News from IUPAC

IUPAC moves to a project-driven system

The organization and management of IUPAC's scientific work will soon begin a transition to a system that emphasizes individual projects, rather than the allocation of Titular Members among a large number of Commissions and Committees. By a vote of 20–0, with two abstentions, the Bureau has approved an integrated programme proposed by the Strategy Development and Implementation Committee (SDIC) and the Committee on Project Evaluation Criteria (CPEC) that will: (i) assign to greatly strengthened Division Committees the primary responsibility for overseeing the initiation, approval and management of scientific projects, and (ii) establish a uniform procedure for evaluating and funding such projects. Some aspects of the new programme will begin immediately, but there will be a gradual phase-in over the next three years, as Division Committees, Commissions and other IUPAC bodies develop plans for long-range implementation of the new system, as well as proposals for specific new projects.

Changes in the organization and management of IUPAC's scientific work

To meet the challenges occurring world-wide in chemistry and the chemical industry, IUPAC has developed a Strategic Plan to redefine its role as the international organization principally responsible for the promotion of the Chemical Sciences. This plan provides guidelines for the Union to respond to the globalization of science, to the expansion of the borders of chemistry in a wide range of scientific fields, to the interdisciplinary nature of modern chemistry and to the service of chemistry to society. The Strategic Plan articulates the policy of the Union and provides general guidance to our operating arms, the Divisions and the Standing Committees.

The present structure of the Union precludes the fulfilment of many of its central scientific functions, as reflected in organizational fragmentation and resulting hindrance in the inception and conduct of horizontal interdisciplinary projects. The founders of IUPAC envisioned and made provision for the organization and action of a dynamic Union. In time, the concept of a changing structure was replaced by the current system of long-term Commissions, with little opportunity for Divisions to plan for scientific renewal and growth. Significant past attempts for the restructuring of IUPAC by the creation of the Pool Titular Members and by the interdisciplinary unification of Divisional activities have not been effective. IUPAC must build on past successes but must aim toward its future accomplishments, impact and image.

The Bureau has now approved a policy and an operational programme based on the conceptual framework that the Union represents and serves the entire world chemistry community. The objective is to improve the quality, relevance, international impact and effectiveness of the Union's scientific work. The integrated programme constitutes a holistic plan, which rests on major changes in the responsibilities of the Division Presidents and Division Committees, in the election procedures on a Division level, in project evaluation, and in the future function of the Commissions.

I would like to articulate explicitly and clearly that these changes are aimed at the enhancement of IUPAC's future contributions and impact, and do not in any way question the accomplishments and dedication of IUPAC's bodies and of the eminent scientists who have collectively contributed, over the decades, to the Union's reputation.

I am delighted that the Bureau has approved the integrated programme, some elements of which will begin immediately. To implement the programme, we will consult closely with our National Adhering Organizations, which collectively constitute the ultimate authority of the Union and are in turn accountable for the public and scientific resources used by all IUPAC bodies. The newly approved programme will shape IUPAC's role towards the 21st century

Professor Joshua Jortner
President, IUPAC

The programme approved by the Bureau is designed to give clear direction for the Union to

- revitalize its scientific activities,
- ensure the selection of only high quality projects to bear the IUPAC label,
- encourage participation by the world-wide chemistry community,
- optimize the use of IUPAC's limited financial resources, and
- simplify management and accountability.

There are five principal components of the new programme:

1 The Union will gradually replace its long-time practice of allocating resources by the assignment of Titular Members to Commissions and Committees, with a system in which funds are directly allocated to carry out approved projects. The purpose of the change is to ensure that high priority projects are adequately funded and can be started and completed as expeditiously as is feasible. Uniform IUPAC-wide procedures will be implemented by January 1999 to evaluate proposed projects for quality and suitability, and to fund them within individual Divisions or from central IUPAC funds. Generally, each project will be carried out by a limited-term Task Group. The new system is designed to simplify management, reduce bureaucratic rules and clarify accountability. The Executive Summary of the report by the Committee on Project Evaluation Criteria can found on page 167.

2 Division Committees have been given the responsibility for seeking out ideas for projects, evaluating proposals and managing approved projects. The Division Committees will be strengthened by new procedures for the nomination of their Members. The Bureau has given approval, effective immediately, for an interim modification of Division Committees as needed to ensure necessary expertise and breadth. Over the next three years, existing Commissions are expected to continue to provide the primary source of new projects, but efforts will start immediately to solicit ideas and interested participants for new Task Groups from the world-wide chemistry community.

3 Beginning in 2002, there will be a major redistribution of funds, with increases in Division budgets, the establishment of a central pool of money to support interdisciplinary projects and projects that require resources beyond the scope of an individual Division or Standing Committee, and the termination of separate budgets for the General Assemblies. Council will be asked to amend Bylaw 4.307, which currently describes the 'right' of Titular Members to receive travel reimbursements, irrespective of responsibility for projects or other activities.

4 The role of Commissions will change drastically beginning in 2002. As an initial step, Council will be asked in 1999 to exercise its responsibility under Bylaw 4.302 to decide not to continue any existing Commission beyond the end of 2001. This action will permit each Division Committee to utilize the period 1999–2001 to take a fresh look at its overall programmes, to consider how best to allocate its resources, and to determine the optimum way to provide for oversight of activities and continuity of programmes. During this period (and thereafter) if a Division Committee believes that a new Commission is needed for a particular purpose, it may request the Bureau and Council to form such a Commission by making a persuasive case under the procedures of Bylaw 4.301, including specification of the life of the proposed Commission. Such a Commission might be established, for example, to generate a long-term strategy and develop IUPAC's role in a new area or to accomplish an important short-term task. Funding will be provided as needed to accomplish the objectives.

5 After 2002, it is anticipated that there will be a substantial reduction in the number of Commissions and a significant increase in the number of short-term Task Groups. These changes will require reconsideration of the 'membership' of the Divisions—currently defined in the Bylaws as the Titular and Associate Members of Commissions and Division Committees. The Secretary General and Division Presidents have been charged by the Bureau to develop proposals that could be acted on by Council in 2001. In addition, the role of National Representatives will be re-examined. The plan approved by the Bureau includes provision for a limited number of nonvoting National Representatives on Division Committees, but additional mechanisms are to be developed to enhance participation by a large number of scientists from both large and small countries.

Secretary General's Report

Edwin D. Becker

As reported in the article on pp. 163, the IUPAC Bureau has approved a policy that will phase in major changes in the organization and management of our scientific work. In this column I would like to provide some information on the discussions that led to the Bureau decision and to answer some questions that have been raised by many members of IUPAC bodies.

Bureau discussion. Every Member of the Bureau recognized the importance of this decision for the Union as it positions itself for the next decade—indeed, the next century. The final vote, 20–0, with two abstentions, came only after a careful analysis of the programme and consideration of its long-range impact. During the last few years, there have been extensive discussions of the reasons why the Union must make major changes in its operations to ensure its survival and enhance its role in world-wide chemistry. The proposals made by the *ad hoc* Strategy Development and Implementation Committee after a year's study and debate, provided an integrated programme to effect the necessary changes.

The SDIC recommendations were widely publicized and elicited many comments, both within and outside the Union. In particular, several Division Presidents received extensive input from members of their Divisions who will initially be the most affected by many of the changes. There was widespread support for most or all aspects of the SDIC programme, but also a number of strong criticisms and suggestions for specific alterations in the proposals.

Future role of Commissions. Probably the most contentious issue was the recommendation by the Bureau that in 1999, Council exercise its responsibility under Bylaw 4.302 to decide not to continue any existing Commission beyond the end of 2001. Several very reasonable questions have been widely asked: (i) 'Since the work produced by most Commissions, Subcommittees and Working Parties has generally been highly regarded, why should the 37 Commissions not be continued indefinitely?', (ii) 'Most ideas for new projects have emanated in one way or another from Commissions. If they are not continued, where will new projects originate?', (iii) 'Without continuing Commissions, who will carry out projects (if good ideas can somehow be generated elsewhere)?', (iv) 'If there are few or no Commissions, how will National Representatives be accommodated?', (v) Without a large cadre of Commission members, who will comprise the membership of the Divisions?, (vi) 'How will members of short-term Task Groups develop the kind of knowledge about IUPAC and the loyalty to the Union that characterizes many Commission members?'

These are all very important issues. Let me try to explain the reasoning behind the SDIC recommendations regarding Commissions, which were endorsed by the Executive Committee and now approved by the Bureau. First, the organizational changes recommended by the SDIC are not intended to demean the accomplishments of the members of Commissions or any other IUPAC bodies, nor should the discontinuance of a Commission be interpreted as indicating lack of support for the discipline or special area that it represents. If individuals and/or a group of chemists are carrying out valuable work under the current organizational framework, there is no *a priori* reason why they cannot carry out equally good (perhaps even more effective!) work under a number of other organizational arrangements. There is nothing essential or unique about our current Commission structure, but it does have a long history and some disadvantages, as well as advantages.

According to the *History of IUPAC, 1919–1987*, Commissions originated in 1922, and for over 25 years a relatively small number of Commissions (of the order of 10) were established, discontinued, and re-established in modified form. The names of some of the original Commissions suggest that they were forerunners of some current Commissions [e.g. Chemical Elements (including Atomic Weights), Reform of Nomenclature, Thermochemical Standards, Preservation of Foodstuffs]. After World War II, chemistry expanded rapidly,

and chemists thought of themselves primarily as specializing in one branch of the field. As a result, in about 1950, IUPAC formed Sections on Physical, Inorganic, Organic, Biological, Analytical and Applied Chemistry, with the existing Commissions assigned to Sections, in some instances only one Commission in a Section. However, the Sections were allowed to form additional Commissions and predictably they did, usually by slicing the discipline into subspecialties. By 1955 a total of 33 Commissions were in existence—many of them continuing to the present. Certainly there have been many changes, but the overall structure has been relatively static for 45 years, in spite of continuing pleas from IUPAC Presidents for more flexibility (including Arne Tiselius, already in 1955; Jacques Bénard in 1973; Heini Zollinger in 1981; and Alan Bard in 1993).

Future division programmes. Now, back to the present. Over the last three years a major initiative of the IUPAC Officers, as endorsed by the Bureau, has been to articulate the long-range mission and goals of the Union and, with the help of the SDIC, to develop a Strategic Plan. This gives a sense of direction to the Union as a whole, but it is only a framework and must be 'fleshed out' in practical terms. So far as IUPAC's scientific work is concerned, no single committee—not the Bureau, not the Executive Committee, not the SDIC—can provide expertise over all chemistry. Moreover, no one in IUPAC wants a 'top-down' directed programme; it is not likely to be very good, and it certainly won't work in a volunteer organization. What we need is to have each of the seven Divisions develop its own coherent programme and to have Divisions jointly determine how they can best address many increasingly important interdisciplinary fields. Each Division needs to take a fresh look at its part of chemistry, without the need to accommodate and/or justify a set of pre-existing Commissions. Permanent Commissions, by their existence, tend to emphasize fragmentation and specialization in chemistry, rather than a coherent whole.

During the next two years, it is anticipated that each Division will consider its future directions—and IUPAC's overall future scientific directions—in a thorough and objective manner. Current Commission chairmen can and should play a major role in this process in their capacities as experts in specific aspects of chemistry, not as advocates for maintaining the structure as it currently exists. We also need the participation of leading scientists throughout the world who are not currently directly involved in IUPAC work but who can help the Union decide on future directions. In some instances a Division, or several Divisions acting together, might well set up *ad hoc* planning and strategy groups or even convene a small working conference to elicit broad advice on how IUPAC programmes can best meet the world's scientific needs in particular areas.

In developing their programmes, Division Committees will have a range of available options. They may appoint *ad hoc* advisory, strategy or planning groups as needed. They may appoint Task Groups to carry out individual projects, which can cover a variety of topics. They may propose augmenting the Division Committee if needed, to ensure continuity and oversight in particular programmes. If a Division Committee believes that a particular area requires a longer term Commission (for example, to develop a programme in a new area of chemistry), it may propose the creation of such a Commission, with a well defined mandate and a termination date. Money, rather than the number of Titular Members, will be the principal resource allocated to Divisions and will be used by Division Committees to support their projects, to obtain advice and to manage their programmes. I do not know what the ultimate mix will be, but I hope that each Division will take advantage of the flexibility and opportunities that will be available under the new system.

A project-driven system. What about ideas for projects and people to serve on Task Groups? Over the next three years, I expect that very many projects will be generated in the existing Commissions, but we will also reach out to the entire chemistry community for specific proposals for projects. I believe that some proposals will eventually come from organized groups, such as National Adhering Organizations, national chemical societies and regional federations, and industry groups. However, most will arise, as they do now, from interested groups of scientists, who discover in the course of their work areas to which IUPAC should contribute. We will make positive efforts to solicit ideas at conferences and symposia and from journal editors. By 1 January 1999 we expect to have a mechanism in place to insure that each proposal is subjected to a critical evaluation; if it is approved, the necessary funding can be made available immediately—not at the beginning of the next biennium, as has usually been true in the past. We will provide more details on the evaluation process at a later date, and Divisions will make arrangements to phase in this procedure. Some Divisions will probably find only small changes in the way projects are evaluated, but I firmly believe that this uniform project-driven system will provide very significant advantages in initiating, managing and completing high quality scientific efforts. Meanwhile, of course, existing projects will continue, and many will be completed during the next three years. The Executive Summary of the report by the Committee on Project Evaluation Criteria can found on the next page.

As is true now, the people who work on projects are those who have the necessary expertise and also the interest to take on and pursue the job. Individuals who are currently members of Commissions, Subcommit-

tees and Working Parties meet these criteria, and will undoubtedly be heavily represented on Task Groups, but other scientists who do not necessarily want to make a long-term commitment to IUPAC can and should participate in Task Groups in line with their interests and expertise.

IUPAC's human capital. The membership of Divisions continues in its present form to the end of 2001, and National Representatives will continue on Commissions during this transition period. The Bureau has not yet decided how best to ensure the continuation of viable Division memberships, and precisely what recommendations to make to Council in 2001 for changes in Bylaws, but there are a several options to consider as we gain experience during the next three years. The new structure of Division Committees allows for a limited number of National Representatives, and we will welcome widespread participation on Task Groups from all countries. However, we must consider additional possibilities to ensure a very wide participation from just as many countries as is feasible. I will be in contact with NAOs regarding these issues.

One very important mechanism for maintaining contact with a large group of people who are interested in IUPAC is the Fellows Programme, established by Council in 1997. Everyone who completes service on an IUPAC Commission, Committee, Subcommittee, Working Party or Task Group is eligible for appointment as a Fellow. Of course, not everyone is interested in continuing contact with the Union, but our experience so far in 1998 is that most recently 'retired' IUPAC members welcome the opportunity. With electronic communication methods, it is easy and relatively inexpensive to provide information on IUPAC programmes and to solicit advice and comments from Fellows. After 2001, we should have over 1000 Fellows, and I anticipate that a significant fraction of future Task Group members will continue involvement with IUPAC.

Problems solved and continuing issues. During the two months before the Bureau meeting, I met individually with several Division Presidents and Vice-Presidents and corresponded extensively with others, in an effort to understand the potential problems that each foresaw in implementing the SDIC recommendations and to develop with them specific ways of overcoming the difficulties. Just prior to the Bureau meeting, the Division Presidents held their annual meeting with the Secretary General, devoted almost exclusively to a joint discussion of the SDIC proposals. In particular, we tried to design procedures by which we can guarantee the continuity of IUPAC's important work and ensure the continued recruitment of talented scientists who volunteer to carry out this work. In the end, as the Bureau vote indicates, there was almost unanimous agreement that this programme should be implemented. However, it was also clearly recognized that not all problems are solved and that all of us in the Union must continue to address the issues of implementation during the three-year period before the new system becomes fully effective.

I have had an opportunity to see many of the very thoughtful comments submitted by members of various IUPAC Commissions and Committees, and my own views have been significantly modified as a result. I have tried here to respond to some points and to explain the underlying purpose of what sometimes may initially appear to be arbitrary or unnecessary changes in traditional modes of organization and operation within IUPAC. There are many other aspects of the new system that can be explored further. I invite questions and suggestions, preferably by email, directly <tbecker@nih.gov> or via the Secretariat <secretariat@iupac.org>.

Committee on Project Evaluation Criteria

Executive Summary of the Report of the Committee on Project Evaluation Criteria

Introduction

The key attributes desired of the Project Evaluation Process are that it provides a simple and rapid method for selecting projects to be carried out by IUPAC and its Divisions. It is expected that most of the steps in the process will be carried out by email. Decisions on funding will be made throughout the course of the year as projects are submitted. Most projects will be evaluated and funded by the various Division Committees from their budgets. Interdivisional, Standing Committee and 'large' projects will be evaluated and funded by the Project Committee of the Bureau from a separate fund.

The two general qualities all projects must have to be funded are that they represent good science and that

they are something that IUPAC, as opposed to some other organization, should do.

Process description—Division Committee projects

Any individual or group that wishes to submit a project for funding by IUPAC will be able to download a Project Submission Form and Instructions from the IUPAC Website, or obtain a printed copy from the Secretariat. After completion, the form, and any supporting material, is sent to the Secretariat for distribution to the appropriate Division Committee. If the Division Committee decides to consider the project further, it chooses three reviewers from those named on the submission form or selects reviewers based on its own experience. The Secretariat then distributes the project materials to the reviewers, assembles the reviewers' comments and distributes them both to the Division Committee and the project submitters. After receiving the comments, if any, on the reviews by the project submitters the Division Committee makes a funding decision.

Process description—Project Committee projects

Interdivisional Projects are first evaluated by the relevant Division Committees. The project materials are then forwarded, along with any comments by the Division Committee, to the Project Committee. They evaluate the materials submitted and make their decision on funding. The same process is followed for projects in the area of a Standing Committee, except that the original evaluation is by the Standing Committee. 'Large' projects are those that would require more than 10% of the budget of a Division. These would also be forwarded by the Division Committee to the Project Committee for a funding decision.

Project management

The technical aspects of all projects would be managed by the Division Committee(s) or Standing Committee, including those funded by the Project Committee. For centrally funded Projects, the Project Committee would review project expenditures. Each project group would submit progress reports at agreed-upon intervals.

Retrospective evaluation

Projects will be retrospectively evaluated by the Evaluation Committee of the Bureau two to three years after completion. The criteria used will be those suggested by the project group in its proposal and others chosen by the Committee. The CPEC has recommended that projects completed in the past few years be evaluated in 1999.

A guest essay

What is the role of science in developing countries?

José Goldemberg*

After the Second World War, a small technical elite arose in developing countries such as India, Pakistan, Brazil and Iraq who had been educated as scientists in the industrialized world. They thought that by pushing for 'Manhattan project'-type enterprises in nuclear energy, electronics, pharmaceuticals or space research they could leapfrog the dismally low level of development of their countries. India, for example, started a nuclear energy programme that mobilized thousands of technicians and cost hundreds of millions of dollars but failed to meet power demands.

What my scientist colleagues and national leaders alike failed to understand was that development does not necessarily coincide with the possession of nuclear weapons or the capability to launch satellites. Rather, it requires modern agriculture, industrial systems and education. The technical elite naively believed that spin-offs from their nuclear energy or space programmes would somehow convert their countries to 20th-century industrialized states. Instead, there were heavy economic and political costs. In India, for example, such programmes led to the development of nuclear weapons—which only encouraged Pakistan to do the same—while many basic human needs such as health and education were not given the support they needed.

In my view, this scenario means that we, in developing countries, should not expect to follow the research model that led to the scientific enterprise of the USA and elsewhere. Rather, we need to adapt and develop technologies appropriate to our local circumstances, help strengthen education, and expand our roles as advisers

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in both government and industry. In this way, we can prevent the 'brain drain' that results when scientists are not in touch with the problems of their home countries or when they face indifference—and poor financial support—from their governments.

In Brazil, the use of ethanol as fuel is one example of how this approach can work.[1] By encouraging the wide use of ethanol produced from sugarcane—a traditional crop in the country—as fuel to replace gasoline, the government of Brazil was able replace half of the gasoline used by automobiles in the country (about 200 000 barrels of ethanol per day) with a renewable energy source. In so doing, Brazil became a pioneer in an area that had been neglected by industrialized countries. The entire technology, from the agricultural to the industrial phase, was developed or improved upon by local scientists and technologists. I and other Brazilian scientists first had to convince the government that this approach was technically feasible, even though it had been ignored in industrialized countries. To do this, we had to address questions regarding motor technology, environmental concerns, and the trade-off between raising crops for food vs. fuel.

In general, the misconceptions held by the technical elite are derived from an idea cherished by many in the developing world, that pure research leads to technological development and then to products that open new markets or conquer existing ones (see Fig. 1, model A). This naive 'linear theory' or 'cradle-to-grave' approach to science and development served as a blueprint for the establishment of the National Science Foundation[2] in the USA and was widely copied throughout the world. However, that model fails to stress the interaction that should occur among the phases. As one moves from pure research to technological development and then to production and marketing, unanticipated problems arise that require re-examination and adaptation at the earlier stages.

More realistic are models B and C.[3] Model B corresponds, generally speaking, to present practices in the USA, where some overlap exists between the successive stages. Model C illustrates the Japanese practice of having the three phases completely superimposed. These are the more realistic models that developing countries should follow. In models B and C, practical needs—that is, demand—influence supply, namely, the type of pure research that is done. For example, after the introduction of solid state devices such as transistors made possible the expansion of switchboarding in telephone services, industrial laboratories such as Bell Laboratories lavishly financed solid-state physics.

In developing countries, government goals and the 'demand side' pull are often lacking. As a result, universities and research centres have become isolated from the rest of the country in an 'ivory tower', more connected to research centres in Europe or the USA than to the obvious needs of industry, agriculture and education in their own countries. Science and technology budgets receive little support from the private sector and instead depend on the national treasury.[4] Heavy government bureaucracies wind up cultivating whatever science and technology is fashionable in the developed countries, waiting indefinitely for the time when such competence would trigger development.

What, then, is a realistic view of the role of basic science in developing countries? After all, many outstanding scientists born and educated in developing countries have contributed significantly to the advancement of science. Talent exists everywhere. What can they do to help their countrymen in solving the problems of development? The answers, in my view, are the following:

1 Help adapt technology to local circumstances. Even when technologies are imported from abroad, research is necessary to make them work. Rather than insisting on developing indigenous technologies, when abundant and well-proven technologies exist, scientists can help choose the right ones, given the local environment and available raw materials, and learn how to use them. An example is given by the 'green revolution.' Despite its shortcomings, this

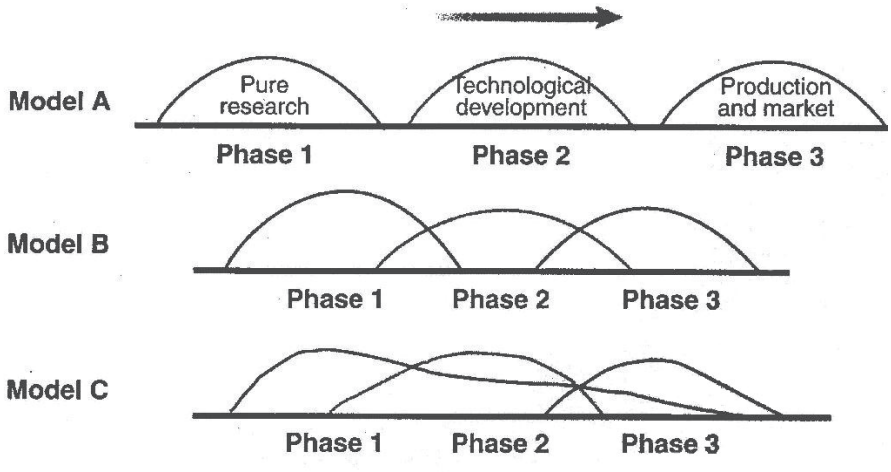

Fig. 1

'imported' technology, when applied properly in the developing world, helped eradicate hunger. Problems with the use of pesticides and fertilizers arose because of abuses by commercial interests and because, owing to a lack of knowledge, users and local scientists failed to provide the expertise or make the adaptations necessary to make the best use of the imported technology.

2 Incorporate new science into education. Development requires a well-trained work force; therefore, high-quality education must be put in place early in development. The teaching of modem science in engineering or medical schools cannot be restricted to the same old classical textbooks but has to be done by active scientists who read the current literature and are capable of conveying the latest advances to their students. This approach worked well in the 19th century during the Meiji restoration, which brought Japan into the modem world.

3 Be involved in government. Science and scientists are an important element in choices and decisions made by governments and can make a difference. For example, at one time the Brazilian government had to set the reservation boundaries for the Yanomamis, a primitive group of some 10 000 indigenous people living in the mineral-rich Amazon basin. The issue was whether to set up one large, or several small, reservations. The military and the mining groups favoured small reservations, as Indian reservations are 'out of bounds' for them according to Brazilian law and could restrict their movements in that region. But anthropologists advised that this solution would destroy the Yanomami civilization, because these Indians were accustomed to long-distance migrations. As the federal Secretary for Science and Technology, I argued for one large reservation, a solution that was adopted.

I also helped to mediate a conflict in Brazil between multinational enterprises that had computer technology and wanted free access to local markets, and local entrepreneurs who wished to preserve the markets for themselves. In the 1980s, the local entrepreneurs convinced the government to establish high import barriers, virtually isolating the region and condemning it to use obsolete technology. I helped resolve this issue by convincing foreign companies and local enterprises to set up joint ventures in which the technology came from abroad but the manufacturing was local.

Scientific research is motivated not only by curiosity or love for science, but also by fashions and the perception that some areas of research are more rewarding than others. The current emphasis given to costly therapeutics for the treatment of AIDS is counterproductive in developing countries, where a vaccine against the disease is the only real hope. It is important that developing countries avoid the allure of costly but ineffective programmes and establish a system that rewards solving practical problems. Although that emphasis may seem to stray from the tradition of academic research, the truth is that many seemingly mundane problems require very sophisticated tools and technologies. Science can also accelerate progress. This has occurred in agricultural research, which is highly advanced in developing countries such as Mexico (corn), Brazil (soybeans and sugarcane), and the Philippines (rice).

In conclusion, my experience has shown that the transition of a country from developing to developed is a complex process that requires facing up to the established interests in society. The impetus for this has to come not only from scientists, but from other sectors of society as well. In a world where globalization and competitiveness are the rule, progress requires that developing countries find areas in which they are significantly better than their competitors because of a better trained work force, favourable natural resources, or scientific and technological capabilities. Science and scientists can play an important role in determining those choices and implementing development strategies.

Acknowledgement

I thank G. Moscati for useful discussions.

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Reports from IUPAC sponsored symposia

Fifteenth international conference on chemical education: chemistry and global environmental change. Cairo, Egypt, 9–14 August 1998

Symposium: tertiary vocational training in chemistry related to health care

The International Conferences on Chemical Education, are held biennially under the auspices of UNESCO and the International Union of Pure and Applied Chemistry (IUPAC). The 15th Conference was held in Cairo from 9–14 August 1998, organized by the Chemistry Department in the Faculty of Science at Ain Shams University, Cairo, Egypt. The theme for this conference was '*Chemistry and Global Environmental Change'*. The pivotal role of IUPAC in the development, and education in, chemistry means that IUPAC has an inevitable and essential role in these conferences. It follows that its Committee on the Teaching of Chemistry (CTC) is the essential interface between IUPAC and the organizers of the International Conferences on Chemical Education.

In 1995, as part of a reorganization within IUPAC, the Clinical Chemistry Division and the Medicinal Chemistry Section were amalgamated into a new Division of Chemistry and Human Health. Up to this point both the Medicinal Chemistry Section and the Clinical Chemistry Division were represented at CTC by Prof. C.R. Ganellin and Dr H.G.J. Worth, respectively. When the theme for the 15th Conference was announced, it was agreed that it would be appropriate for the new Division (which was in a gestational stage at this point), to make a contribution. Professor Ganellin and Dr Worth agreed to organize a joint symposium on behalf of the new Division. Their programme, which was endorsed by both the CTC and the Chemistry and Human Health Division, is shown in the Appendix. The symposium was presented on the morning of Wednesday 12 August 1998.

Both Clinical Chemistry and Medicinal Chemistry are important areas of science, where chemistry graduates can (and do) make major contributions in the application and development of the science. They are areas that are not always well understood by teachers of chemistry, and consequently students are not always encouraged to embark upon careers in these challenging areas. This was the general theme of the symposium with specific areas highlighted in each of the individual presentations. Dr Worth defined the role of the clinical chemistry department within the hospital laboratory service, and indicated the interrelation between chemists and other professional groups, particularly medical graduates, and the role of the chemist within this. Dr Khatami's presentation indicated the difficulties of the development of clinical chemistry within developing countries. These problems are often similar to those in so-called developed countries, but perhaps more intense. Finally, Dr Duffus considered toxicology as a speciality within clinical chemistry, and indicated the particular problems that there are in training in toxicology for chemists. With the increasing awareness of the relationship between chemicals and the environment, it is the chemist whose advice is frequently sought, but who is often poorly educated in this respect, as toxicology does not feature in the curriculum of many chemistry graduates.

In the section on Medicinal Chemistry, Professor Ganellin indicated the essential role that is played by chemists in the development of drugs within the pharmaceutical industry. It is well recognized that pharmaceutical companies prefer to recruit competent organic chemists with good potential and train them in medicinal chemistry. This emphasizes the importance in training good synthetic organic chemists and to include some insight into the requirements of medicinal chemistry in order to encourage the good chemists to look for careers within the pharmaceutical industry. Dr Kobayashi gave a comprehensive overview of the pharmaceutical industry world-wide, and indicated the role of Asia within that context. This includes conventional medicinal chemistry as practised by the pharmaceutical industry, but also Chinese and herbal medicines based upon traditional Asian practices. Medicinal chemistry has an important role in combining these approaches, particularly in identifying active components in herb medicine. In Latin America there is perhaps less output for medicinal chemists within the pharmaceutical industry, as it tends to concentrate its research and development in other geographical areas. However, there is an important role in the teaching of medicinal chemistry within university faculties and these are concentrated primarily in chemistry departments and schools of pharmacy. Professor Gupta described a major programme throughout Latin America where data on curricula for the teaching of medicinal chemistry is being correlated across about 30 institutions.

Unfortunately, Dr Khatami was unable to attend the conference and could therefore not make her presenta-

tion. This was read on her behalf by Dr Worth.

The overall attendance of the symposium was about 30–40 participants, which the speakers felt was disappointing, but in fact was typical of most of the symposia. However, some useful discussion was generated which may well lead to further discussion and developments outside the conference.

On of us (H.G.J.W.) would like to acknowledge the support of the British Council.

H.G.J. Worth

Appendix

Clinical chemistry—Chairman Prof. C. R. Ganellin

Postgraduate Curriculum for Training in Clinical Chemistry
Dr H.G.J. Worth, Department of Clinical Chemistry, The King's Mill Centre for Health Care Services, Sutton in Ashfield, Nottinghamshire, NG17 4JL, UK.

Clinical Chemistry Training in Developing Countries
Dr Z. Khatami, Officer in Charge of QC and Biochemistry Department, WHO Collaborating Centre, National Reference Laboratories of Iran.

Toxicology for Clinical Chemists
Dr J.H. Duffus, The Edinburgh Centre for Toxicology, 43 Mansionhouse Road, Edinburgh, EH9 2JD, Scotland, UK.

Medicinal chemistry—Chairman Dr H.G.J. Worth

Training Medicinal Chemists for Research in Industry
Prof. C.R. Ganellin, Department of Chemistry, University College of London, 20 Gordon Street, London EC1H 0AJ, UK.

The Situation for Educating Medicinal Chemists in Asia
Dr T. Kobayashi, Lilly Research Laboratories, Eli Lilly, Kobe, Japan

Teaching of Medicinal Chemistry in Latin America
Prof. M.P. Gupta, College of Pharmacy, Pharmacognosy Research Center, Estafeta Universitaria, University of Panama, Panama, Republic of Panama

7th International chemistry conference in Africa and 34th convention of the South African Chemical Institute. University of Natal, Durban, 6–10 July 1998

The 7th International Chemistry Conference in Africa (7ICCA) combined with the 34th South African Chemical Institute (SACI) Convention was held at Natal University, Durban (Shepstone Building) from 6 to 10 July 1998. It was the first time that an ICCA meeting had been held in South Africa.

It was the largest chemistry conference ever held in Africa, and attracted over 600 delegates. The Plenary lecturers included Nobel Laureate, Prof. Jean-Marie Lehn of France, Prof. Peter Day, FRS, Director of the Royal Institution of Great Britain, Prof. Peter Atkins, the well known Physical Chemist and Philosopher from Lincoln College, Oxford, and Prof. Krishna V. Sane of the Jawaharlal Nehru Centre for Advanced Scientific Research in Bangalore, India. His work on cost effective education in science in the 21st century is relevant to Africa today. The keynote speakers included Prof. David King, FRS, Head of Chemistry at the University of Cambridge, UK.

The conference was sponsored by the International Union of Pure and Applied Chemistry (IUPAC) and was

Delegates at the opening ceremony, 7ICCA. From left to right: Prof. Ernst Breedt, President of the South African Chemical Institute, Prof. Paul Walter, President of the American Chemical Society, Dr. L.P.H.M. Mtshali, Minister of Arts, Science, Culture and Technology, Republic of South Africa, Prof. Trevor Letcher, Chairman of the Organizing Committee and Prof. Joshua Jortner, President of IUPAC.

attended by the President of IUPAC, the eminent chemist, Prof. Joshua Jortner of Israel and the Secretary General, Dr Ted Becker.

Financial support for the conference came from many sources including the American Chemical Society, whose President, Prof. Paul Walter, and Director of the Office of International Activities, Dr J. Malin, attended the conference.

The 12 plenary and two keynote lectures were the highlights of the conference. One hundred and thirty-five oral presentations in the form of parallel sessions were also given and two hundred and fifty posters were presented in two sessions.

Opening ceremony of the 8th International Symposium on Solubility Phenomena. From left to right: Prof. Hideo Akaiwa, Chairman of the Symposium; Prof. John Lorimer, Representative of IUPAC; Prof. Koske Izutsu, President of the Japan Society for Analytical Chemistry; Prof. David Shaw, Chairman of the Commission on Solubility Data, IUPAC; Prof. Masaaki Arakawa, President of Niigata University.

The conference was organized by a team of chemists from the University of Natal, Durban (UND) and local Universities and Technikons and was chaired by Prof. Trevor Letcher and Dr Bice Martincigh of UND. The theme of the conference was 'Chemistry for the Development of Africa in the 21st Century'. An exhibition of books, chemicals and equipment was presented and was well patronized by the delegates. The conference was honoured in having Beilstein, the well known German chemical information service company, display their products.

The conference was also host to a number of other meetings, including a special meeting of the International Organization for Chemical Sciences in Development (IOCD), an historic meeting of IUPAC and the African Association of Pure and Applied Chemistry (AAPAC), a session given by the Chemical and Allied Industries Association on Responsible Care: Managing Health, Safety and Environmental Performance in the Chemical Industry, and a special meeting on low cost chemical education for local educators.

T. M. Letcher

8th International Symposium on Solubility Phenomena 5–8 August 1998, Niigata, Japan

The city of Niigata, due north of Tokyo on the Sea of Japan, was the site of the *8th International Symposium on Solubility Phenomena.* The Symposium was chaired by Hideo Akaiwa, President of Gunma University, with Hiroshi Miyamoto of Niigata University as Vice-Chairman and Kyoshi Sawada of Niigata University as General Secretary. Joint organizers were IUPAC Commission V.8 (Solubility Data), The Japan Society for Analytical Chemistry and Niigata University. The Symposium also welcomed the sponsorship of IUPAC, The Science Council of Japan, The Chemical Society of Japan, The Japan Association of Solution Chemistry and the Japan Society of Coordination Chemistry. Financial support from The Ministry of Education, Science, Sports and Culture, Japan, four other foundations and two industries is acknowledged.

One hundred and fifty-four participants from 22 countries (Australia, Austria, Bulgaria, Canada, China, Czech Republic, Egypt, Finland, France, Germany, Hungary, Israel, Japan, Poland, Portugal, Russia, Sweden, Switzerland, Tunisia, Turkey, UK and USA) took part. Of the scientific participants, 102 were from Japan and 40 from elsewhere. There were also 12 accompanying persons. The Symposium was reported in the local Niigata newspaper, with a photograph and mention of IUPAC.

Two days before the Symposium, Niigata was hit by a record 25 cm of rain in a few hours, flooding the storm sewer system and making many streets impassable, including that in front of the Bandai Civic Hall, the venue of the Symposium. Fortunately, everything but the elevator had dried out in time, and the main disruptions were to the annual meeting of Commission V.8 preceding the Symposium and the opening mixer.

Those taking part in the opening ceremonies were Hideo Akaiwa, President, Gunma University and Symposium chair; Masaaki Arakawa, President, Niigata University; Kosuke Isutsu, President, The Japan Society for Analytical Chemistry; David Shaw, Chair of IUPAC Commission V.8; and Jack Lorimer, IUPAC representative.

Plenary lectures were given by George H. Nancollas (USA), 'The dissolution and growth of sparingly soluble inorganic salts: a kinetics and surface energy approach', and Kosuke Isutsu (Japan), 'Studies on the electrochemical approach to ion solvation'. Eight invited lectures were given by Mihaly Beck (Hungary), Hotoshi Watarai (Japan), Boris Spivakov (Russia), Pirketta Scharlin (Finland), Mark Salomon (USA), Heinz Gamsjäger (Austria), Jean-Claude Bollinger (France) and Masaaki Tabata (Japan). In addition, there were 37 contributed papers and 68 posters. H.L. Clever (USA) presented a special poster on the history of the Solubility Data Project. The invited lectures, contributed papers and posters covered the general areas of: chemistry of crystallization and dissolution; analytical chemistry related to phase transfer; thermodynamics and kinetics in solution; biomineralization; and compilation and evaluation of solubility data. Lectures and contributed papers were given in six sessions, and there was a very lively half-day poster session. It is planned to publish the plenary and invited lectures in *Pure and Applied Chemistry* under the editorship of Peter Fogg (UK).

Opening Ceremony of the 14th IUPAC Conference on Physical Organic Chemistry. From left to right: interpreter; Sergio Gargoni, Director Superintendent of the Institute Euvaldo Lodi; Francisco E. Viera, General Director of the Foundation of Science and Technology of the State of Santa Catarina; Prof. Rodolfo Pinto da Luz, Rector of the Federal University of Santa Catarina; Prof. Eduardo Humeres, UFSC, Organizer of the Conference; Prof. Thomas T. Tidwell, representative of IUPAC; and Prof. Carlos Alberto Kuhnen, Director of the Center of Physical and Mathematical Sciences, UFSC.

Participants enjoyed an evening reception and the Symposium banquet, as well as a rainy and foggy half-day excursion to Yahiko Shrine and Mountain followed by a seaside barbecue. Accompanying persons were well looked after, with tours to a wealthy farmer's house and of Niigata City, as well as taking part in the traditional Japanese arts of flower arranging and the tea ceremony.

The organizers are to be congratulated on providing an excellently organized meeting that provided valuable new information on many aspects of solubility phenomena. The informal, friendly atmosphere during both the scientific meetings and social events left the participants with a deep appreciation of Japanese hospitality.

J. Lorimer

The 14th IUPAC International Conference on Physical Organic Chemistry

The 14th IUPAC International Conference on Physical Organic Chemistry (ICPOC-14) was held from the 16th to the 21st August 1998, in Florianopolis, Santa Catarina, Brazil, with an attendance of 260 people from 43 countries. With 14 meetings since 1972, ICPOC is one of the longest-running conferences sponsored by IUPAC, and has now met in Asia, New Zealand, the Middle East, North and South America, and Europe, and fulfills the IUPAC mandates of globalization and diversification.

The plenary lectures at the Florianopolis Conference illustrated the breadth of this field. By way of example, the keynote lecture by Professor Ronald Breslow (USA) 'The Hydrophobic Effect as a Mechanistic Tool' and others lectures by Professors Norma Nudelman (Argentina) 'The Role of Complexing Effects in Defining the Mechanisms of Some Organometallic Reactions', and Jose Riveros (Brazil) 'Recent Advances in the Energetics and Mechanisms of Gas Phase Ionic Reactions'. Other plenary lectures by K. Houk (USA), H. Iwamura (Japan), U. Tonellato (Italy), L. Radom (Australia), and D. Reinhoudt (the Netherlands), dealt with theoretical studies of molecules and reactions, reactions in aggregates, magnetic properties of radicals, and supramolecular chemistry.

The broad scope of the field has been presented in the Symposium-in-Print 'Physical Organic Chemistry for the 21st Century' (*Pure Appl. Chem.* 1997, 69, 211–292), and copies of this report were distributed at this meeting, as has been done already at Conferences in Italy, Japan, Belgium and the USA, in addition to Internet posting <http://www.iupac.org>.

The Florianopolis Conference had 216 scientific contributions which were submitted from 43 countries. The Chair of the National Committee was Professor Eduardo Humeres of the Universidade Federal de Santa Catarina, the host institution of the meeting. There were also Pre-conference and Post-conference Symposia in Mexico City and Puerto Iguazu (Argentina), respectively.

Together, these meetings showed not only the worldwide dynamism of Physical Organic Chemistry, but also the strength and maturity of the chemical sciences in Latin America.

Prof. Thomas Tidwell

Reports from Commissions

Nomenclature Committee of IUBMB (NC-IUBMB) and IUPAC-IUBMB Joint Commission on Biochemical Nomenclature (JCBN)

Report of current activities, May 1998

As stated in the committees' web page <http://www.chem.qmw.ac.uk/iubmb/nomenclature/>, 'the purpose of the committees is to coordinate recommendations to aid communication of biochemical information by encouraging scientists to use generally understood terminology'.

At our meeting in Prague on 16–18 May 1998, two large projects occupied most of our time, bioinformatics, and listing enzymes, the first two of the following topics.

1. Bioinformatics

On bioinformatics, we are already participating in the scheme that Berendson has put to ICSU. But we are more excited by the ideas Cantor had produced on forming an International Network of Protein Databases. He pointed out the need to collect experimental work on proteins over the last 50–100 years, and put it into computer-readable form, so that the knowledge could readily be accessed. This is precisely within the function of the Unions to spread scientific knowledge. He outlined how this could be approached.

The aim would be a database for each protein or type of protein. To be widely useful, standards would need to be similar for each. Laying these down would be the first phase. Berman has done some pilot work with students. This phase would need to be tried with several different proteins so as to develop a robust procedure. This would be followed by an educational phase, finding local editors for each database, and teaching them, e.g. by running workshops. Much of this could be in relatively undeveloped countries, and many of the databases could be located there. Quality control procedures would need to be set up.

Members raised many difficulties, but agreed that these could probably be overcome, and that the whole project was worthwhile. It would involve inter-Union collaboration, and would commission much work in less developed countries, where it would give opportunities to those interested in bioinformatics who have no lab.

A working party was set up, headed by Cantor, with Apweiler, Bairoch, Berman, Cammack, Cornish-Bowden, and Tipton. They could call on others; all members of the committees were willing to help. They would:

(i) lay out a preliminary set of guidelines for (a) standards for the databases, and (b) standards for the types of data to be included;
(ii) run a pilot study on a few proteins; and
(iii) try to obtain sponsorship.

Cantor would seek IUPAB participation, so that it would be inter-Union from the start.

2. Enzymes

The listing of enzymes remains a large part of the committees' work, since the accurate and unambiguous description is used in many fields and is needed in databases. Most of the points had been raised by correspondence before the meeting, and this made it possible to go through a large supplement to the list.

2.1. We approved complete descriptions for listing 151 new enzymes. Two clarifications are awaited before these can form a supplement for submission to *Eur. J. Biochem*. and publication on WWW pages. We were interested in how often authors made errors in submitting enzymes for listing, one even giving a chiral descriptor to an achiral substrate.

2.2. We modified the descriptions of 38 previously listed enzyme in major ways. These will be added to the new entries in the supplement.

2.3. A very large number of existing entries received minor modifications, and these will appear in the next general update of the list.

2.4. In addition to enzymes generally, peptidases required special treatment. The entries for about 250 enzymes were modified by adding further information about the classes they belonged to.

2.5. We agreed to that the whole list now needs revision, and that we would examine it, one subclass at a time, using a closed website for circulation within the committees.

2.6. We identified specific groups of enzymes in urgent need of updating, including GTPases, initiation and elongation factors, transporting ATPases and protein kinases. Advice is being obtained from groups of experts in each case.

2.7. Linkage is proceeding of Enzyme Nomenclature to other databases, including those for thermodynamics (GOLDBERG), enzyme properties (BRENDA), metabolic properties (KLOTHO, DRAGON, etc.), clinical chemistry (CPNU) and structural features (SWISSPROT, TREMBL, etc.).

2.8. We agreed to seek advice on formulating procedures for dealing with multifunctional enzymes.

2.9. We are working on the classification of catalytic antibodies, ribozymes, mutated and synthetic enzymes, protein kinases.

3. Metabolic pathways

Don Nicholson has generously transferred the copyrights on his metabolic charts and Inborn Errors of Metabolism to IUBMB. The nomenclature committees give high priority to presenting the charts in computer-readable form on the web, and are keen to contribute to this by working with him. They will therefore be delighted to learn that negotiations with Sigma are proceeding, and that there is the prospect that Sigma will support the web version.

4. Transport proteins

Kotyk pointed out that the coverage of transport proteins in *Enzyme Nomenclature* was poor. He was appointed to form a panel to advise on these and Apweiler, Cantor and Dixon were willing to serve on it, and M. Ashburner and Apweiler would try to raise financial support for the work.

5. Biotechnology

Schmid told the committees of the work of the IUPAC Commission on Biotechnology (COB), which is presented on <http://www.itb.uni-stuttgart.de:8080/IUPAC/homepage/iupac.html>. Several items of common interest emerged, and the committees will work with COB on them.

6 Published recommendations and web access

Nomenclature-of-Carbohydrates, published in *Pure Appl. Chem.* 1996, **68**, 1919–2008; *Adv. Carbohydr. Chem. Biochem*. 1997, **52**, 43–177; *Carbohydr. Res*. 1997, **297**, 1–90; *J. Carbohydr. Chem*. 1997, **16**, 1191–1280, is now available on the web <http://www.chem.qmw.ac.uk/iupac/2carb/>. It is being consulted about 140 times per week. Apart from organic class names <http://www.chem.qmw.ac.uk/iupac/class>, at 450 per week, it is more consulted than any other IUPAC document, though closely followed, at 130 per week, by our recommendations on Nomenclature-and-Symbolism-for-Amino-Acids-and-Peptides <http://www.chem.qmw.ac.uk/iupac/AminoAcid/> and (100 per week) the section of Enzyme-Nomenclature on peptidases <http://www.chem.qmw.ac.uk/iubmb/enzyme/>, which is about to be updated (see 2.4 above). (These figures exclude local access to the sites.) Our steroid recommendations <http://www.chem.qmw.ac.uk/iupac/steroid>, added in 1996, receives 80 visits per week.

Nomenclature-of-Glycolipids was published (*Pure Appl. Chem.* 1997, **69**, 2475–2487) and will appear in *Eur. J. Biochem*. 1998; it is now also on the web at <http://www.chem.qmw.ac.uk/iupac/misc/glylp.html>

The following recommendations of ours have been added to the website since 1 May 1997. The URL is always <http://www.chem.qmw.ac.uk/>, followed by that given below. The final column gives the approximate weekly visiting over the last few weeks:

Nucleic acid sequences	iubmb/misc/naseq.html	20
Branched nucleic acids	iubmb/misc/bran.html	5
Multienzymes	iubmb/misc/menz.html	5
Newsletter	iubmb/newsletter	30
Polypeptide conformation	iupac/misc/ppep1.html	20
Polynucleotide conformation	iupac/misc/pnuc1.html	10
Glycoproteins	iupac/misc/glycp.html	15

Total usage of IUPAC's and our recommendations on the web is 1300 per week and comes from 95 countries.

7. Other needs

We are contacting previously appointed working parties, setting up new working parties, and seeking advice from individuals, in order to assess needs and the progress being made to meet such needs.

H.B.F. Dixon
Chairman of JCBN
28 May 1998

Commission on Toxicology—VII.C.2

Minutes of Commission Meeting in Edinburgh. University of Edinburgh, 10–13 September 1998

Reports from sponsored scientific meetings and proceedings

Assessment of Carcinogenic Risk of Inorganic Substances, Luxembourg. The proceedings were published in 1997 by the Royal Society of Chemistry, Cambridge: J.H. Duffus (ed.) *Carcinogenicity of Inorganic Substances*.

1st International Conference on Trace Element Speciation, Munich. This conference was attended by Drs Duffus, Templeton and Cornelis, who was a member of the scientific committee. The excellent 3-day conference was attended by 120 participants. The proceedings will be published in the *Fresenius Journal on Analytical Chemistry*.

5th International Symposium on Metal Ions, Munich. The conference was attended by Drs Duffus, Cornelis, Heinrich-Ramm and Templeton, who was on the scientific advisory board. A book of abstracts has been published.

Conference on Chemical Education in Cairo, August 1998. Dr Duffus attended the well organized conference and gave a presentation on the Curriculum on Toxicology as part of the Clinical Chemistry Symposium. At a meeting with CTC during the conference Dr Duffus presented the status of ongoing joint activities. A short report on the conference symposium: 'Tertiary vocational training in chemistry related to health care' was prepared by Dr Howard Worth and can be obtained from the ComTox secretary (Dr Birger Heinzow, e-mail <bheinzow@lanu.landsh.de>) upon request (see page 171).

Status report on publications of the Commission and Co-operation with other Committees

As a joint project agreed upon with CTC at the General Assembly in Geneva, Dr Duffus has prepared a draft 'Toxicology: an Introduction'. The manuscript was favourably accepted by the CTC and is under circulation. ComTox members should send their comments to Dr Duffus within 3 months. The final version should be ready for publication by CTC at the next General Assembly in Berlin. This educational material should be made available as a download from the Internet and the *PowerPoint* graphics can easily be adapted to other languages. The material aims at courses of an introductory level, e.g. teaching in high schools, and might be especially useful for developing countries. Sponsorship will be sought.

The co-operation with the IPCS will continue as outlined at the meeting in Geneva with Dr Mercier, An advanced toxicology textbook for schools is in the process of publication by IPCS following a review stage involving Dr Duffus. Further co-operation with ComTox is appreciated by IPCS.

Dr Duffus will represent IUPAC (observer status) at the forthcoming IPCS Programme Advisory Meeting, Berlin, 5–8 October 1998.

The manuscript on *Sample Collection Guidelines for Trace Elements* by Dr Cornelis, published in *Pure and Applied Chemistry* has been reprinted in *Clin. Chem Acta* and *Eur. J. Clin. Chem. Clin. Biochem*.

Status report on forthcoming IUPAC ComTox sponsored or supported meetings

6th ComTox Symposium 2001, Uppsala. Dr Sunderman Jr will be contacted to obtain the latest status of the organization of the planned conference. The Commission welcomes and encourages the conference, Dr Sunderman is asked to contact Drs Hans Tjälve and Monica Nordberg to clarify the process at his earliest convenience.

3rd Congress of the Cuban Chemical Society, 1–4 December 1999, Havana. Dr Heinzow was approached by the organising committee from Cuba seeking support for the conference. It was suggested that they organize, as a course, a symposium on risk assessment and environmental chemistry , and make inquiries concerning external funding. The organising committee welcomed the proposal, and will discuss it at its next meeting in October 1998. When it is accepted, Dr Heinzow and Dr Duffus will finalize the programme for the course; several experts from Europe have expressed their support and interest in participation.

Status report of ComTox Working Parties and Projects

Biomonitoring of VOCs: Dr Heinrich-Ramm presented the final draft, which has been circulated before to the ComTox members. The paper was thoroughly revised during the Copenhagen meeting and was accepted by the Commission. After a clarification of copyright issues for the graphs, the paper will be handed on to the IUPAC review process.

Exposure assessment and decision rules in compliance testing for implementation of exposure limits. Dr Christensen explained the title change to *Rules for stating when a limiting value is exceeded*, and planned a

revision related to the experience of the ISO-guide working party referring to the draft ISO 10576-1 and a statistical paper by E. Holst. The statistician Peter Wilrich from Berlin has joined the working party. Suggestions by the ComTox members were made, outlining the scope and practical aspects in more detail in the introduction and adding a glossary and a list of symbols and abbreviations as an appendix. The manuscript will be re-circulated by the end of November and finished by the next General Assembly.

Combined effect. Dr Heinzow reported that a first draft has been prepared and that a meeting will be held at forthcoming ICCEF in September in Baden/Vienna and the status will be given thereafter by Drs Poech and Herzig.

Dr Herzig reported in the meanwhile that his proposals were positively accepted and that a nucleus working party will prepare a completely revised draft by the end of 1998. A meeting of 10 experts is planned, Dr Herzig will try to get the necessary funding; otherwise the next group meeting will not be possible before the next ICCEF conference in Finland (in 2000)

Exposure assessment using the Logbook Method. The status of the project was presented by Erik Olsen. A preliminary draft version was circulated that had been prepared by Erik Olsen, Erik Holst, Robert Herrik and Patricia Stewart. The document outlines the logbook method from a practical viewpoint and will be valuable for a realistic estimate of exposure on an individual basis.

Risk assessment, educational material. A document 'Risk assessment for occupational exposure to inorganic compounds' was prepared by Rob Herber and John Duffus; the group will convene in October in Amsterdam. Comments and additional information should be forwarded to John Duffus. It was suggested that there be an expansion on of the section on general aspects of risk assessment and that it should not focus merely on inorganic matter.

Modelling outdoor exposure. The project will be delayed by several months for unforeseen personal reasons.

Risk assessment of particulate matter. The project was delayed; the group will meet in New York in December. The issue is at present under active discussion. The document should include the more recent knowledge on cofactors of particulate toxicity such as iron content and redox cycling.

Status report on manuscripts and reports

The document: 'Toxicology: an Introduction' prepared by John Duffus, with input by Howard Worth, was circulated. Comments are invited and should be forwarded to John within the next 2 months. Regine Heinrich-Ramm will provide educational material from the German Chemical Society (GDCh).

The joint IUPAC–IFCC Technical report on *Properties and Units in the Clinical Laboratory Sciences* has been re-published: IX. Properties and Units in Trace Elements, prepared by R. Cornelis, X. Fuentes-Arderiu, I. Bruunshuus and D. Templeton. *Clin. Chim. Acta* 1997, **268,** S75–S89, and *Eur. J. Clin. Biochem.* 1997, **35**(10), 833–843.

A draft (6th edition) of *IUPAC Guidelines for Terms Related to Chemical Speciation and Fractionation of Trace Elements: Definitions, Structural Aspects and Methodological Approaches*, by D. Templeton, F. Ariese, R. Cornelis, L-G. Danielson, H. Muntau and H.P. van Leeuwen has been completed. The definitions were discussed and minor modifications suggested including a cross-check with the 'Gold Book'. The project is close to completion; comments should reach Rita Cornelis by 10 October.

New Commission members

On behalf of the Irish National Committee for Chemistry, Dr Iona Pratt was nominated as National Representative, replacing Dr William King who has served for 12 years.

Dr Pratt will be contacted by the secretary and informed about the ongoing activities and invited to join existing projects.

IUPAC reorganization

Dr Cornelis and Dr Duffus informed the Commission about the planned reorganization of IUPAC; details were also given in the last issues of *Chemistry International* (*Chem. Intl.*, 1988, **20**, no. 2, 21–24 and no. 3, 55–76). Briefly the new approach will reduce or abolish Commissions and favour limited time-funded working parties, and will introduce external evaluators. Although the ComTox members have some doubt as to whether the new process will prove to be more productive than the existing system, they look forward to the restructuring and will provide their continuing support to IUPAC as required. The issue of risk assessment and decision rules, including statistical aspects, will remain the main focus for the forthcoming activities of ComTox until restructuring occurs, and it is believed that this will also continue to be important to IUPAC after this time. ComTox is convinced that there will be a need for a continuing IUPAC concern for toxicology and Dr Duffus undertook to prepare a case for this.

Preparation for the next General Assembly in 1999

The next General Assembly will be held in Berlin. Dr Heinzow will supply Commission members with information on hotels/guest houses in Berlin for accommodation and travel, as well as public transport in Berlin.

Miscellaneous/Website activities

Dr Duffus introduced the proposal of a ComTox website, providing information about ongoing projects and existing educational material on the Internet. The site could be operated free of charge for ComTox within the Edinburgh University website on Health, Environment and Work, with a link to the IUPAC website.

A photograph of the commission members at the University of Edinburgh can be found under <http://www.med.ac.uk/hew/tox/>. In addition, a self study course entitled 'Introduction to Applied Toxicology' prepared by Dr Duffus is available from <http://www.med.ac.uk/hew/tox/>.

B. Heinzow
Secretary of Commission VII.C.2
and
J. Duffus
President of Commission VII.C.2
September 1998

Commission on Separation Methods in Analytical Chemistry—V.3

Report of the Meeting in El Escorial, Madrid, 5-6 September 1998

Future of IUPAC—Discussion of SDIC report

Implications for projects and Commission
The Secretary reported on the meeting in Idstein and on some of the implications for the Commission in the SDIC report. The clearest description was given in a recent *Chemistry International* (May 1998).

The principal effect was that the Commission would be dissolved in 2001 but as yet, the structure(s) which would replace it were not yet clear. The comments followed those concerns expressed in Idstein that continuity would be lost and that the Analytical Division Committee, even if it were greatly expanded, would have limited ability to generate projects and less capacity to execute them. The Analytical Division operated over a wider range of activities than many other Divisions. A version of advisory panels linked to Commission members was one possible alternative.

The view was expressed that it was important that the details of how continuity would be achieved were available before the Berlin General Assembly so that they could be discussed. Unless it was clear where we were going, little new activity could be initiated in Berlin and the programme of activities would rapidly start to die out. The 2001 meeting should not be the final one, but a transitional meeting to a new format.

No strong views were expressed on the project-driven formula, except that the generation of projects in a top-down sequence would be unlikely to be successful. What is needed was the interest from the members carrying out the projects. The concept of NAO organizations generating projects was also thought to be unlikely to succeed unless the project was also felt to be of importance by the Division members

A concern was expressed that by the time project proposals had passed through the acceptance procedure, the original proposers would have lost interest. Rather like many other aspects of IUPAC, the time scales are too long.

To some extent, the proposals are still at a very nebulous stage and what was needed was much more detail of how they would affect the work that is currently carried out by Commissions and what new structure would be put into place.

Action to be taken—priority projects
The Secretary proposed a list of priority areas which the Commission should concentrate on completing in the next three years (or less). In most cases these were already in place, except for the more major revision of the General Nomenclature. He would make more detailed proposals for Berlin.

Any response to Division/Secretariat
The need for more details of replacements to be discussed in Berlin rather than in 2001.

Discussion of current projects

'Mobile phases for liquid chromatography'. Part I Descriptive terminology, Project 530/9/95, Author: Siskos and co-workers

Part I. Terminology and definitions. A draft paper had been circulated—some terms such as eluent/mobile phase needed complementary definitions to the stationary phases definitions recently adopted. R.M.S. to revise and return to authors.

Part II. Discussion paper on mobile phase properties: to be developed as a critical review of mobile phase properties directly related to chromatography. It was thought that this could be developed as a critical data compilation paper on the properties of compounds commonly used as eluents in HPLC which would provide values relevant to chromatographic applications. To be proposed as a project in Berlin and a working party established

'Nomenclature for Analytical electromigration techniques', Project 530/10/95, Author: Riekkola

A paper was presented by Prof. Riekkola. A detailed discussion examined a number of the criteria and particular concern was felt about the distribution constant related to micellar methods because it was effectively the inverse of the conventional use of distribution in chromatography. k_{mc} was proposed to make the distinction.

It was felt that the paper should concentrate on capillary methods and the title of the final proposals would reflect this. (Where possible definitions and terms applicable to other electromigration methods would be used.) M.L.R. to revise, and the paper would be circulated by email for comment.

'Nomenclature for chromatography of polymers and related substances'. Author: Berek, Commission IV project.

A working party had been established but so far no paper had been produced—a joint Commission meeting would be organized in Berlin.

Field flow fractionation—Project 530/11/97, Jönnson). The authors (Beckett) had agreed to produce a shortened paper of 5–10 pages but a copy was still awaited.

Definition of dead volume in chromatography—Project 530/12/97 (Garcia-Dominguez). Draft papers have been circulated for comment, The 4th version was discussed in detail and some additional practical results on exchanges between static and bound mobile phase was reported which will lead to a further revision being produced. All the mobile phase in the column appeared to be involved.

It was suggested that the paper should include a conclusion from the comparisons, and recommend methods or a discussion of best practice where the conclusion is ambiguous.

Retention parameters in gas chromatography—Project 530/13/97, Author: Prof. Davankov. Draft paper circulated for comment. Discussed and some revisions proposed. Extension to ~ zero outlet pressure was discussed to take GC-MS method into account. V.A.D. to revise and send to R.M.S. for comments on English.

Projects in Draft stage

1 *Sample preparation methods* (Jönnson to prepare paper). Felt to be a useful topic but needs a cross Commission structure because it overlaps into different areas. To be discussed in Berlin—it might gain from a new style cross Commission working party.

2 *Updating of Chromatography Nomenclature*. Following a discussion of problems present in Nomenclature for Chromatography document related to the definitions of retention volumes in gas chromatography it was agreed to initiate a project which would include:

- Updating of GLC nomenclature (J.V.H.)
- Detector definitions (R.M.S.) coupled detectors (K.J.)
- Definition and description of Modes of chromatography
- The Secretary will try and bring together a paper for Berlin of topics needing additional work.

3 *Integrators and quantitation*. This was felt to be an important area but also to have cross-Division implications, therefore a wider working party might be needed. As above, the topic was of interest in a number of areas. It was suggested that this might be an area where a practical round robin study was needed. Difficult under present structure but might be a future IUPAC activity.

4 *Definition of calculation of asymmetry*. This was a particular area of confusion and it was felt that a agreed proposal might be useful (J.A.J. to examine)

Report on revision of Orange book (Marton)

The Chairman reported that the Orange book had now been published and details were in *Chemistry International*.

Next Meeting at General Assembly, Berlin, 7–14 August, 1999. Year 2000 meeting to be decided. Final Meeting 2001 combined General Assembly and Congress—all current Commissions will be abolished December 2001.

The meeting ends with thanks to the local organizers for their assistance with the hotel, meeting facilities and their hard work in ensuring that all the members were transported from and to Madrid airport and had information on local travel.

Priority projects for 1999–2001

1 Analytical electromigration methods—Nomenclature (M.L.R.)

2 Hold-up time in LC and GC. A fundamental definition (J.G.D., V.A.D.)

3 Up-date of General nomenclature (R.M.S.)
(a) Gas chromatography—terms related to capillary chromatography (J.H.)
(b) Mobile phase terminology—many new terms since (P.S.)
(c) Detector definitions—generally omitted—much more needed many usage terms also in other Commissions. (R.M.S.) coupled (K.J.)

4 Data collection—some broader across Division
5 Integration
Peak shapes
Asymmetry
6 Definition of sample preparation terms—general across Division (J.A.J.)

Useful projects
1 Field flow fractionation (J.A.J.) (limited application)
2 Macromolecular separations (D.B., V.A.D.)
3 Definition of modes of chromatography (broad terms)

Less urgent aspects
1 Mobile phase properties (reviewed material—not definitions)

All for completion by 2001—plan full draft paper by 1999.

R. M. Smith
Secretary of Commission V.3

Commission in Microchemical Techniques and Trace Analysis—V.2

Minutes of Commission Meeting in Geneva, 24–25 August 1997

Status of Current Projects

All of the current projects and their status were thoroughly discussed in the commission. Several papers were cancelled, given to the Division or to press and others made good progress; the updated list of projects follows (see Table p. 182).

New Projects

The following new projects were initiated, and drafts presented at the meeting:
1 *Application of Inductively Coupled Plasma Mass Spectrometry to Speciation Studies* by D.T. Heitkemper, B.S. Zimmer, K Wolnik and J.A. Caruso, draft available, comments to L.G. Danielsson by 1 October 1997.
2 *Electrophoresis of metal species* by A. Timerbaev, comments to author or Boris Spivakov by 1 December 1997.
3 *Speciation Analysis for Metal-Biomacromolecule Complexes using Hyphenated Methods* by Rychard Lobinski, Comments to author by 31 December 1997.
4 Report *Enhancement of Environmental Analytical Laboratories in Third World Countries* by Prof. Lars Reutergardh *et al.*; this report has been sent to the Division.

in *statu nascendi* without draft

Direct derivatization of Organic Compounds at Trace Level Concentrations for Fluorescence Detection and Capillary Electrophoresis by Staffan Folestad

New structure of Commission V.2

A new structure of the Commission was adopted after thorough discussion of the options at hand. The results are as follows: all the working groups will be abandoned and only groups for smaller projects will be set up (such as the authors of a report)

The following position papers shall provide the outlines for future activities; the list of participants reflects the situation of the Commission after the elections of new members:

1 Hyphenated techniques for metal specific detectors, ***W. Lund****, L.G. Danielsson, A. Timerbaev, J. Edmonds, R. Lobinski, K. Fujiwara*

2 Quality Assurance and Quality Control. ***E. Maier****, J. Hlavay, W. Cofino*

3 Surface Characterization and Materials Science. ***G. Friedbacher****, Yunsoo Kim, D. Hercules*

4 GC/MS for Organic Trace Analysis. ***W. Cofino****, S. Pergantis, R. Morabito, R. van Cleuvenbergen*

5 Fractionation and Sequential Leaching. ***J. Hlavay****, R. Morabito*

W. Cofino agreed to make a format for the preparation of the position papers (enclosed as an appendix). The papers are to be discussed at the meeting next year in Vesprem, Hungary.

The chairman thanked all leaving members for the scientific and personal contributions they have made over the past years. He expressed the hope that the contacts will not be terminated completely!

The venue of the next meeting was planned to be Vesprem, Hungary at the weekend following Euroanalysis in Basel.

M. Linscheid
Secretary of Commission V.2

Commission V.2—Current Projects

Status report—1 september 1997

Project no.	Title	Coordinator	Start	Review/ compl. date	Status (flowchart)
OTA521/9/89	Analytical Techniques for Trace Organic Compounds VII Extraction and Preconcentration of Some Environmental Trace Pollutants by Supercritical Fluid Extraction	L. Reuterg Drdh/ M. Linscheid	1990	1997	ready for the Commission in 1997
OTA 521/11/91	Analytical Techniques for Trace Organic Compounds/VII Applications of Negative Ion Chemical Ionization Mass Spectrometry	M.W. Linscheid/ D.G. Westmoreland	1992	1997	ready for the Commission in 1997
OTA521/12/95	Derivatization Reactions for Trace Analysis in HPLC	L.-G. Danielsson	1995	1998	in progress (8), draft in 1998
SAN 522/8/95	Classification of Scanning Probe Microscopies	G. Friedbacher	1995	1997	paper to commission secretary for Division
STE 523/2/89	Determination of Trace Elements Bound to Soils and Sediment Fractions	H. Muntau	1989	1997/ 1998	if not published, need complete update and approval by commission
STE523/3/89	Determination of Mercury Species in Environmental and Biological Samples	M. Morita	1989	1997/ 1998	revised draft available final draft with secretary
STE 523/4/89	Determination of Tin Species in Biological and Environmental Samples	M. Leroy	1989	1997	to the division via secretary
STE 523/6/91	Determination of Selenium Species in Biological Samples	J.S. Edmonds/ M. Morita/ M. Leroy	1991	1997	with the chairman for formal approval
STE 523/7/91	Determination of Phosphorus Species in Environmental Samples	H. Muntau/ B. Ya Spivakov	1991	1997	final version for publication before Geneva, available
STE523/8/93	Speciation Terminology	M. Morita (joint project)	1993	1997	progress made, 2nd draft in 1997
STE523/10/95	Determination of Selenium Species in Environmental Samples	C. Camara	1995	1997	J.S. Edmonds and R.Lobinski will continue
STE523/11/95	Determination of Iodine Species in Environmental and Biological Samples	J. Edmonds	1995	1997	with chairman for approval then to division (12)
	The QA projects will be merged into a Book: 'Quality management in chemical laboratories'	W.P. Cofino/ E.A. Maier	1997	1999	
QA524/2/91	Quality Improvement Programmes	E.A. Maier	1991	1996	draft available (9–10), input from commission expected
QA524/3/91	Method Development and Validation	C. Camara	1991	1997	draft available (9–10)
QA524/4/91	Quality Assurance of Environmental Sampling	J. Hlavay	1991	1997	draft available
QA524/5/91	Quality Control in Daily Practice	W.P. Cofino	1991	1996	draft available (9–10)
520/22/95	Enhancement of Environmental Laboratories in Third World Countries	W.P. Cofino/ L. Reuthergardh	1995	1997	L. Reutergardh agreed to continue with W.P. Cofino as responsible TM. Project to be terminated if no progress is made in 1999.
	New Projects				
	Speciation of Antimony	C. Camara			contact to C. Camara

Conference announcements

16th IUPAC Conference on Chemical Thermodynamics, Halifax, 6–11 August 2000, Nova Scotia, Canada

This conference brings together scientists who participate in thermodynamic research, in order to discuss the most recent research, and to stimulate new lines of research. A special goal of this conference is to include participants who make use of thermodynamic data, in order to guide research in areas where thermodynamic data are required and not presently available. This is especially important because the number of active thermodynamic researchers has decreased dramatically in the last few decades. This is an international problem, and it is hoped that this conference will address this problem, both through research interactions and through the symposium on teaching of thermodynamics. It is expected that the audience will be very international; the 1996 conference attracted participants from 39 countries.

Several subsections are planned; the following are (approximate) titles to date:

- Symposium on Standards (for NIST's 100th anniversary)
- Symposium on Thermodynamics of Materials (batteries, superconductors, etc.)
- Symposium on the Relationship between Theoretical Chemistry and Experimental Chemical Thermodynamics (highlighting areas in which experimental data are needed)
- Symposium on Thermodynamics Education
- Symposium on Biological Thermodynamics.

Novel Porphyrinoids and their Metal Complexes, Berlin, 17 August 1999

'Novel Porphyrinoids and their Metal Complexes', A Micro Symposium, will be held on 17 August 1999, during the 37th IUPAC Congress/27th GDCh General Meeting, 14–19 August 1999, Berlin, Germany. The main theme of the Congress is: 'Frontiers of Chemistry—Molecular Basis of Life Sciences'. The Micro Symposium is being jointly organized by the GDCh and the Biomolecular Chemistry Committee of the IUPAC. It will feature: Chemistry, Photophysical Properties and Biomedical Aspects.

Chairs: U.K. Pandit, Amsterdam, (Netherlands) and E. Vogel, Koeln (Germany). Speakers: R. Guilard, Dijon (France); T.D. Lash, Normal IL (USA); L.Latos-Grazynski, Wroclaw (Poland); J.S. Lindsey, Raleigh NC (USA); A. Osuka, Kyoto (Japan); J.L. Sessler, Austin TX (USA); E. Vogel, Koeln (Germany); N.G. Vorozhtsov, Moscow (Russia).

Further Information will be available in the Second Circular and the updated webpages <http://www.gdch.de/tagung/1999/iupac_hv/index.htm> in Spring 1999. Gesellschaft Deutscher Chemiker, IUPAC 99, PO Box 90 04 40, D-60444, Frankfurt am Main. Germany. Tel.: +49 69 7917 358/360/366; Fax: +49 69 7917 475, Email: <tg@gdch.de>, Homepage <http://www.gdch.de>.

IFCC–WORLDLAB

17th International and 13th European Congress of Clinical Chemistry and Laboratory Medicine, Firenze, Italy, 6–11 June 1999

The Programme for this event is given below. The 3rd Announcement can be found on the Internet at <http://www.worldlab99.it>.

Opening lecture

Arthur Kornberg—1959 Nobel Laureate in Medicine, Stanford University, Stanford, CA, USA.

- Achievements and Perspectives in Medical Biotechnologies

Plenary lectures

Apoptosis—Prof. Shiegakazu Nagata, Department of Genetics, Osaka University Medical School, Osaka, Japan

The T helper 1 (Th1) and T helper 2 (Th2) Paradigm in Human Diseases—Prof. Sergio Romagnani, Head of the Institute of Internal Medicine and Immunology, University of Firenze, Firenze, Italy.

Proteome Research and its Impact on Laboratory Medicine—Prof. Denis Hochstrasser, Head of the Central Clinical Chemistry Laboratory, Geneva University Hospital, Geneva, Switzerland.

Genetics and Environment—Prof. John Burn, Head of the Department of Human Genetics, University of Newcastle, Newcastle upon Tyne, UK.

From Genome Sequence to Protein Functions—Prof. C. Thomas Caskey, Senior Vice President Merck Research Laboratories West Point, PA, USA.

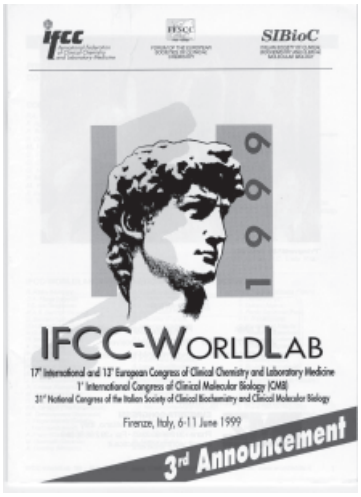
Symposia—tentative programme

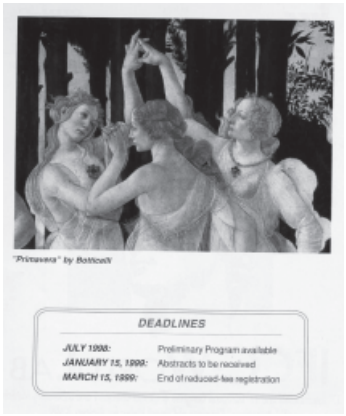
Clinical Molecular Biology Symposia

1 New Tools in Genetic Analysis: the Emerging Biochip Technologies
2 Standardization and Quality Control of Molecular Biological Techniques in Clinical Laboratory (in collaboration with the International Union of Biochemistry and Molecular Biology—IUBMB)
3 Diagnostic Molecular Microbiology: Current and Future Trends
4 Molecular Markers in Solid Tumors
5 Molecular Diagnostic and Prognostic Markers in Haematological Malignancies
6 From Genotype to Phenotype
7 Genetic Analysis of Common Diseases
8 Gene Therapy: Promise and Reality
9 Genetic-Based Drug Responses

Clinical Chemistry and Laboratory Medicine Symposia

10 Robotics, Automation and the Virtual Laboratory
11 Biosensors and Non-Invasive Technology
12 Advanced Mass Spectrometry as a Diagnostic Tool
13 Electrophoresis and High Resolution Separation Techniques
14 Animal Models on Human Diseases
15 Endothelial Cells—Functional and Diagnostic Aspects
16 Receptors and Other Surface Markers
17 Novel Aspects of Haemostasis and Thrombosis
18 Computer-assisted Decision-making Activated by Clinical Laboratory Finc
19 Assessment of Male Fertility and Infertility
20 New Trends in Obesity and Diabetes
21 Environmental Risks for Human Health
22 Standardization and Reference Materials for Immunoassays
23 High Sensitivity and Multi-analyte Immunochemical Methods





24 Microbial Agents and Cardiovascular Diseases
25 Critical Care (AVL Awards Session)
26 Ion Channel Diseases
27 Assessment of Nutritional Status
28 Oxidants and Antioxidants in Clinical Biochemistry
29 Ageing and Neurological Diseases
30 Role of the Laboratory in Medical-Assisted Fertilization—I (confirmation pending)
31 Regulation of Gene Expression in Inflammation: Tool and Target for Therapeutic Applications
32 Biochemical and Genetic Markers of Atherosclerosis
33 Standardization in Clinical Chemistry
34 Therapeutic Drug Monitoring and Clinical Toxicology
35 Biochemical and Genetic Tumor Markers

Economics & Management Symposia

38 Organizational Structure of Laboratories in Europe
39 Accreditation in Clinical Chemistry
40 The Laboratory Influencing Clinical Practice—Past, Present and Future
41 The Changing Face of Laboratory Medicine
42 External Quality Assessment Programmes
43 Projects for Quality Improvement in Developing Countries
44 The Role of the Laboratory in Evidence-Based Medicine
45 PUSH (Public Understanding of Science and Health)

The 30th annual one-week short course, 'Advances in Emulsion Polymerization and Latex Technology', will be offered at Lehigh University during the week of 7–11 June 1999

This course is designed for engineers, chemists, other scientists and managers who are actively involved in emulsion work and for those who wish to develop expertise in the area.

The course is an in-depth study of the synthesis and properties of high polymer latexes. The subject matter includes a balance of theory and applications as well as a balance between chemical and physical problems. Lectures, given by leading academic and industrial workers, begin with introductory material and review, and progress through recent research results. The course fee is $1000 for the entire week or $350 per day for any part.

Further information can be obtained from: Dr Mohamed S. El-Aasser, Emulsion Polymers Institute, Lehigh University, I 11 Research Drive, Bethlehem, PA 18015, USA. Tel.: (610) 758-3082; Fax: (610) 758-5880; E-mail: <mse0@Iehigh.edu>

International Dairy Federation Symposium Laboratory Accreditation & Proficiency Testing, 19 April 1999, Convention Centre, Ottawa, Canada

This symposium will be held during the IDF/ISO/AOAC Analytical Week, which will take place from 18 to 23 April 1999.

Objectives

The symposium will deal with the subject of Laboratory Accreditation and Proficiency Testing. In a relatively short time Laboratory Accreditation has become essential for every laboratory involved in enforcement and an invaluable asset for any laboratory selling its services to other clients. Proficiency Testing is a recognized tool for maintaining accreditation.

The objectives are:

- to harmonize analytical methods & test results,
- to monitor laboratory & analyst performance on an on-going basis,
- to provide users with increased confidence in the test data,
- to ensure mutual acceptance of test results in import & export of products.

Special emphasis will be given to the following items:

- importance of Laboratory Accreditation on a more International basis
- compliance of International standards for Laboratory Accreditation impact of International requirements
- International guidelines for Proficiency testing
- equivalency determination

But Laboratory Accreditation is very time-consuming for laboratory managers. It must be carried out successfully. The object of the seminar is to consider the mechanisms, pitfalls and advantages of Laboratory Accreditation, the documentation available to guide the accreditee and the essential requirements for Proficiency Testing to be useful in Laboratory Accreditation.

31st International Chemistry Olympiad, 4–11 July 1999, Bangkok

Thailand will play host to about 60 nations participating in the 31st International Chemistry Olympiad. Further information can be obtained from the Chairman, Dr Bhinyo Panijpan; E-mail: <icho31@ku.ac.th>; Fax: (662) 942-8715.

AACC Oak Ridge Conference, 23–24 April 1999

Call for abstracts

AACC's highly respected 31st Annual Oak Ridge Conference will take place in San Jose, California, USA, on 23 and 24 April 1999. The title of the conference will be 'On the Road to Non-Invasive Testing: The New Millennium of Minimally Invasive and Non-Invasive Technologies in Clinical Settings'.

The conference committee is inviting abstract submissions on the following topics: immunoassay technologies, DNA/RNA-based technologies, biosensors, minimally and non-invasive testing, and point-of-care testing. Abstracts may be submitted via the AACC website <http://www.aacc.org www.aacc.org/meetings/oakridge> or via post.

Contact: AACC Customer Service, 2010 L Street, NW, Suite 202, Washington, DC 30037-1526, USA. Tel.: (202) 857-0717, fax: (202) 833-5093 , e-mail: <custserv@aacc.org> for more information. Deadline for submission is Friday, 30 October 1998.

1st Workshop on Global Phase Diagrams, Walberberg near Cologne, Germany, 21–24 March 1999

Global Phase Diagrams, as introduced by van Konynenburg and Scott, are maps providing an overview of the phase behaviour of binary fluid mixtures. The investigation of Global Phase Diagrams is a powerful method for understanding phase equilibrium phenomena of mixtures in general. The objective of the workshop is to report achievements and recent developments in this area and its extension to new fields of application.

Theoretical or experimental papers are invited that deal with the systematic investigation of:

- the influence of interaction parameters on mixing phenomena
- equations of states or lattice models for pure, binary or multicomponent mixtures
- the influence of interaction or geometry parameters on adsorption phenomena or separation factors
- interference of solid and fluid phases in mixtures

- phase phenomena in reacting systems
- classification of phase diagrams

For details and registration see the workshop web page at: <http://van-der-Waals.pc.uni-koeln.de/1stGPD/register.html>

Prof. Dr Ulrich K. Deiters and Priv.-Doz. Dr Thomas Kraska Thermodynamics Center, Institute of Physical Chemistry, University at Cologne, Luxemburger Str. 116, D-50939 Köln, Germany.

Dr Leonid Z. Boshkov, State Academy of Refrigeration, Odessa, Ukraine. Tel.: + 49 221470 4543, fax: + 49 221470 4900, e-mail: <deiters@stthd0.pc.uni-koeln.de> or <Kraska@stthd0.pc.uni-koeln.de>

EMRS-99 Spring Conference June 1–4, 1999, Strasbourg, France

First call for papers

Conference Programme:
<http://www-emrs.c-strasbourg.fr/99prog.htm>

Symposium A	Photo-Excited Processes & Applications ('3-ICPEPA')
Symposium B	Protective Coatings & Thin Films 99
Symposium C	Progress in Computational Materials Science
Symposium D	Plasma & Ion Surface Engineering
Symposium E	Advances in Silicon Substrates
Symposium F	Process Induced Defects in Semiconductors
Symposium G	Material Physics Issues & Applications of Magnetic Oxides
Symposium H	Strain in Materials: Analysis, Relaxation & Properties
Symposium I	Microcrystalline & Nanocrystalline Semiconductors
Symposium J	Materials for Coherent Optics
Symposium K	Materials, Process and Technology for Optical Interconnect
Symposium L	*Ab-Initio* Approaches to Microelectronics Materials and Process Modelling
Symposium M	Basic Models to Enhance Reliability in Si-Based Devices and Circuits
Symposium N	Molecular Optoelectronics: Materials, Physics and Devices
Symposium O	Chalcogenide Semiconductors for Photovoltaics
Symposium P	Optical Characterization of Semiconductor Layers and Surfaces

News and notices

37th IUPAC Congress—travel grants

Young scientists from developing countries and less developed countries may apply for travel and accomodation grants to participate in the 37th IUPAC Congress. These grants are co-sponsored by IUPAC, UNESCO and the German Chemical Society (GDCh). Applicants for grants are encouraged to participate actively with a poster contribution (deadline 1 March 1999; see details on the Internet <http://www.gdch.de>) . There will be a special programme to bring together grantees and young host scientists from European countries. Details can also be found on the conference web pages.

New observer countries

The applications of the Cuban Chemical Society and the Pancyprian Union of Chemists for Observer Country status have been approved by the EC/Bureau.

Roland Andersson Named Executive Director of Chemical Institute of Canada

Terry Rummery, Chair of the Board of the Chemical Institute of Canda (CIC), is pleased to announce the appointment of Roland Andersson, as Executive Director. Roland graduated from the University of Winnipeg in 1976 with a 4-year BSc in chemistry. He has over 20 years of management experience in the chemical field, acquired through responsibilities in research and development, operations, marketing and administration, in both chemical manufacturing companies and non-profit organizations.

He became involved early on in his career with the Canadian Manufacturers of Chemical Specialties Association (CMCS). Roland participated in the development and communication of industry positions to government on such issues as the Canadian Environmental Protection Act (CEPA) and Workplace Hazardous Materials Information System (WHMIS). He was active on the Board from 1985 to 1994, which included his 1990–1991 term as Chair.

His operational and marketing experience in the chemical field led him to the Major Industrial Accidents Council of Canada (MIACC) in 1994 in the newly created position of Marketing Director. In a membership campaign, more than 15 trade associations and 80

companies joined the MIACC in three years, an accomplishment that Andersson credits to the Board's strong team spirit. He became Director of Technical Programmes in 1995. Through the voluntary efforts of a Technical Management Committee, supported by the Board and membership, Roland coordinated the development and implementation of a national programme for the voluntary control of major hazards.

Forming Andersson & Associates in 1997, he has undertaken national and international projects with The Canadian Chemical Producers' Association (CCPA) on climate change, for Environment Canada on promoting Accelerated Reduction and Elimination of Toxics (ARET) to industry, and for the Intergovernmental Forum on Chemical Safety (IFCS) in the development of an international marketing and funding strategy.

A new name for the International Federation of Clinical Chemistry

The scientific, technological and organizational changes in health care that are taking place in most countries challenged the IFCC Executive Board to consider the advantages of updating the name of the federation. The basis for this proposal arose during the development of the IFCC strategic plan. While the IFCC will continue to strive for excellence in the profession of laboratory analysis—two considerations about the organization's role have emerged. On the one hand, there is increasing use of techniques of chemical and molecular biology in related fields, which are not strictly subsumed in clinical chemistry. On the other, there is a huge increase in the potential use of laboratory data and diagnostic possibilities in preventive medicine. This requires substantial integration of demographic and clinical-medical information regarding the patient.

These reasons supported the decision of the IFCC Executive Board to ask the national societies affiliated with the IFCC to vote on extending its name to the International Federation of Clinical Chemistry and Laboratory Medicine. A majority of those voting approved this proposal in September 1997.

The Executive Board of the IFCC noted that it must be made clear that this name change in no way implies that laboratory sciences are the exclusive province of medical doctors. While it is clear in all countries that only physicians can provide therapy, diagnostic process today require the integration of skills in biochemistry, physiopathology, chemistry, physics, and so forth. These professional contributions are then used by some physicians for the final diagnosis and by other physicians in prescribing treatment.

Isotope geochemists—Website

Those of you who are interested in the use of stable isotopes in geochemistry should be aware of a website server ISOGEOCHEM at <http://geology.uvm.edu/isogeochem.html>. It is a useful way of getting information on any isotopic problem through its 'chat-line', and also provides information on conferences, positions vacant, short courses, student opportunities, suppliers and stable isotope laboratories. A particularly useful aspect is the 'archive' link which allows you to search for discussion on any previous item. ISOGEOCHEM has over 1100 subscribers in some 40 countries.

Obituary

Prof. O. Wichterle, the father of soft contact lenses, died on 18 August 1998 in the Czech Republic. Prof. Wichterle was the first President of the Macromolecular Division, 1967–71.

Recent reports

Recent reports published in *Pure and Applied Chemistry*

pH measurements in non-aqueous and mixed solvents: Predicting pH(PS) of potassium hydrogen phthalate for alcohol–water mixtures (Technical Report)

Synopsis: Predictive equations for estimating pH(PS) (PS = Primary Standard) of the potass ium hydrogen phthalate buffer in any aqueous–alcoholic mixture are given as functions of the alcoholic moiety mole fraction, x, in the mixture and of the relative permittivity, ε, and the autoprotolysis constant, pK_{ap}, of the pure alcohol at 298.15 K. The two equations, one valid for 298.15 K and the other covering the 263–318 K temperature range, have been optimized by using the experimental data for pH(PS) in aqueous mixtures with the following alcohols: methanol, ethanol, propan-2-ol, ethane-1,2-diol, 2-methoxyethanol ('methylcellosolve'). The equations, tested on subsets generated from the full set by removing an entire co-solvent at a time, provide predicted pH(PS) values which differ from the 'true' ones by less than 0.1 pH over the entire range of co-solvent

composition: $0 < x \leq 0.75$. The predictive equations are recommended for calculating pH(PS) only in those aqueous–alcoholic media for which the corresponding experimental values are not available, and not as smoothing equations for water and its mixtures with the above-mentioned solvents.

This report was prepared for publication by: S. Rondinini, P.R. Mussini, T. Mussini and A. Vertova. Department of Physical Chemistry and Electrochemistry, University of Milan, Via Golgi 19, 20133 Milano, Italy. The full details are to be found in Pure Appl. Chem. *1998, **70**(7), 1419–1422.*

IUPAC Reports on Pesticides(40). Bound xenobiotic residues in food commodities of plant and animal origin (Technical Report)

Synopsis: In order to assess the dietary risk resulting from the use of pesticides or veterinary drugs, the nature of the chemical residues on food commodities needs to be determined. Elucidation of the nature of the chemical residue is carried out using radiolabelled studies, where the radiolabelled xenobiotic is applied or dosed in a manner which reflects its conditions of use. Food commodities are exhaustively extracted to remove the individual components of the residue. Once extracted, the identity and toxicological significance of the components can be assessed and, where appropriate, analytical methods developed to quantitatively determine the amount of the components in food items.

Depending on the characteristics of the components of the residue, the extraction regime may not remove all the chemical residue from the sample matrix. These residues are frequently characterized as being 'bound', however, the amount and nature of this residue will be highly dependent on the extraction regime used. To provide guidance and standardization, a definition of the term 'bound residues' is recommended. This definition builds on a previous IUPAC definition, but takes account of the current availability of enzyme systems, which effectively solubilize the entire matrix rather than extracting the residue. It is also recommended that where the extraction falls short of the full definition, then the residues should be termed as 'unextractable' and the conditions of the extraction should also be defined.

Where residues are bound, the assessment of dietary risk cannot be directly assessed, thus raising issues relating to the significance of the bound residue. The overall toxicological significance of a bound residue will depend primarily on its bioavailability and the level of exposure. In order to determine the bioavailability, study design is crucial in order to perform a critical safety assessment.

This report was prepared for publication by: M.W. Skidmore[1], G.D. Paulson[2], H.A. Kuiper[3], B. Ohlin[4] and S. Reynolds[5]. [1]Zeneca Agrochemicals, Jealotts Hill, Bracknell, UK. [2]State Institute for Quality Control of Agricultural Products, Wageningen, Netherlands. [3]US Department of Agriculture, ARS, Fargo, ND 58105, USA. [4]National Food Administration, Uppsala, Sweden. [5]Central Science Laboratories, York, UK. The full details are to be found in Pure Appl. Chem. *1998, **70**(7), 1423–1447.*

Critically evaluated propagation rate coefficients in free radical polymerizations—II. Alkyl methacrylates (Technical Report)

Synopsis: Propagation rate coefficients, k_p, with confidence ellipses of the Arrhenius parameters, are reported for bulk free-radical homopolymerizations of *n*-butyl and *n*-dodecyl methacrylate at ambient pressure and low conversion. The data, which are from independent experiments in two laboratories, were obtained by the pulsed-laser polymerization/size-exclusion chromatography method. They obey the consistency criteria established for this technique. Plotting the *n*-butyl and *n*-dodecyl methacrylate k_p data, together with the benchmark k_p values for methyl methacrylate and recent data for four other linear and branched alkyl methacrylates, clearly shows a pronounced family type behaviour of alkyl methacrylate k_p.

This report was prepared for publication by: Sabine Beuermann and Michael Buback. Institut für Physikalische Chemie der Universität Göttingen, Tammannstr. 6, D-37077 Göttingen, Germany. The full details are to be found in Pure & Appl. Chem. *1998, **70**(7), 1415–1418.*

Spectroelectrochemistry. A survey of *in situ* spectroscopic techniques (Technical Report)

Synopsis: In this technical paper a summary of the available *in situ* spectroelectrochemical methods, their basic principles, their typical applications, and their limitations is given. With respect to the names of the methods and usual abbreviations, the paper follows the literature as far as possible, but tries to point out inconsistencies. An introductory section gives a summary of the basic equations and introduces the IUPAC recommendations for quantities and symbols.

This report was prepared for publication by: W. Plieth[1], G.S. Wilson[2] and C. Gutiérrez de la Fe[3]. [1]Institut für Physikalische Chemie und Elektrochemie, Technische Universität Dresden, Bergstr. 66b, D-01062 Dresden, Germany. [2]Department of Chemistry, University of

Kansas, Lawrence, KS 66045, USA. [3] *Instituto de Quimica Fisica 'Rocasolano', Calle Serrano 119, Madrid 28006, Spain. The full details are to be found in* Pure Appl. Chem. *1998,* ***70****(7), 1395–1414.*

Analytical aspects of chemically modified electrodes: classification, critical evaluation and recommendations (IUPAC Recommendations 1998)

Synopsis: Analytical aspects of chemically modified electrodes (CMEs) are critically reviewed. Effects of analyte and/or reagent accumulation, chemical transformation, electrocatalysis, permeability, ionic equilibria, controlled release and change of mass, as well as combinations of these effects are evaluated and classified. In addition, relevant definitions are provided and recommendations formulated for the most effective CME operation.

This report was prepared for publication by: Wlodzimierz Kutner[1]*, Joseph Wang,*[2] *Maurice L'her,*[3] *and Richard P. Buck*[4]*.* [1] *Institute of Physical Chemistry, Polish Academy of Sciences, Kasprzaka 44, 01-224 Warsaw, Poland.* [2] *Department of Chemistry and Biochemistry, New Mexico State University, Las Cruces, NM 88003, USA.* [3] *Faculté des Sciences et Techniques, URA CNRS 322, 6 avenue V. Le Gorgeu, B.P. 809-29285, Brest Cedex, France.* [4] *Department of Chemistry, University of North Carolina at Chapel Hill, Chapel Hill, NC 27599, USA. The full details are to be found in* Pure Appl. Chem. *1998,* ***70****(6), 1301–1318*

Glossary of terms used in medicinal chemistry (IUPAC Recommendations 1998)

Synopsis: The objective of this glossary is to provide, in a single document, a consistent terminology and concise definitions of terms covering the various aspects of medicinal chemistry. This was felt necessary with regard to the rapid changes occurring in medicinal chemistry and also by the need to establish international definition standards. Effectively the possibility exists that in different countries certain terms may not have the same meaning, in such a case the creation of an internationally accepted definition is particularly justified.

A Working Party belonging to the IUPAC Section on Medicinal Chemistry has therefore been assembled which prepared the present glossary. Concise but sufficiently explanatory definitions have been formulated for about one hundred commonly employed terms which can be considered of particular interest to the medicinal chemistry community. The glossary has been compiled in part from definitions proposed by the Working Party, in part from earlier IUPAC glossaries, and in part from well-accepted definitions taken from the literature but which were sometimes published in journals or books that may not be readily accessible.

This report was prepared for publication by: C.G. Wermuth[1]*, C.R. Ganellin*[2]*, P. Lindberg*[3] *and L.A. Mitscher*[4]*.* [1] *Faculté de Pharmacie, Université Louis Pasteur, Strasbourg, France.* [2] *University College London, London, UK.* [3] *Astra Hässle AB, Mölndal, Sweden.* [4] *School of Pharmacy, University of Kansas, Lawrence, Kansas, USA. The full details are to be found in* Pure Appl. Chem. *1998,* ***70****(5), 1129–1143.*

Guidelines for presentation of methodological choices in the publication of computational results. A. *Ab initio* electronic structure calculations (IUPAC Recommendations

Synopsis: Guidelines are presented to assist authors in preparing manuscripts that describe the results of *ab initio* computation. These guidelines are not intended to recommend how *ab initio* calculations should be done, but rather to ensure that the reader can have a clear understanding of what was actually carried out. They are written in a form to facilitate reprinting in original research journals and as information sheets that can be distributed to authors and reviewers.

This report was prepared for publication by: James E. Boggs, Department of Chemistry, The University of Texas, Austin, Texas 78712, USA. The full details are to be found in Pure Appl. Chem. *1998,* ***70****(4),1015–1018.*

Guidelines for calibration in analytical chemistry—Part 1: Fundamentals and single component calibration (IUPAC Recommendations 1998)

Synopsis: This IUPAC nomenclature document has been prepared to establish a uniform and meaningful approach to terminology, notation and formulation for calibration in analytical chemistry. In this first part, the general fundamentals of calibration are presented, namely for both relationships of qualitative and quantitative variables (relations between variables characterizing certain types of analytes and measured signals in certain positions of a measured function on the one hand and between variables characterizing the amount or concentration of the chemical species and the intensities of the measured signals, on the other hand). On this basis, the fundamentals of the common single component calibration which models the relationships

$y = f(x)$ between the signal intensities y and the amounts or concentration are represented. Additional papers will be prepared dealing with extensive relationships between several signal intensities and analyte contents, namely with multivariate calibration and with optimization and experimental design.

This report was prepared for publication by: K. Danzer and L. A. Currie, The full details are to be found in Pure Appl. Chem. *1998,* ***70****(4), 993–1014.*

Definitions of terms relating to the non-ultimate mechanical properties of polymers (IUPAC Recommendations 1998)

Synopsis: The document gives definitions of terms related to the nonultimate mechanical behaviour of polymeric materials, in particular bulk polymers and concentrated solutions and their elastic and viscoelastic properties. The terms which have been selected are those met in the conventional mechanical characterization of isotropic polymeric materials. They have additionally been limited to those which can be defined precisely and with mathematical rigour. They are arranged in sections dealing with basic definitions of stress and strain, deformations used experimentally, stresses observed experimentally, quantities relating stress and deformation, linear viscoelastic behaviour and oscillatory deformations and stresses used experimentally for solids. An index, an alphabetical list of terms and a glossary of symbols are included for ease of reference.

This report was prepared for publication by: A. Kaye (UK), R.F.T. Stepto (UK), W. J. Work (USA), J. V. Alemán (Spain), A. Ya. Malkin (Russia). The full details are to be found in Pure Appl. Chem. *1998,* ***70****(3), 701–754.*

Nomenclature, symbols, units and their usage in spectrochemical analysis—XIV. Laser-based atomic spectroscopy: Proposal for a new notation (IUPAC Recommendations 1998)

Synopsis: This report is the 14th in a series on Spectrochemical Methods of Analysis issued by IUPAC Commission V.4. Because of the complexity and the lack of uniformity of the present nomenclature (e.g. '2 step excited resonance fluorescence', 'resonance enhanced multiphoton ionization', etc.) a new way is needed to describe these transitions. The aim of this document is therefore to present a new notation, the IUPAC Notation, to describe the various processes involved in atomic laser spectroscopy. Using a few assumptions, this notation has the advantage of being simple and systematic. States and processes can be described in a general way irrespective of the type of laser spectrometry.

This report was prepared for publication by: N. Omenetto,[1] J.-M. Mermet,[2] G.C. Turk,[3] and D. S. Moore[4]. [1]Joint Research Centre, Ispra Establishment, I-21020 Ispra (Varese), Italy. [2]Department of Spectroscopic Analysis, Université de Lyons, Lyons, France. [3]Inorganic Analytical Research Division, NIST, Gaithersburg, MD 20899, USA. [4]Chemical Science and Technology Division, Los Alamos National Laboratory, Los Alamos, NM 87544, USA. The full details are to be found in Pure Appl. Chem. *1998,* ***70****(2), 517–526.*

History of the recommended atomic-weight values form 1882 to 1997: A comparison of differences from current values to the estimated uncertainties of earlier values (Technical Report)

Synopsis: International commissions and national committees for atomic weights (mean relative atomic masses) have recommended regularly updated, best values for these atomic weights as applicable to terrestrial sources of the chemical elements. Presented here is a historically complete listing starting with the values in F.W. Clarke's 1882 recalculation, followed by the recommended values in the annual reports of the American Chemical Society's Atomic Weights Commission. From 1903, an International Commission published such reports and its values (scaled to an atomic weight of 16 for oxygen) areused here in preference to those of national committees of the UK, Germany, Spain, Switzerland and the USA. We have, however, made scaling adjustments from Ar(^{16}O) to Ar(^{12}C) where not negligible.

From 1920, this International Commission constituted itself under the International Union of Pure and Applied Chemistry (IUPAC). Since then, IUPAC has published reports (mostly biennially) listing the recommended atomic weights, which are reproduced here. Since 1979, these values have been called the 'standard atomic weights' and, since 1969, all values have been published with their estimated uncertainties. Few of the earlier values were published with uncertainties. Nevertheless, we assessed such uncertainties on the basis of our understanding of the likely contemporary judgement of the values' reliability. While neglecting remaining uncertainties of 1997 values, we derive 'differences' and a retrospective index of reliability of atomic-weight values in relation to assessments of uncertainties at the time of their publication. A striking improvement in reliability appears to have been achieved since the commissions have imposed upon themselves the rule of recording

estimated uncertainties from all recognized sources of error.

This report was prepared for publication by: T. B. Coplen and H. S. Peiser, U.S. Geological Survey, 431 National Center, Reston, VA 20192, USA. The full details are to be found in Pure Appl. Chem. *1998,* ***70****(1), 237–257.*

Isotopic compositions of the elements 1997 (Technical Report)

Synopsis: The Commission's Subcommittee for the Isotopic Composition of the Elements (SIAM) has carried out its biennial review of isotopic compositions, as determined by mass spectrometry and other relevant methods. This involves a critical evaluation of the published literature, element by element, and forms the basis of the table of isotopic compositions of the elements as determined by mass spectrometry presented here. New guidelines have been used to arrive at the uncertainties on the isotopic abundances and there are numerous changes to the table since it was last published in 1991. Atomic weights calculated from this table are consistent with Ar(E) values listed in the T*able of Standard Atomic Weights 1997*.

This report was prepared for publication by: K.J.R. Rosman[1] and P.D.P. Taylor[2]. [1]Department of Applied Physics, Curtin University of Technology, GPO Box U1987, Perth 6001, Australia. [2]Institute for Reference Materials and Measurements, European Commission-JRC, B-2440 Geel, Belgium. The full details are to be found in Pure Appl. Chem. *1998,* ***70****(1), 217–235.*

Nomenclature of fused and bridged fused ring systems (IUPAC Recommendations)

Synopsis: These recommendations constitute a comprehensive documentation for naming fused ring systems and bridged fused ring systems. It expands and extends the recommendations given in rules A-21, A-22, A-23, A-34, B-3 of the IUPAC Nomenclature of Organic Chemistry, Sections A, B, C, D, E, F and H, 1979 and rule R-2.4.1 of A Guide to IUPAC Nomenclature of Organic Compounds, 1993. Any ring system with two or more rings ortho- or ortho- and peri-fused together may be named by these recommendations. Two rings which are ortho-fused together have only two atoms and one bond in common. The nomenclature of spiro systems and von Baeyer nomenclature will be considered in separate recommendations.

This report was prepared for publication by: G.P. Moss. Department of Chemistry, Queen Mary and Westfield College, Mile End Road, London, E1 4NS, UK. The full details are to be found in Pure Appl. Chem. *1998,* ***70****(1), 143–216.*

Recommendations for the presentation of NMR structures of proteins and nucleic acids (IUPAC Recommendations 1998)

Synopsis: The recommendations presented here are designed to support the easier communication of NMR data and NMR structures of proteins and nucleic acids through unified nomenclature and reporting standards. Much of this document pertains to the reporting of data in journal articles; however, in the interest of the future development of structural biology, it is desirable that the bulk of the reported information be stored in computer-accessible form and be freely accessible to the scientific community in standardized formats for data exchange. These recommendations stem from an IUPAC-IUBMB-IUPAB interunion venture with the direct involvement of ICSU and CODATA. The Task Group has reviewed previous formal recommendations and has extended them in the light of more recent developments in the field of biomolecular NMR spectroscopy. Drafts of the recommendations presented here have been examined critically by more than 50 specialists in the field and have gone through two rounds of extensive modification to incorporate suggestions and criticisms.

This report was prepared for publication by: John L. Markley[1], Ad Bax[2], Yoji Arata[3], C.W. Hilbers[4], Robert Kaptein[5], Brian D. Sykes[6], Peter E. Wright[7] and Kurt Wüthrich[8]. [1]Department of Biochemistry, University of Wisconsin-Madison, Madison, WI, USA. [2]Laboratory of Chemical Physics, NIDDK, National Institutes of Health, Bethesda, MD, USA. [3]Water Research Institute, Tsukuba, Japan. [4]Laboratory of Biophysical Chemistry, University of Nijmegen, the Netherlands. [5]Department of Chemistry, University of Utrecht, the Netherlands. [6]Department of Biochemistry, University of Alberta, Edmonton, Alberta, Canada. [7]Department of Molecular Biology, The Scripps Research Institute, La Jolla, CA, USA. [8]Institut für Molekularbiologie und Biophysik, ETH Hönggerberg, Zürich, Switzerland (convenor of the task group to whom correspondence should be addressed).The full details are to be found in Pure Appl. Chem. *1998,* ***70****(1), 117–142.*

Books and other publications

New Approaches in Polymer Synthesis

Macromolecular Symposia, Vol. 128, pp. 1–254, March 1998.
Invited lectures presented at the IUPAC International Symposium on New Approaches in Polymer Synthesis and Macromolecular Formation held in St. Petersburg, Russia, 16-20 June, 1997.

Symposium Editors: A. Yu. Bilibin and S.S. Skorokhodov

The International Symposium 'New Approaches in Polymer Synthesis and Macromolecular Formation' was organized by the Institute of Macromolecular Compounds of the Russian Science Academy and the Chemistry Department of Saint-Petersburg State University. It appeared to be a logical continuation of the St. Petersburg Polymer Meetings, well known due to the 1st and 2nd IUPAC Symposia 'Molecular Order and Mobility in Polymers'.

The final programme included 21 plenary lectures. The Symposium was divided into four sections:

A New approaches in chain-and step-growth polymerization
B Catalysis in polymer synthesis
C New macromolecular architecture
D Non-traditional methods of macromolecular formation.

The above division is somewhat arbitrary, reflecting the interconnection and interpenetration of the branches of contemporary polymer chemistry. The present volume includes the texts of 21 plenary and oral lectures.

Modified Polyolefins

Macromolecular Symposia, Vol. 129, pp. 1–172, March 1998.
Invited lectures presented at the 12th Bratislava IUPAC International Conference on Polymers: Modified Polyolefins for Advanced Polymeric Materials held in Bratislava, Slovak Republic, 25-28 August, 1997. Symposium.

Editor: E. Borsig

The aim of the Conference was to bring together scientists from academia and industry to stimulate the exchange of ideas on recent advances in chemistry and physics of modified polyolefins leading to advanced polymeric materials.

More than 120 scientists, from 23 countries of the five continents presented 10 invited lectures, 22 contributed papers and 51 posters.

The Conference covered the two main kinds of effective chemical modification of polyolefins: the catalytic systems in polyolefin production and during polyolefin processing using extruders as reaction vessels. New catalysts tolerating known catalyst poisons such as carbon monoxide in the co-polymerization with ethylene or methyl methacrylate and other vinyl-functional esters can be incorporated into polyethylene. They allow the control of molar mass, end groups, stereochemistry, monomer incorporation and morphology. In addition to isotactic poly(propylene) also syndiotactic, hemiisotactic poly(propylene)s are available in high yields. Polyethylene short-and long-chain-branching is controlled either by uniform ethylene copolymerization with 1-olefins using 'single-site' metallocene catalysts or by migratory polyinsertion of ethylene, respectively.

An alternative variation of the polyolefin structure by catalysts is the preparation of elastomeric poly(propylene), the properties of which are influenced by variation of the length of isotactic and atactic segments.

The incompatibility of polyolefins with other, mainly polar polymers, requires the adjustment of their apolar chains to more polar blend components using peroxide-initiated grafting of acrylic and maleic anhydride derivatives on to polyolefin chains. Many Conference contributions were also devoted to other kinds of functionalization of polyolefins, mainly poly(propylene), which could extend the possibilities of the preparation of entirely new materials, including polymer blends.

New effective methods of grafting of vinyl monomers on to polyolefins, mainly on poly(propylene) were also reported. The grafting of styrene on to poly(propylene) with more than 50% yield in the solid state seems to be very advantageous.

The results obtained in the preparation of polyolefin blends showed that reactively compounded polymer blends have generally better mechanical properties than the blend prepared only by mechanical mixing. It was illustrated in PP rubber blends and also during UHMW-PE spinning with reactive solvents. The presented contributions on interaction between polymer components in polyolefin blends like dispersion forces, the influence of the crystalline part on the miscibility and morphology of the blend, and adhesive properties of modified polyolefins on to metal have a practical importance for the development of the new advanced polyolefin materials.

The Impact of Electronic Publishing on the Academic Community—available online

The Proceedings of the International Workshop organized by Academia Europaea and the Wenner-Gren Foundation which took place in April 1997 is now freely available. Contact: Adam Marshall, Head of Marketing: +44 171 580 5530.

Information Technology affects all aspects of academic activity, whether in research, scholarship or education. A major revolution is taking place on how knowledge is being held and by whom. In the past, the main guardian of knowledge has been the academic community, with its related institutions of universities, libraries, learned societies, scholarly publishers, etc. That responsibility is rapidly being transferred to others, and yet the voice of academia is hardly being heard in this process.

In *The Impact of Electronic Publishing on the Academic Community*, experts from a wide variety of backgrounds discuss the plans for implementing electronic publishing in their specific subject areas. Topics covered include:

- The present situation and the likely future
- Legal and political issues
- The content and quality of academic communication
- Social and cultural issues
- Digital libraries and archiving of electronic information
- Access to scientific data repositories

The online version of this book is fully searchable with links from the text to references and hot links to other web sites and email addresses. There is a complete list of contributors and participants of the Workshop including contact details.

Edited by Ian Butterworth, Imperial College, London, UK, Wenner-Gren. ISBN 185578 122 0 hardback, 200 pages, GBP 75.00/USD 127.50.

Conference Calendar

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

1999

Functional dyes

31 May–4 June 1999
4th International Symposium on Functional Dyes, Osaka, Japan.
Prof. Yasuhiko Shirota, Faculty of Engineering, Osaka University, Yamadaoka, Suita, Osaka 565-0871, Japan. Tel.: +81 6 879 7364, fax: +81 6 877 7367, e-mail: isfd@chem.eng.osaka-u.ac.jp

Polymer systems

7 –10 June 1999
3rd International Symposium on Molecular Mobility and Order in
Polymer Systems, St. Petersburg, Russia.Symposium Chairman: Prof. A.A. Darinskii, Symposium Coordinator: Mrs I. Kovalenko, Institute of Macromolecular Coumpounds, Bolshoy pr. 31, St. Petersburg, 199004 Russia. Tel.: +812 213 2907, fax: +812 218 6869, e-mail: IMC@macro.spb.su

CHEMRAWN

20–25 June 1999
CHEMRAWN XII—African Food Security and Natural Resource Management: The New Scientific Frontiers, Nairobi, Kenya.
Dr Pedro Sanchez, International Center for Research in Agroforestry, PO Box 30677, Nairobi, Kenya. Tel.: +254 2 521003, fax: +254 2 520023, e-mail: p.sanchez@cgnet.com

Memorial K.I. Zamaraev

28 June–2 July 1999
International Memorial K.I. Zamaraev Conference on Physical Methods for Catalytic research at the Molecular Level, Novosibirsk, Russia.
Prof. V.N. Parmon, Boreskov Institute of Catalysis, 5, Prosp. Akad. Lavrentieva, Novosibirsk, 630090, Russia. Tel.: +7 3832 343269, fax: +7 3832 343056, e-mail: parmon@catalysis.nsk.su

Biodiversity and Bioresources

11–15 July 1999
2nd International Conference on Biodiversity and Bioresources—Conservation and Utilization, Belo Horizonte, Minas Gerais, Brazil.
Prof. Alaide Braga de Oliveira, Faculdade de Farmacia—UFMG, Av. Olegario Maciel 2360, 30.180-112 Belo Horizonte, Brazil. Fax: +55 31 337 9076, e-mail: fernao@dedalus.lcc.ufmg.br

Polymerization methods

12–15 July 1999
39th Microsymposium, Advances in Polymerization Methods: Controlled Synthesis of Functionalized Polymers, Prague, Czech Republic.
Dr Jaromir Lukas, Institute of Macromolecular Chemistry, Academy of Sciences of the Czech Republic, Heyovskeho na. 2, 162 06 Praha 6, Czech Republic. Tel.: +420 2 360341, fax: +420 2 367981, e-mail: sympo@imc.cas.cz

Advanced materials

15–18 July 1999
1st IUPAC Workshop on New Directions in Chemistry. Workshop on Advanced Materials: Nanostructured Systems (IUPAC-WAM-1), Hong Kong. Professor M.A. El-Sayed, School of Chemistry and Biochemistry, Georgia Institute of Technology Atlanta, GA 30332-0400, USA. Tel.: +1 404 894 0292, fax: +1 404 894 0294, e-mail: mostafa.el-sayed@chemistry.gatech.edu

Organo-metallic Chemistry

18–22 July 1999
10th International Symposium on Organo-Metallic Chemistry Directed Towards Organic Synthesis (OMCOS 10), Versailles, France.
Prof. J.P. Genet, Laboratoire de Synthese Selective Organique et Produits Naturels, E.N.S.C.P.—UMR CNRS 7573, 11 rue Pierre et Marie Curie, 75231 Paris Cedex 05, France. Tel.: +33 1 44 276743, fax: +33 1 44 071062, e-mail: genet@ext.jussieu.fr

Carotenoids

18–23 July 1999
12th International Symposium on Carotenoids, Cairns, Australia.
Prof. George Britton, School of Biological Sciences, The University of Liverpool, Crown Street, Liverpool, L69 3BX, UK. Fax: +44 (151) 794 4349.

Rheology of polymer systems

19–22 July 1999
19th Discussion Conference on the Rheology of Polymer Systems, Prague, Czech Republic.
Dr Jaromir Lukas, Institute of Macromolecular Chemistry, Academy of Sciences of the Czech Republic, Heyovskeho na. 2, 162 06 Praha 6, Czech Republic. Tel.: +420 2 360341, fax: +420 2 367981, e-mail: sympo@imc.cas.cz

Ionic polymerization

19–23 July 1999
International Symposium on Ionic Polymerization, Kyoto, Japan.
Dr Shiro Kobayashi, Department of Materials Chemistry, Graduate School of Engineering, Kyoto University, Kyoto 606-01, Japan. Tel.: +81 75 753 5608, fax: +81 75 753 4911,e-mail: kobayashi@mat.polym.kyoto-u.ac.jp

Analytical science

25–30 July 1999
Analytical Science into the Next Millennium (SAC 99), Dublin, Ireland.
Prof. Malcolm R. Smyth, Faculty of Science, Dublin City University, Dublin 9, Ireland. Tel.: +353 1 704 5308, fax: +353 1 704 5032, e-mail: smythm@ccmail.dcu.ie

Solution chemistry

26–31 July 1999
XXVI International Conference on Solution Chemistry, Fukuoka City, Kyushu, Japan.
Prof. Hitoshi Ohtaki, Department of Chemistry, Faculty of Science and Engineering, Ritsumeikan University, 1-1-1 Noji-Higashi, Kusatsu 525, Japan. Tel.: +81 775 61 2777, fax: +81 775 61 2659, e-mail: ohtaki@bkc.ritsumei.ac.jp

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IUPAC General Assembly

7–13 August 1999
IUPAC Secretariat. Tel.: +1 919 485 8700, fax: +1 919 485 8706, e-mail: secretariat@iupac.org

IUPAC Congress

14–19 August 1999
Frontiers in Chemistry: Molecular Basis of the Life Sciences, Berlin, Germany.
Gesellschaft Deutscher Chemiker–GDCh, PO Box 90 04 40, 60444 Frankfurt Am Main, Germany. Tel.: +49 69 7917 358/360/366, fax: +49 69 7917 475, e-mail: tg@gdch.de

Colloquium Spectroscopicum Internationale

5–10 September 1999
31th Colloquium Spectroscopicum Internationale 1999, Ankara, Turkey.
Prof. Dr. O. Yavuz Ataman, Department of Chemistry, Middle East Technical University, TR-06531 Ankara, Turkey. Tel.: +90 312 210 3232, fax: +90 312 210 1280, e-mail: xxxicsi@rorqual.cc.metu.edu.tr

Macromolecule–metal complexes

6–10 September 1999
8th International Symposium on Macromolecule–Metal Complexes (MMC–VIII) Tokyo, Japan.
Prof. Eishun Tsuchida, Waseda University, Tokyo 169-50, Japan. Tel.: +81 3 5286 3120, fax: +81 3 3209 5522, e-mail: w169988@mn.waseda.ac.jp

2000

Bio-organic chemistry

30 January–4 February 2000
5th IUPAC Symposium on Bio-Organic Chemistry (ISBOC-V), New Delhi, India.

Prof. S. Ranganathan, Biomolecular Research Unit, Regional Research Laboratory, Trivandrum 695 019, India. Tel.: +91 471 491 459, fax: +91 471 490 186.

High temperature materials chemistry

4–10 April 2000
10th International Conference on High Temperature Materials Chemistry, Aachen, Germany.
Prof. K. Hilpert, Forschungszentrum Julich GmbH, Institut fur Werkstoffe der Energietechnik (IWE 1), 52425 Jülich, Germany. Tel.: +49 2461 61 3280, fax: +49 2461 61 3699, e-mail: k.hilpert@fz-juelich.de

Mycotoxins and Phycotoxins

21–25 May 2000
10th International IUPAC Symposium on Mycotoxins and Phycotoxins, Sao Paulo, Brazil.
Dr Myrna Sabino, Instituto Adolfa Lutz, AV Dr Arnaldo 355, Sao Paulo, Brazil, 01246-902. Fax: +455 (11) 853 3505, e-mail: Myrna@Sti.COM.BR

Organic Synthesis

1–5 July 2000
13th International Conference on Organic Synthesis (ICOS-13), Warsaw, Poland.
Prof. M. Chmielewski, Institute of Organic Chemistry, Kasprzaka 44, 01-224 Warsaw 42, PO Box 58, Poland. Tel.: +48 22 631 8788, fax: +48 22 632 6681, e-mail: ichos@ichf.edu.pl

Macromolecules

9–14 July 2000
38th International Symposium on Macromolecules (MACRO 2000), Warsaw, Poland.
Prof. Stanislaw Penczek, Polish Academy of Sciences, ul. Sienkiewicza 112, 90363 Lodz, Poland. Tel.: +48 42 81 9815, fax: +48 42 684 7126, e-mail: spenczek@bilbo.cbmm.lodz.pl

Coordination Chemistry

9–14 July 2000
34th International Conference on Coordination Chemistry (34-ICCC), Edinburgh, Scotland.
Prof. P. Tasker, Chairman, Dr John F. Gibson, Secretary, The Royal Society of Chemistry, Burlington House, London W1V OBN, UK, Tel.: +44 171 440 3321, fax: +44 171 734 1227, e-mail: gibsonj@rsc.org

Polymers In Medicine

17–20 July 2000
40th Microsymposium Polymers In Medicine, Prague, Czech Republic.
Dr Jaromir Lukas, Institute of Macromolecular Chemistry, Academy of Science of the Czech Republic, Heyovskeho na. 2, 162 06 Praha 6, Czech Republic. Tel.: +420 2360341, fax: +420 2367981, e-mail: sympo@imc.cas.cz

Chemical Thermodynamics

6–11 August 2000
16th IUPAC Conference on Chemical Thermodynamics, Halifax, Nova Scotia, Canada.
Dr Peter G. Kusalik, Department of Chemistry, Dalhousie University, Halifax, Nova Scotia B3H 4J3, Canada. Tel.: +1 902 494 3627, fax: +1 902 494 1310. e-mail: kusalik@is.dal.ca

Natural products

1 September 2000
22nd International Symposium on the Chemistry of Natural Products, Sao Paulo, Brazil.
Dr M. Fátima das G.F. da Silva, Universidade Federal de Sao Carlos, Depto. de Quimica, Via Washington Luiz, km 235, CP676, Sao Carlos, Brazil. Tel.: +55 16 274 8208, fax: +55 16 274 8350, e-mail: dmfs@power.ufscar.br

Biotechnology

3–8 September 2000
11th International Biotechnology Symposium, Berlin, Germany.
Prof. G. Kreysa, DECHEMA eV—c/o 11th IBS, Theodor-Heuss-Allee 25, 60486 Frankfurt/Main, Germany. Tel.: +49 69 7564 205, fax: +49 69 7564 201, e-mail: info@dechema.de

Food Packaging

8–10 November 2000
2nd International Symposium on Food Packaging—Ensuring the Safety and Quality Food, Vienna, Austria.
Dr L. Contor, ILSI Europe, 83, Avenue E. Mounier, Box6, B-1200, Brussels, Belgium. Tel.: +32 (2) 762 0044, fax: +32 (2) 771 0014, e-mail: laura@ilsieurope.be

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.

Index

International Union of Pure and Applied Chemistry

Principles of Chemical Nomenclature: A Guide to IUPAC Recommendations

G.J. Leigh, H.A. Favre and W.V. Metanomski
Blackwell Science, 1998, 144 pages, 130 illustrations
ISBN 0 86542 685 6
This slim volume is the absolutely current account of a growing and changing subject. It provides a handy reference guide for experienced chemists, but also an introduction to nomenclature for undergraduate students. It explains the systematic naming of chemical compounds, relates 'trivial' names to systematic nomenclature.

Compendium of Chemical Terminology

'The Gold Book'
A.D. McNaught and A. Wilkinson
Blackwell Science, second edition, 1997, 464 pages
0 86542 684 8 paperback
This classic now fully updated and significantly expanded , is an essential reference resource including around 7000 entries that cover not only all the traditional areas of chemistry, but also growing fields such as stereochemistry, photochemistry, catalysis and bioanalytical chemistry.

Compendium of Analytical Nomenclature (definitive rules 1997)

'The Orange Book'
J. Inczedy, T. Lengyel and A.M. Ure
Blackwell Science, third edition, 1998, 288 pages
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