Item 7: IUPAC Vice-Presidential Critical Assessment Pieter S Steyn [April 2001]

I. INTRODUCTION

IUPAC was established in 1919 as a global, non-governmental, non-profit, scientific organization. As such, it is the only worldwide organization covering all fields of the chemical sciences. It is an honor and privilege to acknowledge and pay tribute to the members of IUPAC, eminent scientists whose sterling contributions have made such a difference to the status and practice of chemistry. Over many years, your commitment and dedication have enabled IUPAC to effectively serve the international educational, research and industrial communities. In fact, IUPAC is unique among the member unions of International Council for Science (ICSU) in its close relationship to an industry.

IUPAC is sailing into new waters: we are changing from a familiar, commission-based organization to one driven primarily by the inception of individual projects, while retaining our absolute commitment to effectively serving the worldwide scientific community. The success achieved in the transformation is the result of concerted, intelligent efforts, relying on the foresight and inspirational leadership of the recent IUPAC presidents, Albert Fischli, Joshua Jortner and Alan Hayes, ably supported by Secretary-General Ted Becker, and the IUPAC Secretariat. I thank all the officers, bureau members, divisional presidents, chairmen of standing committees, divisional managers and all the scientists for their commitment and unstinting loyalty to IUPAC; the *new* IUPAC will require even more dedication and commitment from all of us.

Most previous Vice-Presidential Critical Assessments (VPCAs) focused on analyzing the various scientific activities of its seven divisions; however, the VPCA of Joshua Jortner also contained a strategic analysis of the scientific policy of the Union. This seminal event in the history of IUPAC culminated in the establishment of the Strategy Development and Implementation Committee (SDIC). The ensuing IUPAC Strategic Plan was accepted by the Bureau at its meeting [Frankfurt, September 1998] and by the IUPAC Council [Berlin, August 1999].

The Strategic Plan was recently updated for 2000-2001. A major outcome of the Strategic Plan is embodied in a fundamentally different approach of IUPAC to its operations, specifically the formal termination of its current commissions at the end of this year and a focus on the execution of top quality internationally and scientifically relevant projects. These actions required the establishment of Project and Evaluation Committees, made up of bureau members and effectively managed by Profs. G den Boef and G Schneider, respectively.

This VPCA will not focus in any detail on the scientific activities of the divisions, since the capable Divisional Committees (DCs) currently assess these functions. Rather, this VPCA is directed to the [II] Management of IUPAC; [III] The challenging areas of the chemical sciences; [IV] The core of the new IUPAC: a review of the project-driven system; [V] Review of IUPAC's contribution to the advancement of research in the chemical sciences; [VI] Assessment of IUPAC's function in the development of effective channels of communication in the international chemical community; [VII] Assessment of IUPAC's role in the service of chemistry in both developed and developing countries, with an emphasis on Africa; [VIII] Conclusion: Highlights of 2000/2001, and recommendations for 2002/2003.

II. MANAGEMENT OF IUPAC

1. Mission Statement and Goals of IUPAC

The management of IUPAC is guided by its mission statement and by ten long-range goals.

IUPAC's mission is to advance the worldwide aspects of the chemical sciences and to contribute to the application of chemistry in the service of mankind. In so doing, IUPAC promotes the norms, values, standards, and ethics of science and advocates the free exchange of scientific information and unimpeded access of scientists to participation in activities related to the chemical sciences.

To further its mission, IUPAC has established a set of long-range goals and has formulated strategic thrusts aimed at achieving each of the goals. In summary:

- 1. IUPAC will serve as a scientific, international, non-governmental body in objectively addressing global issues involving the chemical sciences. Where appropriate, IUPAC will represent the interests of chemistry in governmental and non-governmental forums.
- 2. IUPAC will provide tools (e.g. standardized nomenclature and methods) and forums to help advance international research in the chemical sciences.
- **3.** IUPAC will assist chemistry-related industry in its contributions to sustainable development, wealth creation, and improvement in the quality of life.
- 4. IUPAC will facilitate the effective channels of communication in the international chemistry community.
- 5. IUPAC will promote the service of chemistry to society in both developed and developing countries.
- 6. IUPAC will utilize its global perspective to contribute toward the enhancement of education in chemistry and to advance the public understanding of chemistry and the scientific method.
- 7. IUPAC will make special efforts to encourage the career development of young chemists.
- 8. IUPAC will broaden the geographical base of the Union and ensure that its human capital is drawn from all segments of the world chemistry community.
- 9. IUPAC will encourage worldwide dissemination of information about the activities of the Union.
- **10. IUPAC** will assure sound management of its resources to provide maximum value for the funds invested in the Union.

Progress made in achieving the ten goals and associated strategic thrusts was reported last year as IUPAC Global Perspectives in Chemistry: Biennial Report, 1998-1999. The biennial publication of achievements works well and should be continued to ensure proper focus on implementing the strategy of the Union.

Over the past four years we gained much experience in the implementation of the new strategy for IUPAC .The strategic goals should now be critically evaluated to provide a better focus on fewer, more clearly stated goals and to insure that a good "customer focus" is provided.

2. Progress achieved with some goals

Goals 2, 6 and 7 received special attention during the current biennium. In the case of nomenclature [Goal 2], a roundtable meeting was held in April 2000 in Washington, DC. The group included both those familiar with IUPAC and its nomenclature and the users of IUPAC nomenclature. From the meeting came a recommendation concerning the desirability of developing a unique chemical identifier suitable for computer use, in particular over the Internet. IUPAC should specifically retain its unique expertise in chemical nomenclature by partnering with the major chemical societies. The activities of the newly constituted Committee on Chemical Identity and Nomenclature Systems [chaired by Dr Alan McNaught] are strongly supported. See Section [V] of the VPCA for IUPAC's involvement in international chemistry conferences.

To promote education in chemistry [Goal 6] a task group called the Education Strategy Development Committee (ESDC) was established, with members from ten countries and chaired by the distinguished chemical educator, Prof Peter Atkins. The committee's in-depth report proposed recommendations for the direction of IUPAC's activities in Chemistry education and, significantly, the public appreciation of chemistry. Key recommendations included the renaming of the current Committee on Teaching of Chemistry (CTC) to the Committee on Chemical Education. A small working group headed by former IUPAC president Prof Joshua Jortner was appointed to evaluate the significant ESDC recommendations and to determine how they can be optimally implemented. The importance of chemistry education within IUPAC has been further recognized by the recent invitation to the chairman of the CTC to serve on the IUPAC Bureau as an *ex officio* member.

The introduction in 2000 of the IUPAC Prize for Young Chemists is a highly commendable development [Goal 7]. The prize is for the best PhD thesis in chemical sciences, as described in a 1000-word essay. The award of the first nine prizes to S. Adhikari (India), Michelle Louise Coote (Australia), A Credi (Italy), H Isobe (Japan), Stephan Link (USA), Teri Wang Odom (USA), V Patil (India), Paolo Samorí (Germany), and C Saravanan (USA) at the Brisbane Congress, is a distinct highlight in the history of IUPAC. The Prize intended as encouragement for outstanding young research chemists at the beginning of their careers is regarded as a significant contribution to the standards of international chemical sciences and to the image of IUPAC. In addition, IUPAC assists young chemists from developing countries to participate in its biennial Congresses. See section [VII] of the VPCA.

IUPAC has achieved great success with the management of its financial resources [Goal 10]. The dedication and commitment of the former IUPAC Treasurer Prof John Ward and the IUPAC Finance Committee is noted and highly appreciated. A sound financial situation enables IUPAC to take on its new strategy with confidence and enthusiasm. The financial benefit of the new strategy of IUPAC is evident from Section [IV] of the VPCA. I recommend that the Finance Committee continue to review the IUPAC investment policy to ensure the effective functioning of the Biennium Operating Reserve Fund, Southern Hemisphere Sinking Fund, Young Scientists Awards Fund and the Endowment Reserve.

3. The establishment of the Inter-Academy Council

Members of IUPAC should take note of the establishment in May 2000 of the Inter-Academy Council (IAC) in Tokyo with co-chairmen Prof Bruce Alberts and Prof Goverdhan Mehta. This new international scientific advisory mechanism was organized by the world's leading scientific academies to provide timely information and scientific judgments to international decision-

makers. The IAC has presented a list of the top ten scientific challenges of the future, among them:

- Sustaining scientific and technological progress through public and private sector research and development.
- Improving the capacity of societies to use knowledge.
- Understanding and preserving critical ecosystem services and natural resources.
- Using science and technology to address the needs of the poor.
- Meeting energy needs without unacceptable environmental or security impacts.

Clearly, some of these scientific challenges overlap with the established functions of IUPAC and ICSU. ICSU, IUPAC and IAC must communicate to make certain the proper functioning and optimal use of scarce resources (particularly human resources), to ensure optimal synergy and to prevent IAC from usurping the proper roles of IUPAC and of ICSU. IUPAC is a member Union of ICSU.

III. CHALLENGING AREAS OF THE CHEMICAL SCIENCES¹

Traditional IUPAC projects were directed at the international standardization of nomenclature and terminology; publication of glossaries in particular fields; setting standards for the presentation of spectral and other data; establishing uniform scales for data; obtaining agreement on analytical methods; and the compilation of quantitative (usually numeric) data in areas of international need such as thermodynamics, kinetics and solubility data. IUPAC in collaboration with IUPAP establishes the priority of discovery/synthesis of new elements. After considerable debate, the transfermium elements 103 to 109 were named in August 1997.

A fundamental property of each element is its atomic weight. IUPAC's work on atomic weights has gained renewed importance since the advent of more accurate isotope measurement techniques, making chemical analyses and other physical measurements equally more accurate. In Geo- and Cosmo-chemistry, all sorts of materials are dated using radioactive isotopes. In Analytical Chemistry, isotope dilution is the most accurate analytical technique for many elements, while stable isotopes are used as tracers in many fields, e.g. the biosynthesis of natural products.

Chemistry is now recognized as the core science, as it provides the molecular understanding of the physical properties of materials. Chemistry similarly interacts with modern biology (chemical biology) and medicine by providing the molecular understanding of living systems.

IUPAC has identified a number of significant areas in chemistry some of which have appeared in the series on *Chemistry for the 21st Century*. The relationship between the series and the areas mentioned below is self-evident. The 1999 Nobel Prize for Chemistry was awarded to Professor Ahmed H Zewail of Caltech for his studies of chemical reactions using femtosecond spectroscopy. IUPAC takes great pride in the contribution by Prof Zewail to the Chemistry for the 21st Century monograph "Ultrafast Processes in Chemistry and Biology" edited by Prof Mostafa El-Sayed *et al.*

Some of the challenging areas of the chemical sciences, not comprehensive at all, are presented. Ideas for IUPAC projects may emerge from these challenging areas. IUPAC's role is directed at projects, e.g. on nomenclature, codification, standards and conferences dealing with these exciting areas.

Sustainable²/**Green Chemistry**: Pressure on resources makes essential the knowledge, implementation and appreciation of environmentally benign chemistry. Sustainable chemistry requires high yields of a single product, an atom-efficient process, renewable energy and recovery of all products. Homo- and heterogeneous catalysts should replace bulk reactions in the production of fine and specialty chemicals. We as chemists must commit ourselves to shaping a more environmentally benign future in which synthetic pathways and industrial processes are reconciled with current societal expectations. IUPAC's contribution to this commitment is evident from the publication of the Special Topic Issue of *PAC* (Vol. 72, No 7, 2000] devoted to Green Chemistry, and by CHEMRAWN XIV's focus: "Toward Environmentally Benign

^{1.} Appreciation to the Presidents of IUPAC Divisions and several eminent chemists for their invaluable inputs.

^{2.} Sustainability implies meeting current human needs while preserving the environment and natural resources needed by future generations.

Processes and Products." CHEMRAWN XIV will be held in Boulder, Colorado in June 2001. (See www.cires.colorado.edu/env-prog/chemrawn.)

Environmental Chemistry: The recent Scientific Committee on Problems of the Environment (SCOPE)/United Nations Environment Program (UNEP) Report "Emerging Environmental Issues of the 21st Century" (ISBN 92-807-1900-9) identifies the major issues in the social and economic, urbanization and natural disasters areas. Urban areas have been gravely affected by the increase in world population from 2.5 billion (1950) to 5.2 billion (1989), and it is estimated that by 2030 8 billion people, primarily in Asia, Latin America and Africa, will have to be supported by our Earth. Two-thirds of them will be living in cities. Hunger and poverty around the globe must be addressed, and the life-support systems provided by the world's natural environment must be maintained. Environmental concerns close to chemistry include global change (climate, ozone layer). IUPAC's publication "Chemistry of the Atmosphere: Its Impact on Global Change" is devoted to this crucial topic. The relevance of this area of science was evidenced by the award of the 1995 Nobel Prize to Profs Paul Crutzen, Mario Molina, and F. Sherwood Rowland for their work in Atmospheric Chemistry, particularly concerning the formation and decomposition of ozone. IUPAC is taking the lead in promoting collaboration among theoretical chemists to develop and evaluate data related to the reactivity of radical species generated in the atmosphere.

The most important current issues in environmental chemistry are endocrine disrupters (see *PAC*, Vol. 70, No 9, 1998 – "Natural and Anthropogenic environmental estrogens: The scientific basis for risk assessment"); genetically modified organisms (see the Royal Society of London report, "Transgenic Plants and World Agriculture", available online at www.nap.edu/html/transgenic); and persistent bio-accumulative toxins. IUPAC has previously made major contributions to the study of mycotoxins and phycotoxins; however, at present prions and some virulent viruses require new chemical inputs.

Organic Synthesis and Method Development: The chemodiversity of nature is fascinating: many novel structures remain to be investigated for possible applications in medicine (HIV/AIDS, cancer, tuberculosis, malaria), pest control and other beneficial processes. The unique products of nature (antibiotics, antiviral agents, antitumor substances, marine natural products) have led to the development of powerful synthetic methodology and to their total syntheses. The ability of organic chemistry to construct new molecular architecture, combined with its crucial involvement in molecular reactivity and molecular interactions continue to be of great significance to the chemical sciences. Combinatorial chemistry is another facet of organic synthesis and is excellently suited to the rapid development of new drugs and materials. Stereochemistry remains the fundamental cornerstone for understanding the processes of life (chemical biology) and the properties of matter at a molecular level. Stereochemistry is the key to modern molecular biology, the rational design of drugs, material design and biophysics.

Supramolecular Chemistry: Supramolecular Chemistry is concerned with the structure and function of complexes formed by intermolecular bonding between two or more chemical species, and has **b**d to the construction of large molecular aggregates with defined structures and specific properties, e.g. cyclophanes, calixarenes, container molecules, crown ethers and cryptands. Progress in this field is crucial to the understanding of molecular interaction and recognition, and for the dynamics of complex molecular aggregates, e.g. those of living systems such as viruses and similar organelles, as well as for the design of materials or products with predesigned properties (host/guest interactions, etc).

Materials: The burgeoning field of inorganic materials chemistry covers areas such as molecular crystals, crystal engineering, nano- and micro-particles, zeolites, refractory materials and novel magnetic materials. Crystal Engineering involves the design and synthesis of crystalline materials based on metal complexes with novel structures, properties and functions.

In Macromolecular Chemistry, an industry favorite, significant progress is being made in biomaterials and their application to controlled drug release to replace the traditional means of synthesizing raw materials, and in radical polymerization involving free radicals for the manufacturing of specific molecular architecture. Of equal importance are gains in the production of fictionalized polymers (e.g. bioactive, conducting, light-emitting and catalytic active) and hybrid polymers (natural/synthetic and inorganic/organic) possessing increased thermal stability. The importance of the conducting polymers is exemplified by the award of the 2000 Nobel Prize in Chemistry for the preparation of electrically conducting plastics to Profs Alan J Heeger, Alan G MacDiarmid and Hideki Shirakawa.

Nanotechnology relates to the preparation of materials whose characteristic dimensions are on the nanoscale, the properties of such materials, and their applications in computers and micro sensors. Interest in these directions in chemistry is reflected in the excellent response to the Workshop on Advanced Materials: Nanostructured systems, organized by Prof Mostafa El-Sayed in Hong Kong (14-18 July 1999) and published in *PAC*, Vol. 72, No 1-2, 2000. Nanotechnology also involves the utilization of a single molecule, cluster or protein for the processing of electrical, optical or chemical signals. This is an avenue leading towards molecular electronics; the significance of this fascinating area of science is illustrated in the Chemistry for the 21st Century Monograph "Molecular Electronics", edited by J Jortner and M Ratner.

Bioorganic Chemistry: In this rapidly expanding field organic chemistry, biochemistry and molecular biology interact to explore enzyme reactions and life processes. The newest directions in the field are seen in the current efforts to incorporate unnatural amino acids in proteins and prepare peptides fom β amino acids. The role of organic chemistry in improving human health is illustrated by the determination of the x-ray structure of a protease enzyme responsible for peptide accumulation in the brains of Alzheimer's patients. Recent advances in combinatorial chemistry, high-throughput screening, and molecular modeling have begun to revolutionize rational drug discovery efforts for primary protozoan parasitic diseases. Rational drug design begins with identification of a validated biological target (usually an enzyme) against which potential pre-clinical drug candidates (e.g. enzyme inhibitors) are directed. Application of molecular modeling recognition and computer-assisted combinatorial chemistry accelerates the drug discovery efforts in a focused manner by engaging in target-oriented synthesis. Cysteine proteases and the anti-oxidative enzyme trypanothione reductase are biological drugs aimed at parasitic diseases, and are becoming popular for target-oriented synthesis.

The theme of the biennial IUPAC Congress held in Berlin in August 1999 was "Frontiers in Chemistry: Molecular Basis of the Life Sciences." Nobel laureates and other leading scientists discussed new aspects of the chemical sciences and their relation to cell biology, neuroscience, immunology, genetics and other biomedical sciences.

Physical techniques for the study of complex reactions and systems: Physical chemists (spectroscopists) have played a key role in determining the human genome and developing cell-based assays for drug screening. Last year scientists witnessed the announcement of the most complex molecular system to be identified to date: the structure of human chromosome 21, in which the sequence of 33,546,361 base pairs of DNA is defined with very high accuracy (Nature, Vol. 405, 18 May 2000, p. 311).

The Physical and Biophysical Chemistry Division of IUPAC places high priority on the use of physical methods, especially spectroscopy, to characterize biological molecules and their reactions, and the importance of chemistry to the biological sciences. The development and application of protein x-ray crystallography and of protein NMR spectroscopy remain a top priority for determining the tertiary structures of certain key enzymes.

The measurement of very fast reactions and those involving single molecules continues to attract attention. New light sources such as x-ray lasers and synchrotron radiation will be important in studies of biological and chemical reactions and of molecular structure. Miniaturization (nanochemistry) of separations finds increasing application. The approach furthermore minimizes or avoids solvents, e.g. in the analysis of the contents of the human cell.

Chemometrics involves the evaluation and extraction of relevant information from a large amount of numerical data. The approach is applied to the design of synthetic routes of complex substances, and in industry to "Process Analytical Chemistry" in which spectrometric (notably infrared and UV-visible spectroscopy and mass spectroscopy) and other data are acquired on-line and chemometrically evaluated to control product quality and processes.

Quantum chemistry: Quantum chemistry holds the key to the deep understanding of chemistry at the atomic level. Quantum Chemistry moves boldly ahead as testified by the 1998 Nobel Prize awarded to Professors Walter Kohn and John Pople. Over the past thirty years, computational quantum chemistry has developed from merely a computational technique to a discipline in its own right, and it is now used to study molecular properties and chemical reactions in virtually all fields of chemistry. CJ Barden and HF Schaeffer provide a sneak preview of the future directions of the method in their article "Quantum Chemistry in the 21st Century" in *PAC*, Vol 72, No 8, pp. 1405-1423, 2000.

Organometallic Chemistry: Organometallic Chemistry bridges several chemical disciplines. Organometallic-based catalytic procedures have provided tools for selective transformations and for novel carbon-carbon bond formations. Thus, catalytic asymmetric syntheses and the generation of optically pure compounds with predictable chirality are areas of rapid development. Single-site catalysts, such as the metallocenes currently find unique applications in chemical industry. Organometallic substances find novel applications in solid-state chemistry and the low temperature manufacture of ceramics. The importance of this area is made evident in the 21st Century Monograph "Transition Metal Catalyzed Reactions", edited by S-I Murahashi and SG Davies.

In conclusion, the activity is exciting and truly international in the new research fields, and they are expected to contribute to high quality, significant scientific developments and to constitute the cutting edge of new technologies, and ultimately the driving force for the development of mankind.

IV. THE CORE OF THE NEW $IUPAC^3$

1. Commissions and Projects

Almost since its inception in 1919, IUPAC vested much of its scientific work in "permanent" Commissions made up of experts in particular subjects. Commissions were formed initially to tackle problems in specific areas needing international standardization; e.g. atomic weights, tables of constants, reform of nomenclature, bibliographic documentation, chemical standards, fuels and ceramics, preservation of foodstuffs, industrial hygiene. With the greatly increased scope and specialization of chemistry, IUPAC formed Divisions [initially called Sections], and each Division proposed additional Commissions, based primarily on sub-specialties of the Division, e.g. thermodynamics, electrochemical data, molecular structure and spectroscopy, microchemical techniques, oils and fats, etc. By 1955, there were about 35 Commissions or their equivalents, a number that remained constant for 45 years. The basic philosophy of this *Commission-based system* has been to appoint experts to Commissions, and delegate to them the responsibility of identifying areas for IUPAC activity and taking appropriate action. The system worked well for many years, providing continuing bodies that met regularly to think about necessary activities in their field of specialization; a great deal of valuable work emanated from the Commissions. However, the system developed several increasingly apparent shortcomings.

IUPAC often appeared from outside the Union to be primarily inwardly directed. Ideas for activities arose principally from discussions within the Commissions, rather than as a result of a wider solicitation of opinions. The "self-selection" inherent in the election of new Commission members by their predecessors often [but not always] resulted in an increasingly narrow focus to a Commission's activities. The fragmentation of chemistry into small, specialized pieces in different Commissions impeded interdisciplinary activities at a time of increasing need for such endeavors. Regular meetings of Commissions consumed a large portion of the Union's financial resources; as a result, many Commissions had inadequate funds to carry out activities in an expeditious manner. Delays in completing many projects and the inability to marshal funds for large projects became a frequent source of difficulty to the Union.

Under this system, individual projects were proposed largely by Commission members, approved by the Commission and carried out by groups usually made up of members of the Commission or its subcommittees and working parties. About 25 years ago, efforts began to record the titles and brief descriptions of projects [initially called programs] in the Secretariat and to provide a numbering system that indicated the year of inception of the project. This record was largely maintained for information, since individual Commissions approved each project, often without specifically assigned financial resources.

The role of DCs was largely administrative, including the approval [usually *pro forma*] of new Commission members and officers; ensuring adherence to IUPAC policy on term lengths of members of Commissions and subsidiary bodies; allocating Division budgets to Commissions; and monitoring general progress of the work of the Commissions. In some instances, however, DCs took responsibility for obtaining review of proposed projects. In addition, from time to time, DCs proposed new Commissions and created subcommittees and working parties, often attached to individual Commissions but sometimes standing alone and reporting directly to the Division Committee (DC).

^{3.} Appreciation to the IUPAC Secretary-General and the IUPAC Secretariat for their contributions.

2. Restructuring and the new Project-Driven System

In September 1998, the Bureau approved an integrated program that is substantially changing the structure of the Union and how it carries out its scientific projects. In 1999, the Council endorsed the program and gave final approval to necessary structural changes. The program has four essential features:

- DCs are now responsible for initiating and managing scientific programs and projects directly, not through Commissions. Thus, the primary focus of DCs has shifted from administration to science and management.
- Existing Commissions, subcommittees and working parties will be discontinued at the end of 2001. Consolidating the management of scientific programs in seven DCs, rather than 35 Commissions, is expected to reduce fragmentation, promote interdisciplinary activities and permit greater financial resources to be directed toward the projects themselves. Bodies may be formed to advise DCs and to assist them in developing programs. Such bodies may include new Commissions formed under a rigorous procedure for a specified initial lifetime and with specific advisory functions.
- Proposals for projects will be solicited from the worldwide chemistry community, not only from already established IUPAC bodies. Projects will be approved and funded by Divisions only after outside review. Each project will be carried out by a task group set up only for the duration of the project. In this project-driven system, the task group is set up as a result of project approval, in contrast to the former system in which the Commission and its subsidiary groups were formed first, and projects emanated from discussions within these bodies.
- In addition to refereeing prospective projects, DCs will review the accomplishments of projects retrospectively, disseminate reports and other outcomes of the project, and assess the impact of the project on international chemistry. The Evaluation Committee, a committee of the Bureau, will carry out retrospective reviews based on project derivation, output, numbers of citations and incorporation into commercial databases, as well as adoption by journals, textbook authors, and other organizations, and conformance to the IUPAC Strategic Plan.

3. Operation of the Project System

The operation of the Project System is straightforward. Since January 1999, proposals for IUPAC projects have been received by the Secretariat, referred to the appropriate Division(s) and/or Standing Committee(s) to ascertain appropriateness for IUPAC, and sent for review to several outside referees. The relevant Committee(s) considers the referees' reports, decide to approve or disapprove the project and, if approved, determine the amount of funding. This process is estimated to take about four months – less if referees' reports are received promptly, but sometimes considerably longer if questions must be answered or if several projects are competing for funding.

DCs fund most projects. There is, however, an additional source of funds for two types of projects: those that are beyond the financial resources of a Division [>25 percent of the Division budget] and those that are interdisciplinary and involve two or more Divisions. Such funding comes from the *Project Committee*, a Bureau committee established as part of the introduction of the project system. This central source of funds is designed to encourage interdisciplinary efforts and to permit IUPAC to undertake occasional projects that would never have been funded under the former system. The Project Committee also provides a source of funds for projects undertaken by one of the Standing Committees. These committees usually have budgets only for

handling their advisory and coordinating roles, but occasionally a project fits better into the mission of a Standing Committee than into that of a discipline-oriented Division.

Table 1 gives a comprehensive insight into the current status of projects in the IUPAC system .It is evident the project management has become a priority within the IUPAC Secretariat and that extraordinary efforts will be required to effectively complete the long outstanding projects by December 31, 2001. See column 6

	1	2	3	4	5	6	7	8	9
Other/all STC						22	1	1	1
ccins			1			-	-	-	-
CPEP	3		1			-	-	-	-
CTC	6	1	4			-	-	-	-
Div I	11	4	5	2	2	35	3	4	4
Div II	9	4	5	1	1	21	3	2	1
Div III	9	5	5	1		20	2	3	
Div IV	12	11	5	4	8	38	10	1	
Div V	15	9	5	3	4	75	6	12	6
Div VI	16	14	1	1	5	38	10	11	
Div VII	5	2	4	1	1	17	2	2	1
TOTAL	87	50	35	13	21	266	37	36	13

Table 1: The status of IUPAC projects as at December 2000

1: Projects submitted since 1 Jan 1999

- 2: Projects submitted since 1 Jan 1999 and approved
- 3: Projects submitted since 1 Jan 2000
- 4: Projects submitted since 1 Jan 2000 and approved
- 5: Projects submitted since 1 Jan 1999 and approved with proposed end date > 31 Dec 2001 [see Table 2]
- 6: Total current projects (approved, not completed* or abandoned)
- 7: Projects approved since Jan 2000 (not abandoned and not completed)
- 8: Projects completed* since Jan 2000
- 9: Projects abandoned since Jan 2000
- * Including publication in PAC up to July 2000 issue

The scope and breadth of the projects are evident from Table 2. The Table depicts the 21 projects approved since January 1999 with completion after 2001.

Table 2: Projects submitted since 1 January 1999 and approved with proposed end date after31 December 2001

Div	Date end	New project no	Title	Chairman
Code				
2	31-Dec-02	1999-049-1-200	Thermodynamic Characterization of	GF Voronin
			High-Temperature Superconductors in	
			the Yttrium-Barium-Copper-Oxygen	
			System	
2	30-Jun-03	2000-022-1-200	Characterization of Carbon Materials	H-P Boehm
3	01-Aug-02	2000-012-1-300	Single molecule spectroscopy	FC de Schryver
4	31-Dec-02	2000-006-1-400	Terminology of polymers with ioniza-	P Kubisa
			ble groups and polymers containing	

Div Code	Date end	New project no	Title	Chairman
			ions	
4	31-Dec-02	2000-005-1-400	University Education in Polymer Science	A Khokhlov
4	31-Dec-02	1999-024-1-400	Polyaniline: recommendations for pre- paration of conducting polymer and its colloidal form	J Stejskal
4	31-Dec-03	1999-020-1-400	Quantifying Scratch Resistance of Commercial Polymers	Rob Bailey
4	31-Dec-02	1999-039-1-400	Structure and properties of cyclic olefin copolymers	Sung Chul Kim
4	31-Dec-03	1999-021-1-400	Round robin test on the molecular characterization of epoxy resins by liquid chromatography	S Podzimek
4	31-Dec-03	1999-048-1-400	Definitions of Terms Relating to Reactions of Polymers and Functional Polymers	K Horie
4 & 2	21-Dec-02	2000-007-1-400	Glossary of terms relating to polyme- ric gels and networks, hybrid inorga- nic polymeric materials and the pro- cessing thereof	R Jones
5	31-Dec-02	2000-003-1-500	Ionic Strength Corrections for Stabi- lity Constants	LD Pettit
5	31-Dec-02	1999-050-1-500	Chemical speciation of environmental- ly significant heavy metals and inorga- nic ligands	S Sjoberg
5	31-Dec-03	1999-038-1-500	Solubility Phenomena - Applications for environmental improvement	D Shaw
5&0	31-Dec-02	2000-004-2-500	IUPAC Stability constants database - completion of data collection up to 2000	LD Pettit
6	31-Dec-03	1999-013-2-600	Soil and water bio-remediation pro- ject: in-situ treatment of polluted soil and water with emphasis on the use of genetically engineered microorga- nisms	R Mandelbaum
6	31-Dec-03	1999-034-1-600	Local radiation balance: the influence of aerosol	S Slanina
6	31-Dec-03	1999-041-1-600	Bio-availability of Xenobiotics in the soil environment	A Katayama
6	31-Dec-03	1999-014-2-600	Airborne and Remote Monitoring of Water Quality: Evaluation of remote sensing techniques for real time con- trol of water quality in surface water bodies	AG Dekker
6	31-Dec-03	2000-016-1-600	Environmental implications of endo- crine active substance	J Miyamoto

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Div Code	Date end	New project no	Title	Chairman
7	30-Oct-02	1999-047-1-700	Immunochemistry of metal sensitiza- tion	DM Templeton

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4. New Role of DCs

The Bureau recognizes that with new and broader responsibilities, each DC must be strengthened to ensure that it has members of international scientific stature who can provide leadership in the relatively broad area of chemistry for which the Committee is responsible. Nominating committees for each DC have been or are being created, composed of well-known chemists with little or no current IUPAC connections, along with representatives of the DC who are familiar with current programs and needs. This nomination process was begun in two Divisions in 1999 and will be implemented in all Divisions by the end of the year. At the moment, the electorate continues to consist of DC and Commission members, but a proposed amendment to the Bylaws would provide a broad-based electorate including members and NRs on the DCs, together with leaders of current and recent project task groups.

Division Presidents and DCs now have very substantial responsibilities in developing and managing IUPAC's scientific programs. Among their most important duties are:

- a. *Developing an overall strategy for Division programs.* To some extent, the DC should serve as a "think tank" to bring together ideas from the broad expertise of its members on general areas [and sometimes, perhaps, on specific projects] in which the Division could contribute to chemistry. In some instances, the Division may wish to solicit advice from other organizations or from *ad hoc* groups formed to help define the needs and prospects in a particular field. In other cases, where continuing bodies are thought to be needed to provide advice or assistance for the longer term, the DC may establish subcommittees and/or recommend the formation of Commissions.
- b. Working with other Divisions and with organizations outside IUPAC to develop interdisciplinary programs. As an extension of intra-Division planning, one or more members of several DCs should interact by e-mail and by meetings [probably at General Assemblies, in part] to develop initiatives in appropriate areas. Examples include materials science, energy, environmental matters and a wide range of biologically relevant issues. [See Section III of the current VPCA] It is important to consider the inclusion of other groups such as scientific unions, ICSU bodies [e.g., Committee on Data (CODATA), SCOPE], IUPAC's associated organizations, industry trade associations international governmental organizations World Health and [e.g., Organization (WHO), Food and Agriculture Organization (FAO), United Nations Educational, Scientific and Cultural Organization (UNESCO), Organization for the Prohibition of Chemical Weapons (OPCW)]. The intent is to stimulate discussions that could lead to good proposals for specific projects and to identify competent and interested task groups to carry them out.
- c. Setting priorities, approving project proposals and forming task groups. Here, the Committee reacts to proposals submitted to it, rather than in a pro-active manner as described above. This continuing activity should normally be conducted by e-mail. The Secretariat is responsible for the administrative aspects of project review, but the Division President and DC should decide on outside referees, evaluate the reports obtained by the Secretariat, decide whether to approve a project and decide what funds to allocate for the project.
- d. Overseeing and managing the Division's portfolio of projects. The Division President and DC are ultimately responsible for the success of projects. The Secretariat is establishing a

system to monitor progress of projects and to keep the Division informed. The Committee may wish to designate one or more members to review the status of projects, to coordinate related projects, and with the Secretariat's help, to provide assistance and encouragement, all aimed at successful progress, timely completion and adequate dissemination of results in reports or other forums.

e. Managing the Division's biennial budget. It is anticipated that most of the money provided in the Division's budget will be used to support projects, but funds may also be spent for operations, including the development of strategies and programs, as well as necessary overhead. As the transition to a full project system proceeds, some reserve funds are expected to be available from the Treasurer. The Secretariat has developed an accounting system to provide timely information on the status of the biennial budget and the budget of each active project.

The Table 3 shows the original allocations for 1998-9 and 2000-1, the actual expenditures for 1998-9 and the adjusted budgets for 2000-1 as of the third quarter. The adjusted allocation for 2000-1 does not include all of the adjustments approved by the SG/Treasurer and the PC. The best estimate is that a total of USD 50 000 has been approved in addition to the amounts shown here. It may be concluded that funding has not been a limiting factor in Divisional activities over the past two biennia.

Divisions	Original Allocation 1998-1999	Actually Spent 1998-1999	Original Allocation 2000-2001	Adjusted Allocations as of 1999/2000
Ι	50,150	50,739	52,700	52,700
II	37,310	64,734	39,200	46,700
III & Biotechnology	46,050	47,986	48,400	40,900
IV	37,850	33,246	35,700	35,700
V	42,300	*83,771	44,400	44,400
VI	52,570	49,199	55,200	80,200
VII	47,150	60,165	49,500	56,500
TOTAL	313,380	389,840	325,100	357,100

Table 3: Allocation of funds to the IUPAC Divisions for 1998-9 and 2000-1

* Division V's overspending was approved by the Treasurer but the allocation was not changed in the accounting reports.

It is anticipated that in the New IUPAC more resources will become available for worthy projects.

5. Current and Potential Problem Areas

The 2000-2001 biennium is a particularly trying period for DPs, as they continue operating under the Commission system while concurrently restructuring their DCs and initiating the new project system. There have been and will continue to be severe problems in motivating members of the Division to continue enthusiastic work on IUPAC matters while making wrenching changes in the long-established structure. There are difficult decisions of a personal nature to be made in maintaining adequate continuity in the DC while creating vacancies to permit the election of new members who are currently outside the Union.

The project system is generally working well in its current limited form. However, during its gradual introduction in 1999-2000, there were many issues for which policy and procedures had to be established, as everyone "learned by doing." Lengthy discussions between the DPs and the Bureau have resulted in a clearer understanding of the meaning of a "project" and of ways in which activities that are not "projects" can be handled with adequate outside review and with maximum flexibility for the Divisions. Details of the project proposal form and guidelines for submission and for review have gradually been improved through the cooperation of the PC, the DPs, and the Secretariat. IUPAC is a learning organization and as always, further improvements can be made.

The system for tracking, monitoring and reporting on project status and milestones is only beginning to be implemented. As DCs and the Secretariat gain experience, it is likely that procedures will need modification. An increase in Secretariat personnel may well be required as the responsibilities of the Secretariat increase in administering a larger project system and in providing staff assistance to DCs.

Everyone involved, from the President of IUPAC to Commission members, is committed to assuring a continuing flow of ideas for good projects and a supply of people who are able and willing to carry them out as members of IUPAC task groups. The Commission system required only passive management by Divisions, Officers and Bureau; project ideas always came from Commission meetings. They may have been narrow and inward looking in many instances, but there were ideas and there were projects. They were, unfortunately, too often not well thought out in the view of many critics, including the Bureau and many NAOs.

The challenge now is to spark ideas for projects that are appropriate for IUPAC and of broad international interest and importance. Proposals for good projects are unlikely to arise spontaneously; there is a need for continuing pro-active efforts at all levels within the Union to encourage the preparation of such proposals. The Bureau and officers of the Union should also actively create and solicit projects, in particular on behalf of industry. Many suggestions have been made regarding sources of ideas for projects, including efforts at IUPAC symposia and other scientific meetings to engage participants in discussions of potential needs. In addition, IUPAC must maintain a network of international scientific contacts to facilitate recruitment of task groups with wide geographic representation.

A workshop will be held at the General Assembly in Brisbane to explore ways to facilitate the operation of the project system, such as:

- sources of ideas for projects
- ways to recruit members of task groups
- *sources of funding outside IUPAC*
- networking with NAOs, national chemical societies and IUPAC's Associated Organizations
- *assistance that can be provided by the Secretariat*

Another matter of concern is how to provide adequate continuity and expertise in activities under a system that relies heavily on time-limited task groups. There seems to be no single mechanism to ensure such continuity. The Divisions have considerable flexibility to organize *ad hoc* meetings as needed, perhaps at suitable scientific conferences, to bring together people currently or formerly working in a particular field. Continuing two-way contacts with IUPAC Fellows

should keep a body of experts aware of the Union's activities, permit them to propose and comment on various topics and return to active participation in projects from time to time. Continuing advisory groups may be needed in some instances but must be organized with care so as not to commit significant portions of the Division's funds and thus deplete resources available for active projects.

In conclusion, one of the most fundamental changes in the function of the New IUPAC is the increased scientific and management importance of the DCs. Extraordinary efforts should be made to attract eminent chemists of international scientific status and with visionary leadership to DCs – scientists with the ability to recognize and define the areas in which IUPAC can uniquely contribute to the global progress of the chemical sciences. I very much support the role of the Nominating Committees in the selection of the DCs.

V. IUPAC WILL CONTRIBUTE TO THE ADVANCEMENT OF RESEARCH IN THE CHEMICAL SCIENCES THROUGHOUT THE WORLD (GOAL 2)

IUPAC does not have the resources to support experimental research as such. The projects carried out by our Divisions and Operational Committees, however, provide significant support for research. This section will focus on IUPAC-sponsored conferences only. The scientific program of the highly successful IUPAC Congress, held in Berlin, August 1999, as well as that of the Brisbane Congress was based on the guidelines approved by the IUPAC Bureau [report of Jortner and Modena]. It is strongly proposed that this protocol should be followed. In Brisbane, the Congress and the GA will take place concurrently. This approach brings science even closer to the GA and should be favorably considered as a good practice for the future.

IUPAC sponsorship is regarded as adding much value to a conference, mainly by ensuring its scientific quality, facilitating national fundraising, and guaranteeing free access to *bona fide* scientists [ICSU principle]. Many of the conferences receiving IUPAC sponsorship are organized by groups with no other IUPAC connection. There were 26 IUPAC sponsored conferences in 1998, 20 in 1999 (including the Congress), and 28 in 2000. There will be 23 in 2001 (including the Congress), and 10 have been approved so far for 2002. The IUPAC-sponsored conferences for 2001 are shown in Table 3.

	Conference	Location	Date
1	Polymer Characterization, 9th International Conference on (POLYCHAR)	Denton, TX	09-Jan-01
2	Green Chemistry, International Symposium on	Delhi, India	10-Jan-01
	Macromolecules and Materials Science, 4th Annual UNESCO School and South African IUPAC Conference on	Stellenbosch, South Africa	09-Apr-01
4	IV International Congress Cuban Chemical Society	Havana, Cuba	16-Apr-01
5	Free-Radical Polymerization: Kinetics and Mechanism, 3rd International Symposium on	Lucca, Italy	03-Jun-01
	CHEMRAWN XIV - World Conference on green Chemistry: Toward environmentally benign processes and products		09-Jun-01
7	High Temperature Superconductors and Novel Inorganic Materials Engineering, 6th International Workshop on (MSU-HTSC-VI)	-	24-Jun-01
	Polymers: Preparation of Nonconventional Polymer Dispersions, 15th Bratislava International Conference on	· · · ·	25-Jun-01
9	Coordination and Organometallic Chemistry of Germanium, Tin and Lead, 10th International Conference on		08-Jul-01
	Scattering Methods for the Investigation of Polymers, 20th Discussion Conference on	Prague, Czech Republic	09-Jul-01

 Table 3: IUPAC Sponsored Conferences in 2001

	Conference	Location	Date
	Plasma Chemistry, 15th International Symposium on (ISPC-15)	Orleans, France	09-Jul-01
12	Polymer Membranes, 41st Microsymposium on	Prague, Czech Republic	16-Jul-01
13	Organometallic Chemistry Directed Towards Organic Synthesis, 11th IUPAC International Symposium on (OMCOS-11)	-	22-Jul-01
14	Phosphorus Chemistry, 15th International Conference on	Sendai, Japan	29-Jul-01
15	Analytical Science 2001, International Congress in (ICAS 2001)	Tokyo, Japan	06-Aug-01
	Macromolecule-Metal Complexes, 9th International Symposium on (MMC-IX)	Brooklyn, New York	19-Aug-01
17	Solution Chemistry, 27th International Conference on (27th ICSC)	Vaals, Netherlands	26-Aug-01
	Hungarian-German-Italian-Polish Joint Meeting on Medicinal Chemistry	Budapest, Hungary	02-Sep-01
19	Ionic Polymerization, 4th International Symposium on	Crete, Greece	22-Oct-01
20	Biodiversity and Bioresources: Conservation and Utilization, 3rd International Conference on (ICOB-3)	Antalya, Turkey	03-Nov-01
21	6th Brazilian Polymer Conference/9th International Macromolecular Colloquium	Gramado, Brazil	11-Nov-01
22	Sweeteners, 2nd International Symposium on	Hiroshima-shi, Japan	13-Nov-01

In addition to the many IUPAC-sponsored conferences, a workshop on Advanced Materials was held in Hong Kong in July 1999 as the first in a series on New Directions in Chemistry, each of which will highlight a unique area in which chemistry plays a vital role. The workshop coincided nicely with IUPAC's initiatives on materials science, and contributed the editorial content for a Special Topic in Chemistry [published in *PAC* Vol 72, no 1-2, 2000]. Carefully selected Workshops may also be a source of new project ideas. I strongly propose that this initiative be maintained, and that the feasibility of a workshop on Chemical Biology be investigated.

Pursuant to its commitment to promote chemistry in developing and economically disadvantaged countries, IUPAC decided last year to support conferences in those countries at \$10 000 per conference for a maximum of two. Requests were considered from India, Hungary, Czech Republic, South Africa, and Brazil. The IUPAC Bureau decided to sponsor the International Symposium on Green Chemistry to be held in Delhi in January 2001. I fully support the program, however, its impact should be regularly assessed.

The CHEMRAWN conferences continue to play an important role, since issues of global political social and technical importance are focussed on. The most recent was CHEMRAWN XI on Environmental Analytical Chemistry, held in Montevideo, Uruguay in 1998. Unfortunately, CHEMRAWN XII, African Food Security and Natural Resource Management, originally planned for Nairobi in 1999, was eventually cancelled. Attempts are made to revive this important conference, possibly in South Africa. CHEMRAWN XIV, on Environmentally Benign Processes and Products, will be held in Boulder, Colorado. CHEMRAWN conferences bring

together academics, industrial scientists, government and business leaders, and representatives of Nongovernmental Organizations. In addition, action plans are produced to address the issues raised by the conferences. Unfortunately, resources are frequently not available to ensure the recommendations are carried out. However, CHEMRAWN conferences fulfill an important international role and significantly contribute to the image of IUPAC. I completely support the continuation of these high profile CHEMRAWN conferences.

VI. IUPAC WILL FACILITATE THE DEVELOPMENT OF EFFECTIVE CHANNELS OF COMMUNICATION IN THE INTERNATIONAL CHEMISTRY COMMUNITY⁴ (GOAL 4)

As an international scientific organization, IUPAC has a unique communications challenge, since its activities impact both chemical organizations and individuals. Ongoing contacts are maintained with the NAOs, with chemists involved in IUPAC activities, and with chemists belonging to the Affiliate Member Program (AMP) and the IUPAC Fellows Program. The AMP was started in 1983, and now has 5061 members in 45 countries that communicate regularly with IUPAC. The AMP is regarded as highly effective and should be continued.

In 1997, the IUPAC Fellows Program was established for scientists who have completed service on IUPAC bodies. Fellowships have been offered to former IUPAC volunteers through Chemistry International (*CI*) and the IUPAC web site. The Program, comprising 461 Fellows, is highly beneficial and should be strongly promoted. Extraordinary efforts should be taken to enroll the current commission members in the Fellows Program upon termination of their commissions; success would contribute to maintaining the important "IUPAC family" even if only in a virtual sense, and would provide access to the richness of the experience and expertise of scientists who served IUPAC with great distinction.

1. PRINTED COMMUNICATION

a. Pure and Applied Chemistry [PAC]

PAC is a vitally important communication medium; it publishes commission/task group reports and recommendations and all plenary lectures presented at IUPAC-sponsored meetings. The *PAC* advisory committee, chaired by Prof Y. Wolman, and CPEP, chaired by Dr Wendy Warr, continues to play an important role in guiding the publication; in addition, they advise the Bureau on policy matters related to *PAC* and *CI. PAC* experiences stiff competition from international chemistry journals; at present *PAC* has a satisfactory impact factor, but is proposed that the index be regularly monitored to evaluate the impact of changing editorial content. *PAC* obtained impact factors of 1.630, 1.971, and 1.677 for 1996, 1997, and 1998, respectively.

Several new initiatives have been taken to broaden *PAC*'s support base among authors and readers. The recent appointment of Professor James Bull as Special Topics Editor gave new impetus to the publication of issues devoted to special topics. Concerted efforts are being made to attract topics that serve the defined goals of IUPAC, particularly those that promote emerging disciplines and aspects of the chemical sciences relevant to society.

Five special topics have been covered in *PAC*. The impact of the first two topics, produced in collaboration with COCI, was enhanced by their complete translation into Japanese:

- IUPAC White Book on Chlorine: A contribution to the debate on the effect of chlorine and chlorine-containing compounds on the environment, Vol. 68, No 9, September 1996.
- Special Issue: Natural and Anthropogenic Environmental Oestrogens The scientific basis for risk assessment, Vol. 70, No 9, September 1998.

^{4.} Appreciation to the IUPAC Secretariat for their contributions.

- Special Project: Review of Oil Spill Countermeasures Technologies and Response Methods, Vol. 71, No 1, January 1999.
- Special Topic Issue on the Theme of Nanostructured Systems, Vol. 72, No 1-2, January-February 2000.
- Special Topic Issue on Green Chemistry, Vol. 72, No 7, July 2000.

In another initiative, authoritative reviews on new and emerging concepts are being published as stand-alone feature articles. In this series, an excellent review entitled Quantum Chemistry in the 21^{st} Century, authored by Christopher J Barden and Henry F Schaefer III (editors), appeared in *PAC*, Vol 72, No 8, pp. 1405-1423, 2000. The task of the Special Topics Editor is regarded as of crucial importance to the ongoing viability of *PAC*. I actively support the publication of special topics in PAC as well as the regular publication of feature articles in PAC.

The technical reports and recommendations from IUPAC Divisions reflect the goals of the Union and significantly contribute to the editorial content of *PAC*. Table 4 summarizes the number of reports published in *PAC* by the seven Divisions in the years 1998, 1999, and 2000.

DC	1998	1999	2000 (through August)
Ι	5	2	1
П	2	4	3
III	3	8	1
IV	3	2	0
V	7	11	5
VI	1	5	4
VII	2	0	5
Total	23	32	19

Variation from year to year is almost certainly due to the biennial GA cycle that drives most IUPAC activities. It is premature to draw any conclusions on the influence of the *new* IUPAC on the number of manuscripts [recommendations and technical reports] submitted by Divisions for publication in *PAC*. The termination and completion of large numbers of current projects by 31 December 2001 could lead to a substantial increase of editorial matter The *PAC*, EAB, CPEP and DCs should take note of changing circumstances and contribute by identifying themes for special topics and feature articles.

After considerable debate and consideration of options, IUPAC chose to self-publish CI from January 1999 and PAC from January 2000. The relevant publication contract with Blackwell Publishers was therefore duly terminated. While it is gratifying that self-publishing has been a modest financial success (*ca* \$100,000), the primary reason for choosing this route was the

intense desire of IUPAC to improve service to its subscribers and to be free to develop an electronic publishing strategy.

Subscribers to *PAC* are fundamentally important to its well-being. The loss of subscribers is unfortunately in line with the decline experienced over the past few years. IUPAC needs new and imaginative ideas on how to maintain current subscribers and recruit new ones. *PAC* is important to IUPAC's communication strategy and the subscription income is needed to ensure its financial viability and well-being.

b. *Chemistry International* [CI]

CI, our news magazine, is published bimonthly by IUPAC itself. The cost to IUPAC of producing CI has substantially decreased versus the charges from Blackwell. More importantly, the magazine is printed and shipped on a regular schedule and is received early in the issue month. IUPAC also benefited greatly from the experience gained in the self-publishing of CI, viz. it served as a model for that of PAC. The production of CI is an important communication vehicle to IUPAC; however, CI has to compete with several well-financed magazines, published by major chemical societies and multinational corporations. A task group, chaired by Dr Mike Bowen previous chairman of CPEP, was formed to make proposals to the IUPAC Bureau on ways of defining the niche for CI. The task group proposed that IUPAC develop CI into an interesting, easily readable and attractive magazine that complements the IUPAC website, PAC, and the regular series of email alerts (IUPAC enews). I fully support the development of a "new look" for CI. IUPAC should continually endeavor to improve its public relations and the image of chemistry.

2. ELECTRONIC COMMUNICATION

a. The IUPAC website

In adopting its Strategic Plan in 1998, IUPAC wanted to improve its channels of communication, internal and external. One way of accomplishing this was to harness the potential of electronic communication. In a sense, the Internet is the new public face of IUPAC. While recognized in the chemistry community, IUPAC and its contributions are virtually unknown and difficult to access for the public. The Web has eliminated these barriers, and it is up to all of us in IUPAC to make the best use of it.

During the last two biennia, IUPAC made public most of its identity and products. In the IUPAC website can be found:

- individual membership information
- Committee and Division activities
- detailed publications including the contents of Pure and Applied Chemistry
- the complete *CI*
- book references
- provisional recommendations
- charts, reports, meeting minutes, symposia, workshop, and conference calendars
- details on all projects including information on the new project-driven system

Ideally, the IUPAC website is a permanent open house, allowing anyone to visit. All around the world, every day, young chemists enter the professional world, and their familiarity with the use of the Web is far higher than that of the previous generation. In some cases, it is becoming their

principal source for information; not having a presence on the Web would be equivalent to IUPAC's retirement after more than 80 years of service to chemistry.

b. Electronic mail

E-mail technology saves time and money, and for an organization like IUPAC, it helps projects get completed. The Secretariat, like other groups within IUPAC, has made extensive use of e-mail as a means of communication, and has saved considerable money.

c. IUPAC e-news

The Internet is a *get technology* while e-mail is a *push technology*. To balance the two, IUPAC June 1999 launched an electronic newsletter, initially distributed to all members and bodies associated with the Union. IUPAC e-news informs members by e-mail of recent additions to the IUPAC website. The e-news membership list is open to all, and currently has about 1380 subscribers.

d. **IUPAC** and the media

No handbook exists on how to present the Union and its activities on the IUPAC website, though there is plenty of discussion within the publishing world about how journals and their online counterparts should or could be managed. Since IUPAC is now self-publishing its flagship journal *PAC*, we should be aware of the key elements of this important debate.

Some of the questions raised by electronic publishing are technical and economic: should the online product be published simultaneously with or subsequently to the printed journal; as a self-published journal, how do we ensure that *PAC* is incorporated and indexed in a searchable and retrievable format by major scientific databases and portals; how do we reconcile and balance the economics of making publications available online and ensuring economic sustainability?

While the IUPAC Secretariat is developing and steadily updating the contents of the website, the IUPAC CPEP is closely following the debate on electronic publishing.

e. Site structure and search

The site now includes more than 4200 html pages (not including the 6189 puff files that comprise the 'Gold Book'), and it relies on a highly structured file organization and a dependable search engine.

The file structure, as originally designed, closely reflects the structure and function of the Union. A site tour and site map were published in *CI*, and are available online at www.iupac.org/general/site_tour.html. From the main directory, the first pages include News & Notices, Organizations & People, Standing Committees, Divisions, Projects, Reports, Publications, Symposia, Affiliate Membership Program, and Links of Interest.

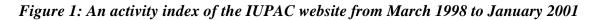
The site search (search engine software ht://Dig -- www.htdig.org/) indexes the entire site and allows for restricted search of specific areas, such as publications and projects. A separate search also allows the user to browse the *Compendium of Chemical Terminology* the 'Gold Book'.

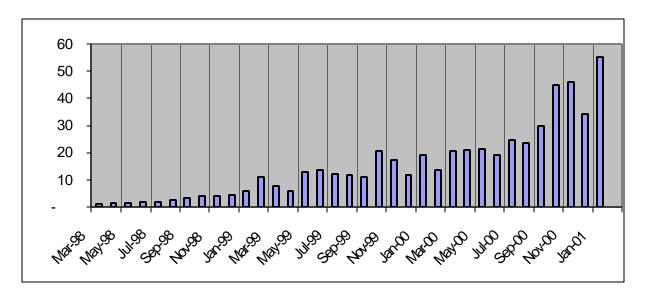
f. Some statistics

The IUPAC site, not including the Gold book, contains 6380 files (4261 html pages) organized in 143 folders, totaling 375.7 MB, as of 1 December 2000. The Gold Book contains 6189 pdf for

a total size of 53.5 MB. The 'home' site, residing in North Carolina, USA, has five mirrors, located in Germany, Japan, Korea, South Africa, and the UK.

An **activity index** has been defined (see Figure 1) that represents the monthly activity relative to the average activity encountered on the site during the first three months of 1998. The corresponding absolute hits are: 3616 for the first three months of 1998, and 199387 for the month of January 2001. This reflects a 55-fold increase.





g. Online workspace

Each year new technologies emerge, challenging our working habits by offering new ways of interacting and sharing information. List servers, for instance, can be employed with or without a moderator to post messages to a membership list that can also be controlled. How should IUPAC use this technology and in what form? The Secretariat and some officers use a simple form to reach a large number of members. Bulletin boards are another tool to exchange questions and answers. These technologies facilitate the work of members focused on a given project. IUPAC must continually evaluate these technologies, comparing their potential benefits to their implementation and maintenance requirements.

h. Electronic Archive

Since volume 1 in 1960, the collection of *PAC* has grown to an average of 2500 pages a year, about half IUPAC reports and recommendations, and half presentations associated with IUPAC-sponsored conferences. Electronic publishing might appear to be the obvious answer for the volumes currently being produced. IUPAC must address the question of electronic archiving, including the entire collection of *PAC*, how much of the collection should be electronically archived and in what format.

i. Publication formats

The technical concepts of electronic publishing go well beyond an online version of a printed publication. The medium requires different thinking about access to and use of documents, illustrated by the most popular IUPAC online publications:

Nomenclature – Searching for a specific rule, naming a chemical compound, and learning *how* to name a chemical compound are three very different reasons that might lead someone to consult IUPAC recommendations on nomenclature. These documents focus principally on defining the rules for naming a given compound and we should ensure that these rules remain easily accessible and searchable. A unified online adaptation of all the nomenclature color books would also be highly desirable. Commercial developers such as Advanced Chemistry Development and Beilstein are writing software that renders a name from a sketch of a molecular structure.

Attempts to address the educational aspects related to nomenclature have been sporadic and traditional, such as the book *Principles of Chemical Nomenclature*. There is no current IUPAC project to develop pedagogic tools for learning nomenclature rules in a non-traditional medium such as a web-based program. Is this a task for IUPAC?

Terminology and Symbols – The large numbers of documents addressing terminology and symbols are usually compiled as glossaries. The online analog should provide enhanced navigation linking to referred terms and related definitions. The most extensive document currently available is the online version of the *Compendium of Chemical Terminology*. The challenge is to keep that document up-to-date and expanded with new and revised definitions as they are published in *Pure and Applied Chemistry*. A unified online adaptation of all such documents is highly desirable, expanding the indexes and updating the search facilities.

j. Databases

IUPAC has long been involved in evaluating data in specific areas of chemistry. The technology is now such that it seems desirable to make those data and supporting databases available online. Technical considerations should be addressed at a level such that once established, standard data formats could be shared and used by different task groups addressing a specific topic. Simple searches should easily point to multiple aspects, multiple databases. Among the questions, IUPAC must address how it should engage in such large and multidisciplinary problems, and the implications of database development and maintenance.

k. Conclusion

IUPAC has greatly benefited from the use of electronic communication. I propose that every effort should be taken to effectively exploit the full potential of this technology

VII. IUPAC'S ROLE IN THE SERVICE OF CHEMISTRY IN BOTH DEVELOPED AND DEVELOPING COUNTRIES (GOAL 5)

At present 44 countries have full membership in IUPAC; 14 countries have ANAO status. IUPAC is well positioned to contribute to their diverse scientific needs. However, the needs for sustainable scientific development and progress are more acute in the developing world; unfortunately, many of these countries do not belong to IUPAC.

IUPAC is dedicated to broadening its geographical base and to ensuring that its human capital is drawn from all segments of the world chemistry community [long-range goal 8]. IUPAC's President sent letters of invitation in July 2000 to 16 chemical societies in 15 countries to become NAOs. Regrettably, few responses have been received to date. I propose that recruiting of members should be done on an individual basis by someone familiar with the country and organization being targeted.

In Latin America and particularly in Argentina, Brazil, Mexico and Venezuela, a remarkable growth in chemical capacity is currently taking place. [See http://www.acs.org/international] Delegates to the XXIV Congresso Latinoamericano de Quimica, heard a presentation on IUPAC by Prof. Steyn last October; Prof G. Infante and Dr E. Wasserman also made remarks. The audience was about 20-30 people, most of them Presidents of Chemical Societies or their delegates. IUPAC Executive Director Dr John Jost had the opportunity to speak to the FLAQ Board and also had private conversations with a number of delegates during the week. There seems to be interest on the part of a number of Latin American chemical societies in becoming ANAOs. The cost of NAO status still seems to be a major stumbling block. FLAQ was encouraged to become an AO; the response was positive, but not definite. Participation in the meetings of the three regional associations, FECS, FACS, and FLAQ, seems to be worthwhile as part of an ongoing program of communication, and should be continued. In all three cases, IUPAC used the opportunity to remind chemical societies about their functions and encourage fellow chemists to participate however they can in the activities, particularly our new project-based approaches.

A world chemistry leadership meeting will be held in Brisbane on July 9 2001 to discuss ways in which the chemical societies of developed countries could assist those from developing and economically disadvantaged countries. Special attention will be directed at the establishment of chemical industry in developing countries and the provision of scientific literature and information. Presidents of chemical societies, presidents of regional associations of chemical societies, and representatives of major chemical trade associations are being invited to participate in this important event. The proposals made at the world chemistry leadership meeting should be critically prioritized and a select few be enacted by IUPAC and related organizations upon.

IUPAC is delighted with the decision of the National Academy of Sciences (NAS) to allow free access to all papers published in PNAS after a four-week delay. IUPAC wishes to discuss similar arrangements with learned societies and publishers on behalf of chemists, particularly those in developing countries. Success in this area would assist in building a global scientific infrastructure, which would in turn benefit the knowledge-based economy and the welfare of mankind.

1. Africa as representative of the developing world

As a scientist, I live and work in Africa. As Vice-President of IUPAC, I am committed to the progress of the chemical sciences in Africa, and the role of chemistry as an enabling science in the development of the continent. On this basis, special emphasis is directed to chemistry in Africa, a continent representative of the developing world. Africa's problems are severe, and its continued reliance on the western world for solutions to its own problems creates an unsustainable scenario. Africa's population growth rate is extremely high: the continent now accounts for 18% of the world's population, compared to 9% in 1950. The ability to feed this growing population will depend upon Africa's success in exploiting its natural resources in a sustainable fashion. Africa is furthermore in the midst of an HIV/AIDS pandemic of unprecedented scale: 70% of the world's cases of HIV live in sub-Saharan Africa, a region which accounts for only 10% of the world's population.

Globalization is regarded as a positive force affecting the world economy; however, for much of the developing world, globalization and knowledge-based economies have had a negative impact on people's lives. Some of these issues relate directly to the chemical sciences:

- **Increasing dependence on intellectual property** owned by the developed world; e.g. pharmaceuticals and agrochemicals.
- A **brain drain** is severely constraining Africa's ability to compete in the global economy. Low levels and loss of intellectual resources make it extremely difficult to succeed in an increasingly knowledge-driven competitive world.

2. Involvement of IUPAC in Africa

At present only Egypt and South Africa are members of IUPAC. Tunisia and Tanzania have the status of ANAOs and the AAPAC is one of IUPAC's Associated Organizations. IUPAC highly values this relationship to the AAPAC.

Analysis of chemical abstracts indicates that Africa's contribution to the world's chemistry literature rose from 3 917 (1987) to 5 369 (1996), an increase of 37%, but dominated by the North African countries, South Africa and Nigeria. External resources are critically important to African educational development: many universities depend on external, usually foreign, support for their basic core functions, while some depend entirely on foreign funding for the execution of research.

IUPAC entered into an agreement with UNESCO to help develop and foster chemistry, with the emphasis on capacity building and research within the least developed countries in Africa. This comprehensive study was published as "Chemistry in Africa's least Developed Countries – an Overview of Capacity Building and Research Support" by CF Garbers (1999). Many African universities are in crisis; their revitalization is among the continent's critical developmental needs. The 1996 report to the President of the World Bank identified several priorities, two directly related to IUPAC and science:

- keeping pace with global changes in scientific information and technology
- revitalization of university research activity

Particular attention is devoted to regional cooperation within Africa: several centers, networks and associations offer and promote postgraduate teaching and research, e.g. AAPAC, Network for Analytical and Biological Services in Africa (NABSA), African Network of Scientific and Technological Institutions (ANSTI), African Biosciences Network (ABN), Association of

African Universities (AAU), Consortium of African Schools of Information Sciences (CASIS), African Academy of Sciences (AAS), Pan-African Union of Science and Technology (PUST), Natural Products Research Network for Eastern and Central Africa (NAPRECA).

In July 1998, Prof Joshua Jortner (then President of IUPAC) and Prof DA Bekoe (then President of AAPAC) co-chaired a meeting in Durban to focus on **Problems facing the chemical enterprise in Africa** [See *CI* Vol. 21 No 1 1999]. The meeting also formed part of IUPAC's response to the challenge of mission-oriented service to mankind through chemistry.

The meeting produced a number of general conclusions and specific roles for IUPAC:

Human capital development is an African priority, with the understanding of chemistry as the conceptual foundation of materials science, physics and biology. The global chemical community should assist Africa in building research and educational capabilities.

Research at the graduate level in the African university system is essential. The professional development of young scientists, graduate students, post-doctoral fellows, and beginning faculty members must remain a top priority. To help in this area, IUPAC will bring 20 young chemists from developing countries to the Brisbane Congress in 2001, as it did to the Berlin Congress in 1999.

Reduction of brain drain: Scientists must be free to pursue research interests at the institutions of their choice. However, African research facilities should take initiatives to bring back young, talented scientists after their training abroad, and to ensure their research career development at African institutions. Imaginative programs should be implemented to foster exchange of personnel in both North-South and South-South directions.

Bridging the gap between donors and developing countries: IUPAC might act as an independent, non-governmental, politically neutral body to help with management and accountability in the distribution of research funds in Africa, and to assist with applications to funding agencies. A CHEMRAWN Symposium aimed at obtaining insight into the funding priorities of donors and the research needs of scientists would greatly promote the practice of the chemical sciences in Africa and the developing world.

Regional and international collaboration is crucial and support must be found for it. An electronic *African Journal of Chemistry* would increase collaboration in Africa and develop worldwide recognition for the chemical sciences on the African continent.

Problems and challenges of the chemical industry in Africa: Concerted efforts should be made to attract environmentally and economically viable chemical industries to Africa. Success in this area would do much to enhance the image of the chemical sciences on the continent.

Environmental chemistry: Africa is confronted with several environmental challenges related to the supply of adequate, safe and affordable food, clean air and water, and associated health problems in their absence. In several regions, mining and industrial development cause severe threats to the fragile African environment and IUPAC can assist in determining the levels of pollution.

Science, society, and government in Africa: The public and their government representatives must understand science to formulate good government science policy. IUPAC can contribute to the interests of Africa's chemical community by organizing governmental and public forums in collaboration with AAPAC.

Electronic communication and access to scientific information: IUPAC is prepared to assist AAPAC in planning an electronic scientific communications highway for Africa. The study of the AAAS of this area, related in the **Report on Online Journals Feasibility Study**

[http://www.aaas.org/international/ssa/ojrep1.htm] is most valuable. Several key factors are involved:

- Bandwidth and its costs.
- The Institution's Internet and LAN facilities.
- The type and location of journal.
- Usage costs and the cost of online journal subscriptions.

Higher education in the chemical sciences in Africa must be strengthened. To do this the full spectrum of information services must be critically evaluated; then the most cost-effective mix can be adopted through the wise use of the Internet.

IUPAC participated in the Workshop of the American Association for the Advancement of Science (AAAS), US and African Chemical Societies [Pretoria, April 1999] aimed at strengthening African chemical societies and creating expanded research opportunities. Four objectives were identified:

- The identification of research areas where there is a mutual significant need for international collaboration.
- The improvement of the technical, financial and managerial capacity of African chemical societies.
- The exploration of ways in which the societies can collaborate and pool resources on value-added initiatives.
- The development and maintenance of regular communication among African chemical societies.

Based on these objectives, three follow-up actions were agreed upon:

- The establishment of a "virtual headquarters" for each society, through a common link to individual society pages. A central website with the domain name [www.africhem.org] was established by AAAS with financial support from IUPAC.
- Creation of a subscription-based electronic newsletter featuring news items contributed by all the African chemical societies, to be coordinated by AAPAC.
- Establishment of a database of African chemists and institutional capacities.

AAPAC through its President, Prof. Trevor Letcher [letcher@nu.ac.za] is coordinating the database with assistance from IUPAC and ACS. A draft report "*Chemically Related Activity across Sectors in Selected Nations of Africa*", prepared by ACS in co-operation with AAPAC, appeared in July 2000 [see http://www.acs.org/international]. There were 41 respondents to 236 questionnaires, a rather disappointing response. Emerging areas identified as significant were food, sanitation, natural products, and pharmaceutical/medicinal chemicals, fine chemicals, environmental remediation, soaps and detergents. The forthcoming conference of the AAPAC, named 8 ICCA, will be held in Dakar, Senegal from July 30 to August 4, 2001 [e-mail: sambac@ucad.sn].

IUPAC collaborates actively with the International Organization for Chemical Sciences in Development (IOCD) in their volunteer service to *chemistry in development* (see http://www.iocd.org). The IOCD/IUPAC joint "Working Party in Environmental Chemistry for Developing Countries" sponsored workshops in Eastern Europe [June 1999] and for sub-Saharan Africa in Potchefstroom [September 2000]. AOAC methodology was used to show that international trade depends on using standard methods of analysis performed in well-managed accredited laboratories. The African meeting facilitated the development of effective channels of

communication among fellow scientists, contributed to the enhancement of education in chemistry, and most importantly promoted the concept of quality of life through chemistry and sustainable development.

Chemistry in Africa, particularly Macromolecular Chemistry, has benefited immensely from the annual UNESCO schools and IUPAC conferences on Macromolecules and Material Science held at the University of Stellenbosch under the direction of Prof. Ron Sanderson [Member of IUPAC Div IV]. The 4th meeting is scheduled for April 2001. In a highly successful development, the Royal Society of Chemistry (RSC), UK and the South African Chemical Institute (SACI) held their first Binational Symposium on Organic Chemistry in Cape Town [Jan 7-11,2001]. The event attracted about 240 delegates; roughly equal numbers from both countries. The meeting attended by the RSC president Prof Steve Ley and organized by Prof James Bull may serve as an example of mutually beneficial collaboration between chemists in developed and developing countries.

3. Chemical literacy in developing countries

One aspect of the service of chemistry to society is the development of "chemical literacy" and public awareness. This is the educational aspect of service, and includes formal, non-formal and informal education. Scientific and technological literacy is widely regarded as important for socio-economic development. In the most developed countries, national chemical societies are usually active in promoting chemical literacy in cooperation with government, educational institutions, etc. In the least developed countries, national chemical societies often do not exist and neither government nor educational institutions have adequate capacity and resources for the task. In both scenarios, IUPAC can help by facilitating exchange of information and crosspollination of ideas. However, it is only in the most developed countries that diffusion and application of ideas and information is likely to take care of itself. In the developing world, the lack of local capacity often totally inhibits this process. Here, IUPAC needs to combine with other agencies in introducing new ideas and facilitating the follow-up. CTC has contributed to this goal accordingly. The traditional mechanism of international conferences has been used, primarily to serve chemistry educators from the more developed countries. The biennial International Conferences on Chemical Education are the principal example of CTC's involvement in this way. To contribute to this goal in developing countries, CTC has worked in cooperation with UNESCO (Basic Sciences). Two successful examples are the introduction and diffusion of small scale, low cost chemistry practical activities and the DIDAC visual educational materials. Initial introduction of such innovations to selected educators in different countries needs to involve only modest funds, to which IUPAC could make a meaningful contribution. If the innovations are favorably received then further diffusion is often requested. This requires much greater financial resources and is dependent on gaining the support of funding agencies or national education departments. IUPAC, in cooperation with UNESCO, can assume the role by bringing the merits of these innovations to the attention of these agencies and government representatives.

In conclusion, it is a great challenge to incorporate new knowledge, information and technology in the developing world. Human capacity remains the key to sustainable development in Africa and the rest of the developing world. 21st century goals must be focused on raising basic education levels, promoting excellence in research, training in science and technology, and preparing young scientists to assume their roles as equal partners in the global community.

VIII. CONCLUSION

1. Highlights

At IUPAC, we take much pride in the following accomplishments:

- The acceptance of the IUPAC Strategic Plan by the IUPAC Council (Berlin), August 1999.
- The introduction of the project-driven system in IUPAC while maintaining the commission-based system. The latter to be phased out by December 31, 2001.
- The election of DCs by the involvement of nominating committees.
- The establishment and functioning of the Project Committee (Prof G den Boef) and the Evaluation Committee (Prof G Schneider).
- The effective and commercially viable self-publishing of *PAC* and of *CI*.
- The creation of a sound financial basis for the introduction of the project-driven system in IUPAC.
- The establishment of the Committee on Chemical Identity and Nomenclature Systems (Dr Alan McNaught) as to position IUPAC in the area of chemical nomenclature.
- The establishment of the ESDC, chaired by Prof Peter Atkins and the ensuing report.
- The effective development of the IUPAC-website and comprehensive use of electronic communication in the Union.
- The publication of two special topic issues of *PAC* in 2000 and the translation of two *PAC* White Books into Japanese.
- The holding of a workshop on Advanced Materials ... the first in the series on New Directions in Chemistry.
- The establishment of the IUPAC Prize for Young Chemists and the award to nine outstanding young chemists at the Brisbane IUPAC Congress.
- The successful introduction of the IUPAC Fellows Program.

2. Recommendations for 2002/2003

- a. The establishment of a task group to evaluate and prioritize the long range goals of the Union as to ensure better focus on fewer, more clearly stated goals, and to insure that a sound "customer focus" is provided.
- b. The establishment of a Division of Systemic Nomenclature and Structure Representation to retain IUPAC's leadership in this area of the chemical sciences.
- c. Concerted efforts should be made to attract eminent chemists to serve on DCs to manage the scientific programs in close collaboration with the IUPAC Secretariat
- d. The provision of the Committee on Chemical Education with sufficient resources to fulfill the important educational functions in the Union.
- e. The sound management of the Investment Policy of IUPAC to ensure sufficient resources for the Biennium Operating Reserve Fund, Southern Hemisphere Sinking Fund, Young Scientists Award Fund, and the Endowment Reserve.
- f. The active promotion of IUPAC-sponsored conferences. The CHEMRAWN program and Workshops on New Areas of Chemistry, e g New Materials and Chemical Biology are highly commended.

- g. The improvement of the image of IUPAC by the IUPAC website and by publishing an interesting, easily readable and attractive CI.
- h. The provision of assistance in chemical information and literacy to developing countries in Africa.
- i. The new IUPAC Vice-President to be tasked to increase the geographic base of the Union, particularly in Eastern Europe, Asia, Africa and South America.

IX. ACR	ONYMS
AAAS:	American Association for the Advancement of Science
AAPAC:	African Association of Pure and Applied Chemistry
AAS:	African Academy of Sciences
AAU:	Association of African Universities
ABN:	African Biosciences Network
ANSTI:	African Network of Scientific and Technological Institutions
CASIS:	Consortium of African Schools of Information Sciences
CI:	Chemistry International
CODATA:	Committee on Data [a component of ICSU]
CTC:	Committee on Teaching of Chemistry
DC:	Division Committee
ESDC:	Education Strategy Development Committee
FAO:	Food and Agriculture Organization
IAC:	Inter-Academy Council
ICSU:	International Council for Science
IOCD:	International Organization for Chemical Sciences in Development
NABSA:	Network for Analytical and Biological Services in Africa
NAPRECA:	Natural Products Research Network for Eastern and Central Africa
NAS:	National Academy of Sciences
NR:	National Representative
OPCW:	Organization for the Prohibition of Chemical Weapons
PAC:	Pure and Applied Chemistry
PUST:	Pan-African Union of Science and Technology
RSC:	Royal Society of Chemistry
SACI:	South African Chemical Institute
SCOPE:	Scientific Committee on Problems of the Environment [a component of ICSU]
SDIC:	Strategy Development and Implementation Committee
UNEP:	United Nations Environment Program
UNESCO:	United Nations Educational, Scientific and Cultural Organization
WHO:	World Health Organization