/symposium/omcos12

Calendar of IUPAC Sponsored Conferences

Visit www.iupac.org for complete information and further links

NEW designates a new conference since the last issue

2002

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: snakahama@aist.go.jp

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 to 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.

Visas

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.

2003

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

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

Heterocyclic Chemistry **NEW**
10–12 March 2003 (Pre-conference 9 March 2003)
4th Florida Heterocyclic Conference, Gainesville, Florida, USA.
Prof. Alan R. Katritzky, University of Florida, Dept. of Chemistry, PO Box 117200 Gainesville, FL 32611, USA
Tel.: +1 352 392 0554
Fax: +1 352 392 9199
E-mail: katritzky@chem.ufl.edu

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

High Temperature Materials
19–23 May 2003
11th International Conference on High Temperature Materials Chemistry

(HTMC XI), Tokyo, Japan.
Prof. Michio Yamawaki, University of Tokyo, Department of Quantum Engineering, 7-3-1 Hongo, Bunkyo-ku, Tokyo 113-8656, Japan
Tel.: +81 3 5841 7422
Fax: +81 3 5841 8633
E-mail: yamawaki@q.t.u-tokyo.ac.jp

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

Ionic Polymerization **NEW**
30 June–4 July 2003
International Symposium on Ionic Polymerization, Boston, Mass., USA.
Prof. R. P. Quirk, Department of Polymer Science, The University of Akron, Akron, Ohio 44325-3909, USA.
Tel.: +1 330 972 7510
Fax: +1 330 972 5290
E-mail: quirk@polymer.uakron.edu

Organo-Metallic Chemistry **NEW**
6–10 July 2003
12th IUPAC International Symposium on Organo-Metallic Chemistry Directed Towards Organic Synthesis (OMCOS-12), Toronto, Ontario, Canada.
Prof. Mark Lautens, Department of Chemistry, University of Toronto, Toronto, ON M5S 3H6, Canada
Tel.: +1 416 978 6031
E-mail: omcos@chem.utoronto.ca

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

IUPAC 39th Congress
10–15 August 2003
—see next page—
and Young Chemists
—see page 18—



August 10-15 août 2003
Ottawa, Canada

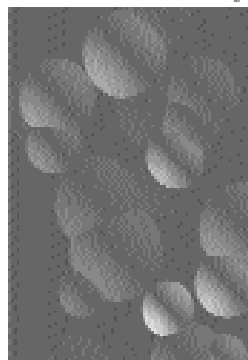
39th IUPAC Congress and 86th Conference of the Canadian Society for Chemistry 39^e Congrès de l'IUPAC et 86^e conférence de la Société canadienne de chimie

Pivotal Speakers / Conférenciers

Jean-Polant, University of California, Berkeley
John C. Polanyi, University of Toronto
Richard C. Smalley, Rice University, Houston

La chimie aux interfaces

Chemistry at the Interfaces



Call for Abstracts

The call for abstracts will appear in the second announcement which will be mailed in November 2002. An abstract submission form will be included in the second announcement.

The deadline for receipt of abstracts will be February 14, 2003. Two abstracts of a complete paper will be published and distributed at the Conference. Further information and the program abstract submission form will be provided in the second announcement.

Appel de communications

L'appel de communications sera publié dans le deuxième avis de conférence qui sera envoyé en novembre 2002 aux personnes qui en font la demande.

Les dates limites de réception des résumés ont lieu en février 2003. Les résumés de toutes les communications complètes seront publiés et distribués à la conférence. De plus, il y aura deux exemplaires de résumés de toutes les communications complètes distribués à la conférence.

Symposia

- 3M Teaching Fellows
- Activation of Small Molecules by Early Transition Metals
- Advanced Spectroscopic Techniques for Characterization of Organometallics
- Biogeochemistry of Metals in the Environment
- Canadian Participation in IUPAC
- Carbohydrates and Chemical Glycobiology
- Catalytic Asymmetric Synthesis
- Chemistry of Nucleic Acids
- Combinatorial Chemistry
- Coordination with Amine as Macromolecular Systems: From Nature to Chemistry to Functional Properties
- Coordination Chemistry: From Hydrogen-Bonding to Metal-Organic Materials
- Crystal Engineering: Supramolecular Synthesis of Advanced Materials
- Designed Surfaces/Interfaces for Catalysis and Separation
- Environmental Quality and Human Health in the 21st Century
- Frontiers in Genomics and Proteomics
- Frontiers of Electrochemistry
- GM0 Analysis-What's Needed? What's Possible?
- Green Chemistry
- Mechanisms in Homogeneous Catalysis
- Metal and Metalloid Containing Macromolecules

- Metalloproteins and Metals in Medicine
- Modeling and Design of Polymers/Carbon Processes
- Nanoparticles and Carbon Nanotubes: Natural and Artificial Chemistry
- New Horizons in Metal Catalysis: Chemistry: From Molecules to Materials
- NMT and NIT of Materials
- Organic Synthesis and Chemical Biology
- Progress in Heterogeneous and Homogeneous Synthesis, Characterization and Device Applications
- Proton Tunneling at Work: Dio, Nano, Opto
- Public Image of Chemistry
- Radicals in Chemistry and Biology
- Recent Advances in Living Polymerizations
- Recent Developments in Physical Organic Chemistry
- Synthetic/Inorganic Organic Synthesis
- Supramolecular Chemistry and Self Assembly
- Surface Phenomena in Polymers
- Syntheses in Process of Airless Early
- Synthesis Radiation and the Canadian Light Source
- Theoretical Chemistry Applied to the Environment
- Water Chemistry: Past, Present and Future

Site and Date

The 39th IUPAC Congress and 86th Conference of the Canadian Society for Chemistry will be held at the Ottawa Congress Centre, as well as at the Westin Hotel, Ottawa, Canada from August 10-15, 2003.

Lieu et date

Le 39^e Congrès de l'IUPAC et la 86^e conférence de la Société canadienne de chimie auront lieu au Centre des congrès d'Ottawa, ainsi qu'à l'Hotel Westin à Ottawa, au Canada, du 10 au 15 août 2003.

Congress President /

Président du congrès:
Alex Murray, University of Victoria

Chair, Program Committee /

Président du comité de programmation:
Dyall Ibbett, University of Guelph

Secretary / Secrétaire

Mail all correspondence to:
Abstracts and program chair:

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Ottawa

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1200 Montreal Road
Ottawa, Ontario, Canada K1A 0R6
Ottawa (Ontario) Canada K1A 0R6

Tel/Fax: (613) 992-0114
Tel/Fax: (613) 992-0760
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www.nrc.ca/confserv/iupac2003



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