International Union of Pure and Applied Chemistry

IUPAC
Project Summaries

The following summaries represent projects, since 2003, for each of the 8 Divisions and Operational Standing Committees:

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June 2005

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I PHYSICAL AND BIOPHYSICAL CHEMISTRY DIVISION

Title: ***Recommended values of the viscosity of molten iron and aluminum***
Number: 2003-005-1-100
Objective:
The widely different data obtained for the viscosity of molten iron and aluminum will be critically reviewed via an interlaboratory comparison and recommended values will be proposed.
Description:
Wide ranges of values of viscosity of both molten iron and aluminum are reported in the literature. The most widely used method is some form of oscillating vessel. For the oscillating cup a number of analytical techniques have been There are two challenges:

1. Agreement about the equations used to determine the viscosity by the oscillating cup method.
2. The widely different data obtained for the viscosity of aluminum and iron need to be critically reviewed and recommended values suggested. This may result in the need for an interlaboratory comparison.

Title: ***NMR chemical shifts: updated conventions***
Number: 2003-006-1-100
Objective:
To update IUPAC Recommendations 2001: NMR Nomenclature, Nuclear Spin Properties and Conventions for Chemical Shifts by addressing several issues still to be resolved in setting standards for chemical shifts, including temperature variation of the NMR signals of reference compounds, the use of magic-angle spinning for both solutions and solids, solvent effects, and magnetic susceptibility corrections.
Description:
Nuclear magnetic resonance has long been an invaluable technique for determining molecular structure and for investigating a wide variety of chemical phenomena. The cornerstone of such applications is the *chemical shift* - a quantity that must be measured relative to an agreed reference. For many years, common practice was to use a separate reference for each nuclide. However, as a result of the above-cited publication, IUPAC is now on record as recommending that chemical shifts for all nuclides be expressed on a unified scale relative to the proton [^{1}H] resonance of tetramethylsilane [TMS] in a 1 percent solution in $CDCl_3$. Since its publication only a year ago, this recommendation has been well received by the international NMR community; has been widely disseminated by republication in NMR journals and presentations at NMR conferences, as detailed below; and has been publicized by one of the three major NMR equipment manufacturers.
The IUPAC publication in 2001 included extensive tables of data on NMR properties, chemical shift values of secondary references for each nuclide, and detailed explanations of factors affecting measurements of chemical shifts.

Title: ***Ionic liquids database***
Number: 2003-020-2-100
Objective:
Create an open-access, free, on-line, comprehensive database for storage and retrieval of metadata and numerical data for ionic liquids, including their syntheses, structure, properties, and uses; lack of this information is impeding progress in a burgeoning field of significant current interest.
Description:
Ionic liquids are expanding dramatically in popularity (see inset figure), and the first industrial application (the BASF BASIL process) was announced at the end of March 2003. Crucial to their implementation on a wider scale (and these are green solvents) is universal access to their physical properties. As there are potentially over one million simple ionic liquids (although fewer than one thousand have yet been reported), the need for a living database, with continuous updating is paramount. This project brings together some of the world leaders in ionic liquid technology with leading thermodynamicists and database technologists.

Title: ***Selected free radicals and critical intermediates: thermodynamic properties from theory and experiment***
Number: 2003-024-1-100
Objective:
The main objective of this project activity is the continued compilation and critical evaluation of published thermodynamic properties, including the computation of accurate thermochemical data for selected free radicals, that are of importance in atmospheric and combustion chemistry. A distinguishing feature of the critical data evaluation is the systematic utilization of all available kinetic, spectroscopic and ion thermochemical results as well as high-level computations.
Description:
Knowledge of accurate thermochemical properties of free radicals is of great importance in many branches of chemistry, in particular atmospheric and combustion modeling. Thermochemical kinetic estimations provide sometimes the only possibility for obtaining rate coefficients and branching ratios for reactions of short-lived intermediates such as free radicals. Thermodynamic quantities for stable molecules are relatively well established. These are typically

obtained from calorimetric determinations, while heat capacities and entropies are derived from the results of spectroscopic measurements. For free radicals and other short-lived intermediates, direct calorimetric measurements are (in most cases) not possible, while spectroscopic investigations require more skill and sophisticated instrumentation. Consequently, thermochemical data for a number of free radicals have a higher uncertainty than the corresponding values of closed shell species. However, computational chemistry has made great progress in reliability and accuracy. A solid basis of thermochemistry now comprises the optimized combination of experimental and computational results.

Title: ***Thermodynamics and non-equilibrium criteria for development and application of supplemented phase diagrams***
Number: 2003-036-2-100
Objective:
The aim of the project is to establish rational links between thermodynamic aspects of phase diagrams supplemented by the non equilibrium curve of the glass transition temperature for mixtures of water with vitrifying agents used in the cryo and dehydropreservation of natural (foods, seeds, etc.) and synthetic products (pharmaceuticals). It will contribute to improve processing and conservation practices of these important materials.It intends not just to compile information that already exists, but to consider all the sort of basic and applied problems that one should consider when managing these phase/state diagrams.
Description:
The present proposal is prepared as to have a very broad and interdisciplinary scope for impacting on many fields related to chemistry and biophysical chemistry. It would permit promoting IUPAC activities and competence to a wider non-chemistry scientific community. It is largely inspired in early activities of the International Symposia on the Properties of Water (ISOPOW). The applicability of state diagrams is recognized in food chemistry and related areas. However, many basic questions are still open and more precise definitions are needed for a correct interpretation of the involved phenomena.The practical aim of the project is to give solid basis to develop supplemented state diagrams of aqueous glassy formers, such as saccharides, polyols, etc., in order to describe the influence of water content, nature of the vitrifying agent and temperature on the physico-chemical stability of natural and synthetic products.

Title: ***Heat capacity of liquids: critical review and recommended values for liquids with data published between 2000 and 2004***
Number: 2004-010-3-100
Objective:
To update and extend two publications that contained recommended data on liquid heat capacities for almost 2000 mostly organic compounds.
Description:
Experimental data on heat capacities of pure liquid organic and some inorganic compounds published in the primary literature between 2000 and 2004 will be compiled, critically evaluated and recommended values provided. Recommended data supplemented with an assessment of their uncertainty and presented in terms of parameters of correlating equations for temperature dependence of heat capacities will be developed by critical assessment of literature calorimetrically determined heat capacities.

Title: ***Categorizing hydrogen bonding and other intermolecular interactions***
Number: 2004-026-2-100
Objective:
To take a comprehensive look at intermolecular interactions and classify them and to give a modern definition of the hydrogen bond, taking in to account all current experimental and theoretical information, and including hydrogen bonded systems both in gaseous and condensed phases as well as in chemical and biological systems.
Description:
Hydrogen bonding has fascinated chemists and biologists for several decades now and it is central to chemistry and biology. The original definition of hydrogen bonding invoked two electronegative atoms (X and Y) interacting through a hydrogen atom as in X-H --- Y. Initially X and Y were found to be mostly N, O and F which led to the mentioning of these atoms as part of the definition of hydrogen bonds in various sources. Hydrogen bonding was inferred by the difference in physical properties between otherwise chemically similar systems such as found between H_2O and H_2S. However, now it is well known that both H_2O and H_2S form a hydrogen bonded $(H_2X)_2$ dimer in the gas phase. Spectroscopic red shift in XH stretching frequency was among the first experimental evidence used for inferring hydrogen bonds. Now there are several hydrogen bonded systems that appear to show blue shift in XH stretching frequency.

Title: ***Establishing recommended data on thermodynamic properties of hydration for selected organic solutes***
Number: 2004-036-1-100
Objective:
The objective of the project is to establish a database of thermodynamic properties of hydration for approximately 200 selected organic solutes at reference condition of 298.15 K and 0.1 MPa and as a function of temperature and pressure up to the near critical region of water. The values of hydration properties for solutes covering different molecular

structures will be calculated from the reliable experimental data for aqueous and pure solutes. The established database will be used as a standard for testing and establishment of new physico-chemical models and methods of molecular simulation as well as for developing semi-theoretical prediction schemes of interest for chemical engineering, environmental chemistry and geochemistry.

Description:

Thermodynamic properties of hydration (TPH) covered in the project are: the Gibbs energy of hydration and its temperature and pressure derivatives (the enthalpy of hydration, the heat capacity of hydration and the partial molar volume at infinite dilution), other TPH result from their combinations; for exact definitions and inter-relationship. TPH express the difference between the property of a solute in the standard state of infinite dilution at a given temperature and pressure and that of an ideal gas at the same temperature and reference pressure of 0.1 MPa. Thus they characterise the transfer of a solute from a state where molecules are not interacting to the state where the solute molecules interact solely with the water solvent. Due to this definition they can be used conveniently in testing and conception of theoretical models and simulation approaches for dilute aqueous solutions developed by physical chemists. At the same time, TPH allow an easy calculation of partition coefficients (such as the Henry's law constant, air-water partition coefficient, relative volatility, etc.) and of the thermodynamic reaction constants for aqueous systems.

II INORGANIC CHEMISTRY DIVISION

Title: ***Isotopic compositions of selected elements***
Number: 2003-031-2-200
Objective:
To design, compile and produce a new Report on the Isotopic Compositions of selected Elements, containing updated data with uncertainties that conform to ISO 9001 requirements.
Description:
The Commission on Isotopic Abundances and Atomic Weights (CIAAW) has produced in the past (last one in 2001) several tables emphasizing the isotopic abundances of the elements. The evaluated data provided on these tables has usually been selected to represent a) the best available measurements and b) that present in representative materials which do not always correspond to the Commission's recommended standard atomic weights for each element. The inconsistencies between some of the recommended isotopic abundances and atomic weights has been requiring our attention for some time which this proposal aims to correct.
The second major aim of this project is to address the increasing importance of isotope ratio measurements in chemistry, geological, environmental sciences, product authentication, forensic and life sciences.

Title: ***Determination of atomic weights using new analytical techniques***
Number: 2003-033-1-200
Objective:
New analytical techniques, including inductively coupled plasma-mass spectrometry, have recently provided atomic weights with unparalleled precision. The purpose of this project is to assess the uncertainties in these new methods in atomic-weights work, evaluate published work, and, if possible, make recommendations to update IUPAC's Table of Standard Atomic Weights.
Description:
New analytical techniques, including inductively coupled plasma-mass spectrometry (ICP-MS), have recently provided atomic weights of chemical elements with unparalleled precision. For example, ICP-MS analyses on boron reference materials distributed by the International Atomic Energy Agency have very low uncertainties in their atomic weights, but the values do not agree well with previous thermal ionization mass spectrometric (TIMS) measurements. In fact, ICP-MS values from different laboratories do not overlap even with 2-? uncertainties. The reasons for the lack of agreement currently are not well understood. The purpose of this project is to assess the uncertainties of these new methods in atomic-weights work.

Title: ***Classification, terminology and nomenclature of borophosphates***
Number: 2003-034-1-200
Objective:
Throughout the literature a variety of systems for the nomenclature of borates are used. On the other hand in recent years numerous compounds were obtained containing boron and phosphorus, which are called borophosphates. These are built with B-O-B or B-O-P linkages where structural information and formula are available. Depending on the formula and structure of the compound, it is observed that different nomenclatures are used by different people or naming of the compound is ignored. There are several examples in recent literature where some difficulties arise in naming borophosphates. The objective of this project is to provide terminology, classification and naming of novel borophosphate compounds depending on structure and linking principles.
Description:
Borophosphates are the intermediate compounds of the $M_xO_y.B_2O_3.P_2O_5$ (H_2O) system which contain complex anionic structures built of BO_4, BO_3 and PO_4 groups and their partially protonated species. Numerous borophosphate compounds have been synthesized by solid state, solution, hydrothermal and microwave techniques. The structure of these is based on the linking principles of the primary building units which should be classified. Borophosphate anions extend from isolated species, rings, chains, oligomers, layers and frameworks like silicates. The main goal of this project is classified as:

1. To investigate some specific structures of boron compounds, containing phosphates, that have close relation to silicates.
2. The publication of such classification and nomenclature would enlighten and stimulate the researchers to synthesize new borophosphates.

Title: ***Towards defining materials chemistry***
Number: 2005-001-1-200
Objective:
To assemble, collate and disseminate information about the scope of the newly-emerging discipline of materials chemistry, leading to an authoritative definition of the subject within the family of chemical sciences.
Description:
The last 10-15 years have seen the emergence and rapid growth of 'materials chemistry' as a distinct discipline within the broad family of chemical sciences. This was a combination of noun and adjective that had not previously formed

part of the chemists' vocabulary. Now a significant fraction of all publications in chemistry claim to form part of this new field. In particular two international journals (*Chemistry of Materials*, published by the American Chemical Society and the *Journal of Materials Chemistry*, published by the Royal Society of Chemistry in Great Britain) are achieving high impact factors and publish work emanating from every continent of the world. Yet there remains no definition of the phrase 'materials chemistry' agreed by the global chemical community. IUPAC being the most appropriate body to sponsor such a debate, the project proposed here aims to address this deficit.

Part of the difficulty in defining the scope of materials chemistry arises from the fact that it transcends the divisions separating the traditional branches of chemistry (e.g. organic and inorganic) or between continuous-lattice and molecular solids.

III ORGANIC AND BIOMOLECULAR CHEMISTRY DIVISION

Title: ***Green chemistry in the Arab region***
Number: 2003-043-1-300
Objective:
This project is aimed at increasing the awareness and interest of university students in Arabic universities and other educational institutes and industrial chemists towards the Green Chemistry activities, by highlighting their general significance and presenting already on-going activities in different regions of the Arab world. The aim of project is to produce and disseminate a book like "Green Chemistry in Africa" and "Green Chemistry in Latin America" and "Green Chemistry in Russia". The Green Chemistry in Africa book is being disseminated in sub-Saharan Universities. Presently, the book "Green Chemistry in Latin America" is being prepared..
Description:
The book will be designed for university students and for industrial chemists and will be written in Arabic. This makes it possible to disseminate the book in all the Arab world that include, Egypt, Syria, Jordan, Palestine, Lebanon, Iraq, Kuwait, United Arab Emirates, Saudi Arabia, Bahrain, Qatar, Yemen, Oman, Sudan, Libya, Tunisia, Morocco, Algeria and Mauritania. The book plans to underline the relevance of Green Chemistry in general, and to elucidate its potential importance for the Arab countries.

Title: ***Workshop for formulation of plans for the establishment of a "Center of Natural Products Research (CNPR)"***
Number: 2003-046-1-300
Objective:
1. Documentation of traditional knowledge of medicine (involvement of traditional healers)
2. Scientific authentication (efficacy, toxicity & dose) of herbal/traditional medicine
3. Value addition to bio-resources (benefit to women and tribal people)
4. Coordination of natural products research for the development of therapeutic agents
5. Conservation of biodiversity: Preservation, Cultivation and Propagation

Description:
Herbal/traditional medicines have been playing an important role in the primary health care of the people around the world, specially in the developing countries. In order to keep pace with the modern medicines, the production of herbal medicines in a standardized way is essential. The World Health Organization in its various forums has stressed upon the need for producing herbal medical preparations in a scientific way to cater the needs of the people for primary health care at a low cost, as many modern medicines are prohibitive to the common people for their high prices.

Title: ***Reference methods, standards and applications of photoluminescence***
Number: 2004-021-1-300
Objective:
IUPAC documents on fluorescence will be updated including advances registered during the last fifteen years. Particular attention will be given to newly developed reference materials and methods.
Description:
Fifteen years ago, David Eaton undertook the task of collecting information on fluorescence methods and materials. Since Eaton's documents were written, new reference materials appeared and the subject evolved rapidly with the incorporation of new areas and methods which were not or only poorly developed at that time. A few examples are single molecule fluorescence, ultrafast fluorescence detection, fluorescence microscopy and so forth. Many of these areas are of utmost relevance in materials science and in biology. In general, the interest shifted impressively to organized, (micro) heterogeneous systems.

IV POLYMER DIVISION

Title: ***Recommendations for data presentation and storage applicable to mechanical and rheological measurements of polymers***
Number: 2003-009-1-400
Objective:
The objective is to simplify the exchange and presentation of data from mechanical and rheological measurements. A document with broadly accepted recommendation based on ISO 67211 will be developed and published in cooperation with instrument manufacturers. The recommendations will be implemented into the software of the participating manufacturers.
Description:
There is a vast number of manufacturers of mechanical and rheological test equipment. Unfortunately, the number of different and incompatible computer programs for data acquisition, evaluation and presentation is just as high. As a consequence, the direct exchange of electronic data files between different laboratories or even between different machines in the same laboratory is cumbersome. Much time is necessary to convert data into a standard ASCII format for exchange. In addition, these ASCII data are often provided without the necessary description of how the measurements were made and/or definition of the applied data manipulation procedures. Furthermore, the data presentation capabilities of the various instruments' software are limited. It would be advantageous if e.g. the diagrams produced could directly be used for transparencies or video presentations without need to improve the readability of legends and axis titles.

Title: ***Structure and properties of polymer/clay nano-composite materials***
Number: 2003-051-1-400
Objective:
To evaluate the relationship between the morphology and the mechanical, rheological and transport properties of the polymer nano-composite materials.
Description:
Recent developments in the technology of intercalating polymer chains in nanoscale layers of clay have produced new types of high performance polymer composites. However, the effects of the higher order structure on mechanical properties are not yet well understood. For example, little is known on the crystallization of polymer chains confined in the nano-scale domains and subsequently occurring morphology formation. Since mechanical properties of the composites are strongly affected by the higher order structure, the control of the higher order structure becomes a key technology to design nano composites with excellent performance and/or functions. The purpose of this study is to clarify the relationship between the higher order structure and properties of commercially available nano-composites composed of polyamide, PMMA and clay. The topics cover a wide range of research from characterization of the components through physical properties in the solid state. Rheological properties of the melts are also an important topic related to the processability of the composites.

Title: ***Guideline for rheological characterization of polyamide melts***
Number: 2004-009-1-400
Objective:
To investigate the influence of the specimen preparation and of the experimental method on the rheological properties of polyamide.
Description:
Rheological characterisation results on polyamide melts strongly depend on sample preparation (e.g. humidity control) and on details of the experimental procedure. As a consequence, data from various laboratories do not agree. Aim of the project is to develop a widely accepted guideline for sample pre-treatment and measurement, both for rotational and capillary rheometry. These guidelines should be in particular be pertinent for industrial laboratories.

Title: ***Data treatment in size exclusion chromatography of polymers***
Number: 2003-023-2-400
Objective:
In spite of the ample use of Size Exclusion Chromatography (SEC) for measuring the molar mass distribution (MMD) of polymers, there are huge variations in the results obtained by different laboratories, when analyzing the same polymer sample. One of the possible reasons for such variations may be the applied data treatment. Thus, it seems indispensable to standardize the SEC data treatment. The objectives are:

1. Develop some novel, more practical, and more efficient procedures for the correction of BB and other sources of error; in order to improve the accuracy of the measured MMD and other polymer molecular characteristics.
2. Compare and critically evaluate the different classical and novel data treatment methods, with the final aim of recommending a standard procedure that may be useful for general SEC user and for the instrument manufacturer.

Description:
SEC is the main analytical technique for determining the MMD of synthetic polymers. In spite of its ample use, the

accuracy of the technique is relatively low, as it is verified by the dispersion of results obtained in round-robin tests. For good quantitative results, not only the equipment must be in good physical shape. Also required are a careful experimental work and a judicious data treatment.

Title: ***Terminology and measurement techniques of starch components***
Number: 2004-022-3-400
Objective:
The aims of this project are (1) to reach agreed definitions of the three types of starches, and (2) to explore reliable and reproducible means of measuring the relative amounts of each in a given sample. At present, different laboratories report different results for what ostensibly is the same quantity.
Description:
There are two well known types of starch in cereals, amylose, or apparent amylose, and amylopectin; research indicates a third. All are polymers of glucose. Amylose, or apparent amylose, is amorphous and contributes to most, if not all, the cooking and processing properties of cereals and tubers. Amylopectin is semi-crystalline and branched and accounts for the greatest proportion of starch in cereals and tubers. The third type is amorphous and branched and its functionality is still unknown.

Title: ***Critically evaluated propagation rate coefficients for free-radical polymerization of water-soluble monomers polymerized in the aqueous phase***
Number: 2004-034-1-400
Objective:
To initiate critical evaluation of propagation rate coefficients for water-soluble monomers polymerized in the aqueous phase. Data from pulsed-laser initiated polymerization in conjunction with polymer molecular weight analysis by size-exclusion chromatography will be considered. The specific role of polymerization conditions with water being the polymerization medium will be emphasized.
Description:
Knowing the kinetics and mechanism of polymerization provides a thorough understanding of polymerization processes and allows for the simulation of polymer properties and polymerization rates. The precise knowledge of rate coefficients was highly insufficient until recently.

Title: ***Towards a holistic mechanistic model for reversible addition fragmentation chain transfer (RAFT) polymerizations: Dithiobenzoates as mediating agents***
Number: 2004-040-1-400
Objective:
To provide the scientific community involved in performing and modeling RAFT polymerizations with appropriate kinetic schemes as well as the best possible and critically evaluated kinetic parameters describing various RAFT processes.
Description:
The reversible addition fragmentation chain transfer (RAFT) polymerization has witnessed a rapid development during the last years. Although being widely used for the generation of both complex and well-defined polymeric materials - especially employing dithioester compounds as the mediating agents -, a complete understanding of the fundamental reaction scheme, which induces the equilibrium between dormant and active radical species, has not yet emerged. A deep understanding of the RAFT process, however, is mandatory to establish structure/rate correlations for a specific RAFT agent, which is essential for rational RAFT agent design delivering novel mediating compounds.

Title: ***Postgraduate course in polymer science***
Number: 2003-041-1-400
Objective:
To enable young university graduates and PhDs from countries with limited research facilities to acquire knowledge on recent advances in polymer science and professional skills needed for promotion of polymer science in their home countries.
Description:
The eighth and ninth runs of the Course were held in the academic years 2003-2004 and 2004-2005 at the Institute of Macromolecular Chemistry, Academy of Sciences of the Czech Republic, in Prague. The Courses are sponsored, mostly without financial assistance, by UNESCO. The Institute with its staff of 240 including more than 100 scientists and with experience of 38 years in educating young scientists from emerging countries offers up-to-date facilities for postgraduate training in polymer science. The Course lasts 10 months and comprises about 50 hours of lectures in modern polymer science, including introduction into the nomenclature and terminology recommended by IUPAC, experimental work on research projects under the supervision of senior scientists of the Institute and participation in all educational activities within the Institute. Young scientists from the following countries graduated from the Course: Bangladesh; Bulgaria; India; Kazakhstan; Poland; Romania; Russia; South Africa; Ukraine; Uzbekistan. The results of their research are published in international technical journals.

Title: ***Design of polymer education material for French speaking countries***
Number: 2004-037-1-400
Objective:
The aim of this project is to provide the French-speaking countries with a standard for polymer education based on various tools such as books, multi-media or databases.
Description:
The need for a standard in polymer education is recognized and expressed by French speaking academics of both emerging and developed countries.
The proposed new materials will be elaborated by partners working in separate task groups, each one focusing on specific medium. The choice of topics to be developed will be made after discussion taking into account the minimum 50-hour program already recommended in France by the French Polymer Group (GFP).

Title: ***Definitions of terms relating to crystalline polymers - revision of IUPAC Recommendations 1988***
Number: 2003-019-2-400
Objective:
To update the previous IUPAC document by accounting for new experimental results, integrating crystallographic, conformational and morphological terminology relating to polymers and providing new, significant examples, harmonising with other documents of the Subcommittee on Macromolecular Terminology.
Description:
The proposed revision will be based on the following points:

1. In view of the rapid development and widespread application of the experimental techniques, explicit reference will be made to results from solid-state NMR, AFM, electron microscopy and diffraction, SANS and SAXS, FT-IR and Raman spectroscopy etc., whenever appropriate.
2. Further examples will be given, especially those that correlate morphology with local conformation of the polymer chains.
3. Reference will be made to biological macromolecules that crystallise as non-globular chains.
4. Some definitions relating to chirality of biological macromolecules and to stereoregularity of synthetic polymers will be compared and harmonised.
5. Definitions of terms belonging to general physical chemistry, such as crystal, unit cell etc. will be avoided as much as possible.
6. Disorder in crystalline polymers will be covered. Some choices are required, such as whether or not to mention the so-called two-phase model and to deal with the issue of static vs dynamic disorder.
7. Wider reference to and fuller integration with other documents of the Subcommittee on Macromolecular Terminology will be attempted, especially with regard to the Liquid Crystal Document, the Glossary of Basic Terms and the Polymer Solutions Document.

Title: ***Terminology on separation of macromolecules***
Number: 2003-060-2-400
Objective:
To revise and elaborate the terminology on the separation of macromolecules in the "Compendium of Analytical Nomenclature'.
Description:
The document deals with the terminology on the separation of macromolecules, which is typical and unique field of activity of the IUPAC organization. The document will include various separation methods widely used in macromolecular separation beyond size exclusion chromatography, which includes interaction chromatography, chromatography at critical condition, temperature rising elution fractionation, field flow fractionation, and so on.

Title: ***Terminology for biomedical (therapeutic) polymers***
Number: 2004-043-1-400
Objective:
Like most of the materials used by humans, polymers and polymeric materials have been tested and occasionally exploited by surgeons and pharmacists to treat trauma and diseases. This project is aimed at proposing a list of terms and definitions to be accepted and respected by academic, industrial and normative people active in the biomedical and pharmacological fields.
Description:
More and more therapeutic problems are relevant to the use of polymer-based therapeutic aids for a limited period of time, namely the healing time related to the outstanding capacity of living systems to self-repair, e.g. bone fracture fixation with screws and plates, of wound closure by sutures and also of drug delivery from implants or similar systems based on polymeric matrices, or on aqueous dispersions or solutions of polymers. After healing the remaining prosthetic materials or devices become foreign residues or wastes that have to be eliminated from the body. Nowadays, biocompatible polymers that can degrade in the body are developed. The degradation and the elimination of degradation by-products depend on rather complex phenomena that are presently reflected inconsistently by terms issued from the tradition because each domain has developed its own terminology almost independently. This is a source of

misunderstandings, confusions and misperceptions among scientists, surgeons, pharmacists, journalists and politicians, the situation being increased by the introduction of degradable polymers in plastic waste management and environmental protection. Therefore, it is urgent to reflect the various phenomena by specific terms, harmonize and enforce their use by the people active in the biomedical, pharmacological and environmental fields, and, last but not least by the publishing media and journalists.

Title: ***Definitions of terms relating to individual macromolecules, their assemblies, and dilute polymer solutions***
Number: 2005-005-2-400
Objective:
To revise and amend the new terminologies on the IUPAC Recommendation: Definitions of Terms Relating to Individual Macromolecules, Their Assemblies, and Dilute Polymer Solutions (*Pure Appl. Chem.* **61**, 211-241 (1989)). The document, published in 1989, deals with terminology in key areas of the physical chemistry of macromolecules as individual macromolecules, their assemblies and dilute polymer solutions; it includes recommended terminology for molecular weight, molecular-weight averages, distribution functions, radius of gyration, the Flory-Huggins theory, viscosity of solutions, scattering of radiation by polymers, fractionation, etc. Since late 70's, there has been a rapid progress in understanding the physical properties of macromolecules in concentrated solution and in bulk, which was not matured enough when the document was prepared. Also, it is (required) desirable to take action against some frequently used improper terms. Therefore, it is urgent to revise and expand the terminology on the physical properties of macromolecules in solution and publish it as a superseding recommendation.
Description:
The document deals with the terminology of macromolecules in solution, individual macromolecules and macromolecular (aggregations) assemblies. Chemical terminology, is (typical and unique field of activity) one of the basic terms of reference of IUPAC. Its update is also of great importance for the recently started project on terminology in separation techniques. The document will include newly introduced terms in the field of physical properties of macromolecules in various states, particularly in concentrated solutions and in bulk.

Title: ***Guide to macromolecular terminology and nomenclature***
Number: 2005-007-1-400
Objective:
To bring to a general and much wider audience, matters of macromolecular nomenclature and terminology in order to foster clear communication in and a deeper understanding of the subject.
Description:
In the early 20th century, the concept of macromolecules was introduced, which led to the foundation of polymer science as a subject of study. With the spread of knowledge of this new type of molecule and the materials thereby formed, the need grew for an unequivocal and universal terminology and chemical nomenclature and its documentation. Initially, small groups and committees were formed to discuss the issues involved. Finally, in 1952 the first recommendations on macromolecular nomenclature were published by IUPAC.
Following this start, many IUPAC recommendations in the fields of macromolecular terminology and nomenclature have been published over the past 50 or so years. They are concerned with the structural representation of macromolecules, terminology related to polymerization, the structure and properties of polymer materials, and chemical nomenclature.
The proposed guide is being written to provide easy access to the most important aspects of these recommendations, with the particular aim of helping newcomers to macromolecular chemistry and physics in order to cope with the particular features of the subject, even though they may be experts in other fields of chemistry and physics. It gives definitions, terms, and nomenclature rules linked with explanatory text, as in a textbook.

V ANALYTICAL CHEMISTRY DIVISION

Title: ***Terminology, quantities and units concerning production and applications of radionuclides in radiopharmaceutical and radioanalytical chemistry***
Number: 2003-015-2-500
Objective:
The current issue of IUPAC Orange Book (1997) does not cover exhaustively the definition of several terms in radioanalytical, radiopharmaceutical, nuclear and radiochemistry and related topics; many terms should be improved and clarified. Radioanalytical techniques are of increasing relevance in the fields of labeled compounds and radiopharmaceuticals to be used in radiodiagnostics, metabolic radiotherapy, radioimmunotherapy.
Description:

1. The following headings will be addressed:
   Glossary
2. Radionuclide Production
3. Radioanalytical and Radiopharmaceutical Chemistry laboratories
4. Analytical and Radioanalytical techniques
5. Quality Control of Radionuclides and Labeled Compounds
6. Interaction of radiation with matter
7. Fields of application
8. Exhaustive and updated list of literature, nuclear databases and international/national electronic links.

Title: ***Optical Biosensors and Bioprobes***
Number: 2003-037-1-500
Objective:
The development of optical biosensors has recently gained increasing interest for important environmental and biological applications. Optical biosensors combine several critical components including a bioreceptor (e.g., enzyme, antibody, gene probe), an excitation light source and an optical detector or optical transducer. Optical biosensors take advantage of the excellent selectivity of the bioreceptor and the outstanding sensitivity of optical detection methods. This project will define terms and nomenclature related to optical biosensors. Collaborative interactions will be pursued with other Commissions and Working Groups which are involved in aspects related to biosensors.

Title: ***Standard definitions of terms relating to mass spectrometry***
Number: 2003-056-2-500
Objective:
To update and extend the definitions of terms related to the field of mass spectrometry.
Description:
Widely accepted standard definitions of terms are necessary for clear communication in the discussion and dissemination of results. This is particularly important for multidisciplinary fields such as mass spectrometry. During the last decade of the 20th century, the field of mass spectrometry has seen a revolutionary change in practice and scope. The introduction of soft ionization methods for the analysis of biological molecules has expanded the scope of mass spectrometry from its early roots in the analysis of inorganic and organic species into the fields of biology and medicine. This expansion in scope and length of time since the last update of standard terms and definitions make it important to undertake a revision of these terms at this time.

Title: ***Comparable pH measurements by metrological traceability***
Number: 2004-005-2-500
Objective:
To implement traceability chains for pH values in routine measurements in order to achieve target uncertainties for specific applications. Also, to develop educational and quality control tools for reference and testing laboratories under the observation of chemical and metrological principles, and to improve the comparability and the assessment of pH values.
Description:
After the production of the IUPAC paper "The Measurement of pH. Definitions, Standards, and Procedures (IUPAC Recommendations 2002)", a workshop “Importance of Traceable pH Measurements in Science and Technology”, revealed priorities and showed a strong request from the concerned community for continuing action on

1. Educational efforts on the calculation of the uncertainty of pH values;
2. Elaboration of recommended protocols for specific applications (*e.g.* quality monitoring and assessment in the different applications of water and in physiological media) by round robin studies, observing the traceability chain, calculating the uncertainty of the sample pH;
3. Critical assessment of the existing methods to calculate the hydrogen ion activities and concentrations, allowing extension of the presently adopted model for a wider range of applications.
4. The proposal aims at covering these objectives. Work is progressing in the frame of the group's research activities and will be submitted to IUPAC for endorsement.

Title: ***Guidelines for potentiometric measurements in suspensions***
Number: 2004-016-2-500
Objective:
To state the causes and natures of the Suspension Effect in potentiometric measurements in suspensions, and to give an unambiguous, experimentally verified definition and interpretation of the Suspension Effect and recommend procedures for pH (pIon) measurements in suspensions.
Description:
The term "suspension effect" (SE) was introduced seventy five years ago. Originally it was defined as the difference between the potentiometrically determined hydrogen ion concentration of a suspension and of the medium pertaining to it. Many interpretations of this difference were published until now but no consensus about its origin or explanation was accepted, though an enormous experimental and theoretical study of these problems was done. Guidelines for practical routine pH (and pIon) measurements in suspensions will be given. The electrodes and the instructions for their use will be described and illustrated with some examples.

Title: ***Standardization of analytical approaches and analytical capacity-building in Africa***
Number: 2004-017-1-500
Objective:
This project seeks to upgrade selected laboratories in Africa, thereby enabling them to produce reliable and internationally accepted analytical results for farmers and enterprises in the private sector that seek to export commodities to markets in the USA, EU, and Japan, where compliance with international standards is required.
Description:
The recent World Bank book *Standards and Global Trade* states that "trade is a crucial driver of growth." The book reveals, however, that farmers and firms in African countries, including Kenya and Uganda, are unable to reap the potential income for the growth of their economies from trade on foreign markets, for their governments fail to provide them the services of a well developed regulatory infrastructure with competent laboratories that can ensure their commodities comply with international standards.
Our project will addresses these constraints that block desired gains from trade by carrying out a pilot activity that first evaluates local needs and then brings appropriate remedial measures to bear on selected laboratories in Kenya and Uganda. Through these two phases, we seek to raise the capability of these laboratories to the level where they produce reliable and internationally acceptable analytical results in testing commodities and thereby facilitate the effort of the farmers and enterprises in the private sector to export their commodities on international markets.

Title: ***Uncertainty estimation and figures of merit for multivariate calibration***
Number: 2004-041-1-500
Objective:
To provide chemists in general, and analytical chemists in particular, with an introduction to uncertainty propagation and figures of merit in multivariate calibration from a chemometrics perspective, and to review the various proposals to generalizing the well-established univariate methodology to the multivariate domain.
Description:
With the ever-increasing sophistication of analytical instruments, multivariate calibration methods are continually evolving, each with its own underlying assumptions and statistical properties. The main purpose of these methods is to produce valid predictions from highly unselective data, e.g. the quantification from near-infrared spectra. A wide variety of multivariate methods have been developed, broadly classified in terms of the tensorial order of the instrumental data. Important conceptual differences exist between first-order methods employing vector data, and second-order methods using matrix data, particularly since the latter make it possible the quantification in the presence of unknown interferents. This is also reflected in the approaches followed for the estimation of figures of merit.
While univariate calibration leads to relatively simple models, and the associated uncertainty estimation and figures of merit are thoroughly covered in several official documents, multivariate calibration does not enjoy a similar status in this regard. Uncertainty estimation and figures of merit for multivariate calibration methods have become subjects of active research, especially in the field of chemometrics.
This work is intended as an introduction to multivariate calibration from a chemometrics perspective and as a review of the various proposals to generalizing the well-established univariate methodology to the multivariate domain.

VI CHEMISTRY AND THE ENVIRONMENT DIVISION

Title: ***A critical compendium of pesticide physical chemistry data***
Number: 2003-011-3-600
Objective:
Establish an IUPAC compendium of critically evaluated values for aqueous solubility, vapor pressure, octanol/water partition coefficient, and acid/base dissociation constant (pKa) for active ingredients of pesticides. Use the procedures and approaches developed by the IUPAC Solubility Data Project as well as pesticide expertise from Industry and the former Agrochemical Commission.
Description:
Solubility in water, vapor pressure, octanol/water partition coefficient, and acid/base dissociation constant (pKa) are basic properties that may be measured with a known precision for any chemical substance. These quantities are of considerable practical significance as they play fundamental roles in describing the pharmacology, toxicology, and environmental fate and behavior of chemicals, as well as being basic input parameters for pesticide risk assessment modeling. Remarkably, few of these parameters have ever been critically evaluated or even exhaustively compiled for the chemical substances that are active ingredients of pesticides.

Title: ***Crop protection chemistry in Latin America: Harmonized approaches for environmental assessment and regulation***
Number: 2003-013-1-600
Objective and desription:
Crop protection chemistry is at a critical juncture in Latin America. The use of agrochemicals and biotechnology for crop protection purposes has increased significantly in recent years, and the region now is one of the world's most important areas for both domestic agricultural production and export of agricultural commodities to North America, Europe, and other regions. The scientific study, evaluation, and regulation of crop protection chemistry is at an early stage of development in Latin America, particularly with respect to environmental considerations. The primary objectives of this project are to:

1. Identify and prioritize the key regional issues related to crop protection chemistry and potential environmental impacts in Latin America.
2. Facilitate exchange of information and ideas regarding harmonized approaches available for the scientific evaluation and regulation of crop protection chemistry.
3. Develop recommendations for advancement of crop protection chemistry in Latin America.

Title: ***Fractal structures and processes in the environment***
Number: 2003-014-2-600
Objective:
The main objective is to provide the scientific community with a novel and valuable approach based on fractal geometry concepts to the chemistry, biochemistry, physical-chemistry and analytical chemistry of structures, properties and processes in environmental systems, with due comparison to classical approaches.
This objective can be extended to the industrial and professional community dealing with practical aspects of environmental systems by providing a fundamental knowledge basis for facing and solving practical environmental problems.
Description:
The project consists in the production of a book having the objectives described above. The book will be published as one volume in the IUPAC Series on "Analytical and Physical Chemistry of Environmental Systems", by John Wiley and Sons, Chichester, UK.

Title: ***Remediation technologies for the removal of arsenic from water and wastewater***
Number: 2003-017-2-600
Objective:
Produce a review of critically evaluated methods used for the removal of arsenic from water and wastewater.
Description:
Arsenic currently threatens millions of people in West Bengal, Bangladesh and Thailand, as a result of their exposure to contaminated groundwater (where concentrations may reach 0.06 mg/L to 1.86 mg/L, a value far in excess of the WHO Maximum Permissible Levels). Major problems have also been identified in some areas in the USA and China and south America.
The WHO and USEPA recommended limit for arsenic in drinking water is currently 10 µg/L. It is not so much the difficulty of removing arsenic from water, as the extremely low levels to which it must be reduced to ensure safety, that presents the challenge to water treatment initiatives, especially in developing countries where the issues of cost and expertise often make 'high-tech' solutions impractical.
Arsenic may be released into natural waters from a variety of hosts, most commonly either iron oxides, organic matter or sulphides. Elevated concentrations of dissolved arsenic may be expected under conditions where these phases are

unstable, or where arsenic is weekly bound (i.e. adsorbed) to the host phase. Arsenic speciation in waters is complex; fundamentally, it is a function of both pH, and Eh, as arsenic occurs naturally in two common oxidation states.
In considering arsenic removal from water, the principal processes of interest are those involving adsorption to particle surfaces, those defined as precipitation reactions and those involving filtration process (e.g. reverse osmosis or electrodialysis).
We propose that a critical review of these processes and technologies will be carried out and will include an evaluation of their appropriateness to different situations.Each process would be reviewed on a case-by-case basis with a literature review, compendium of the data available and critical analysis. Draft publication will be provided on the web and final publication as an IUPAC volume.

Title: ***Glossary of atmospheric chemistry***
Number: 2003-030-1-600
Objective:
Prepare a glossary along the recommendations given by the ISO and ICTNS.
Description:
A comprehensive Glossary of Terms pertinent to atmospheric chemistry was prepared and reviewed and published by IUPAC more than a decade ago. This activity will update that glossary to include terms that have become important subsequent to publication of that document (as well as omissions) and as necessary amend or elaborate previously presented definitions. Widely used or generally accepted acronyms will also be included.

Title: ***Air pollution models in environmental management and assessment***
Number: 2003-058-1-600
Objective and desription:
Air pollution models are strong and necessary tools in environmental management. The aim is to describe the methodology behind application of mathematical models in various assessments of air pollution impacts. The book provide guidelines for avoiding incomplete or even incorrect answers when models are applied.

Title: ***Glossary of terms related to pesticides***
Number: 2004-002-1-600
Objective:
1. To develop a new glossary of the more than 300 terms relating to pesticides.
2. To publish it electronically to facilitate better international communication among researchers, regulatory authorities, toxicologists, agriculturalists and students.
Description:
Pesticides are a broad group of biologically active chemicals and organisms that are important for pest management and human health. Differences in the use of pesticide terminology still exist. These differences are an impediment to the increased international efforts to harmonize the regulation of pesticides on a world basis.
The current Glossary of Terms Related to Pesticides will be ten years old by the time this new glossary of terms can be published.

Title: ***Biophysico-chemical processes of heavy metals and metalloids in soil environments***
Number: 2004-003-3-600
Objective:
To provide the scientific community with a critical evaluation by world-renowned international scientists of the state-of-the-art on the biophysico-chemical processes of metals and metalloids in soil environments including their interactions with soil components (clay minerals, organics, microorganisms). Specifics of heavy metal and metalloid mobility in different soil environments, including the rhizosphere, as influenced by physics, chemistry and biology of soil and their interactions will be examined. Finally, their speciation, mobility, bioavailability and toxicity and innovative restoration strategies of polluted soils will be addressed.
Description:
Pollution induced by heavy metals and metalloids in soils is a very dangerous environmental problem because, as compared with other kinds of pollution (atmosphere and water), the soil environment has a much lower ability to recover. Furthermore, over 99% of environmental pollutants are bound with soil and sediment particles.
Heavy metals are well recognized as potentially toxic to plants and other living organisms.
The present project is to prepare a book by a multidisciplinary group of soil and environmental scientists to provide the scientific community with a critical evaluation of the state-of-the-art on the processes of these elements in soil environments, their speciation, mobility, bioavailability and toxicity and their impact on the development of innovative restoration strategies. Biogeochemical processes operating in soil environments that affect the fate, behavior, and bioavailability of metals and metalloids is currently an area of active research. Yet, a comprehensive and detailed book of the state-of-knowledge is absent from scientific literature.

Title: ***Development of simplified methods and tools for ecological risk assessment of pesticides***
Number: 2004-011-1-600

Objective:
1. To develop simplified methods and supporting tools that can be used by developing country governments to perform ecological risk assessments of pesticides.
2. To make these methods and tools easily available to those desiring to use them for pesticide evaluation.

Description:
All countries use pesticides for protection of agricultural crops and for safeguarding public health. Pesticides, however, may have unintended adverse impacts on non-target organisms and any such potential impacts should be assessed before these chemicals are approved by governments for use. Many countries have developed methods for pesticide ecological risk assessment, but the complexity of the techniques and the overall amount of work required to use them has reached a level beyond the capacity of the majority of governments. As a result, only about 25 of the world's more than 180 countries routinely perform pesticide risk assessments in terms of the accepted procedure of comparing measured toxicity concentrations to estimated exposure concentrations. Countries besides these few would also benefit greatly from having the capacity to quickly perform a scientifically valid pesticide ecological risk assessment prior to approving use.
The project will develop pesticide ecological assessment methods and tools based on simplifying some of the methods and tools that have been established in other countries, establishing developing country scenarios for simulation models or employing the simplifying assumptions of relative (comparative) risk assessment.

Title: ***Environmental colloids: behavior, structure and characterization***
Number: 2004-015-1-600
Objective:
The objective of this book will be to examine, through critical reviews, some of the important novel techniques for characterizing colloidal/ particulate systems. The focus of the book will be on techniques that were not examined in previous books in addition to techniques for which major advances have been made in the last decade.

Description:
The project consists in the production of a book having the objectives described above. The book will be published as one volume in the IUPAC Series on "Analytical and Physical Chemistry of Environmental Systems".
To our knowledge, there are no other books currently available which deal directly with current state-of-the-art techniques in colloidal characterization.

VII CHEMISTRY AND HUMAN HEALTH DIVISION

Title: ***Explanatory dictionary of concepts in toxicokinetics***
Number: 2003-001-2-700
Objective:
IUPAC has the world authority on chemical nomenclature and terminology and experience in critical evaluation of data. In order to incorporate chemistry and merge toxicology into the terminology used in toxicokinetics in various scientific disciplines a project was initiated to create a glossary of terms used in toxicokinetics (project #2000-034-2-700).
The objective of this new project is to create an *Explanatory Dictionary of Concepts in Toxicokinetics* consisting of about 40 terms chosen from the glossary of terms used in toxicokinetics (referred to above) with full explanations of the meaning of the terms and the underlying concepts. Such a project will improve the IUPAC impact in a number of scientific fields and improve the image of chemistry in society. It will serve the needs of the chemists in the world, who increasingly require an understanding of toxicology, and thus be of global interest.
Description:
The terms in toxicokinetics will be selected on the basis of their importance for human health. The "Explanatory Dictionary of Concepts in Toxicokinetics" will play an important role in helping chemists to meet the increased requirement from society and government for risk assessment of chemicals produced by the chemical industry. It is designed to help chemists to understand fully the meaning of terms used in toxicokinetics which they will met in the literature related to risk assessment. Better risk assessment will result helping to ensure that the practice of chemistry remains safe and continues to benefit human health.

Title: ***Glossary for chemists of terms used in toxicology - revision and updating***
Number: 2003-028-1-700
Objective:
IUPAC is the world authority on chemical nomenclature and terminology. Toxicology is a subject area dependent on good chemistry and itself influences chemistry through its impact on legislation for chemical safety. The objective of this project is to create a revised "Glossary for Chemists of Terms Used in Toxicology". The revised glossary will incorporate essential terms from the new Glossary of Terms in Toxicokinetics, review existing definitions, and add new terms which have come into common use since the original glossary was compiled.
Description:
This Glossary in its revised version will cover all terms relevant to toxicology and bring them together in one source document for ease of use. It will include new terms and more terms in toxicokinetics identified and defined in the recent project which produced a glossary of terms in toxicokinetics. It will also cover essential terms relevant to risk assessment of chemical use.

Title: ***Glossary of terms used in combinatorial chemistry***
Number: 2003-044-1-700
Objective:
To prepare a Glossary for the field of Combinatorial Chemistry, and to provide an authoritative, on-line resource for Combinatorial Chemistry nomenclature.
Description:
This project is intended to capture and define terminology used in the field of Combinatorial Chemistry. An initial Technical Report on this subject was published in 1999[1] In the intervening period this relatively new field has continued to innovate and produce new terminology. In addition, a reasonable period of time has elapsed for the earlier definitions to be revised in light of comments received and the current status and direction of the field.

Title: ***Quantifying the effects of compound combinations***
Number: 2003-059-1-700
Objective:
To recommend standard descriptions and reference models for quantifying the effects of compounds in combination.
Description:
The past three decades have seen considerable debate on how to describe the effects of compound combinations. Much of the discussion was focused on which is the best reference model for combination response surfaces, as predicted from the single agent dose-response curves.
We propose to prepare an IUPAC recommendation endorsing the nomenclature resulting from the Saariselskä agreement. We further propose to recommend a predictive response surface approach to quantifying combination effects, based on a simple system of target connections, and to present some sets of models that are appropriate to networks of biological reactions.

Title: ***Glossary of terms used in biomolecular screening***
Number: 2004-019-3-700

Objective:
To provide standardized definitions of terms and technologies used in biomolecular screening supporting drug discovery.
Description:
Over the past 15 years, high throughput screening (HTS) of small molecules has become a mainstay in the drug discovery process both in lead discovery and lead optimization. In both HTS and routine screening to optimize lead structures, new technologies, techniques and terminology have emerged. A definitive glossary of biomolecular screening terms will be broadly useful to scientists involved in the drug discovery process. The glossary will be generated in collaboration with the Society for Biomolecular Screening.

Title: ***Internationally agreed terminology for observations in scientific communication***
Number: 2004-023-1-700
Objective:
Most scientific disciplines, not only laboratory medicine, rely to some extent on observations in addition to measurable quantities. An integrated explanatory treatise and vocabulary explaining and exploring the conceptual relationship between observations and measurements is the main outcome of this project. The proposed project should be used to explain and extend the systematic description of properties to observable properties.
Description:
Scientists of disciplines in laboratory medicine has long recognized the need of a common language for efficient and safe request of investigations, report of results, and communication of experience and scientific achievements. To achieve this, the IFCC and the IUPAC in a joint project have developed a metrologically based coding scheme based on progress in modern classification science. In collaboration with professionals in a series of medical specialties a coding scheme has evolved that fulfils the needs in electronic communication and data presentation.
The present project is aimed at developing a common framework for a project meant to integrate and also explain to the laboratory medicine workers the meaning of and usefulness of such an integrated view of the concepts property and in a more restricted sense quantity.

Title: ***Compendium of targets of the top 100 commercially important drugs***
Number: 2004-025-1-700
Objective:
To provide a compendium of the biological targets of the top 100 drugs.
Description:
A recent article indicated that the 100 best selling drugstarget 43 gene products. However there does not appear to be a resource where compiled target information is readily available in a single source. The intention is to provide a resource containing the following information on commercially important drug targets: type of target (enzyme, receptor etc); brief description of relevance to disease treated; reference to knockout information, if available; reference to structural information, if available; listing of the marketed drugs that interact with the target along with potency and relevant selectivity information.

Title: ***Practical studies for Medicinal Chemistry - An integrating approach for developing countries***
Number: 2004-028-1-700
Objective:
To provide the developing countries with a practical textbook containing practical experiments to assist studies in Medicinal Chemistry. It should take into account the special characteristics of these societies, such as taking advantage of the natural resources, lack of economic means for obtaining reagents, materials, etc. The idea is to also provide a foundation for post graduate studies that will facilitate the training of medicinal chemists so that they can conduct research into the discovery and development of drugs to treat indigenous diseases, such as tuberculosis, malaria, leprosy, and Chagas. Since these diseases principally affect the developing countries and receive little attention in the pharmaceutical industry of the developed countries, it is important to assist the developing countries to tackle their own problems.
Description:
The text will be written in English but some texts will also be in Spanish and Portuguese, when provided by the authors. This allows accessibility to students who are not fluent in English. The text would be of integrating character, from disciplines that converge in R&D of Medicinal Chemistry: organic synthesis, natural product, isolation, structural identification, and structure-activity relationships; biological activities. The experiments provided would be such that they could be carried out with easily accessible starting materials (natural products from the area, for example) and economic reagents, and low-cost instrumentation and techniques.
These practical texts would be applicable to diseases which are indigenous to the developing countries, for example, isolation of products with antimalaria activity, based on products of natural origin; low-cost synthesis of antituberculosis products, etc.

Title: ***Training of school children on pesticides and health***
Number: 2004-045-1-700

Objective and desCription:
Infants and children are particularly vulnerable to pesticides and other toxic chemicals because their bodies are smaller and still developing. Children also face greater exposures than adults due to their hand-to-mouth behaviors. Children living in farming areas or whose parents work in agriculture suffer greater pesticide exposure than other children. The aim is to contribute to the enhancement of chemistry education, and the public appreciation of chemistry by information and appropriate handling based on informed risk assessment.
Despite some non-chemical methods of pest control there is at present no alternative to chemical control. Pesticides are essential to farming economies, especially in developing countries and economies in transition, where adverse effects caused by weeds, diseases and pests are of greater concern. However there is a need to optimise the beneficial use of pesticides by minimising harm through better education about the risks of toxic substances. The project will improve the image of chemistry by associating IUPAC with educational material to reduce careless use of pesticides. The material should also enhance or even help to provide basic education in chemistry and basic toxicology in the classroom. The material will be targeted to chemistry/science teachers in the early years of secondary school. A main objective is to produce training materials for school children aged 9-13 on pesticides to teach them to understand the action of pesticides and the principles of safe handling and to protect themselves and others from harmful effects of pesticides.

VIII CHEMICAL NOMENCLATURE AND STRUCTURE REPRESENTATION DIVISION

Title: ***Extension of IUPAC rules for stereo descriptors to include coordination numbers 7-12***
Number: 2003-025-1-800
Objective:
The set of stereo descriptors in the IUPAC Red Book extend only as far as coordination number 6. There have been recent desriptions as to how these might be extended to face-capped octahedra, and this project is an attempt to provide a unified method for descriptors for all higher coordination numbers 7-12.
Description:
The project aims to present a unified treatment for higher coordination numbers. This involves defining appropriate idealised polyhedra with rules on how to assign them to real structures, determining unambiguously principal axes, deriving a consistent method for defining planes, and finally deciding rules for numbering. The whole would need to be consistent with the principles laid down for lower coordination numbers, and would also have implications for boron nomenclature and possibly for cluster nomenclature, which is almost non-existent The absence of rules for higher coordination numbers is a gap in the current nomenclatures, and the project would also enable us to determine how far the current rules can be extended.

Title: ***Source-based nomenclature of single-strand organic polymers***
Number: 2003-042-1-800
Objective:
To provide systematic and practical recommendations for source-based nomenclature of single-strand organic polymers.
Description:
Among many issues to be reconsidered, some examples are briefly shown in the following.

1. Issues relevant to both homopolymers and copolymers:
   Establish the rules for choosing the name(s) of a monomer from two or three different names. Select one preferred name among plural names all conforming to the rules to have only one preferred name for one polymer as far as possible. Expand the definition of the source-based name to be able to cover PET (polyethylene terephthalate) type names.
2. Issues relevant only to homopolymers:
   Find better generic names for the isomeric regular homopolymers and irregular homopolymers such as polyisoprenes, for which the generic convention allows to distinguish isomeric plural homopolymers, e.g., polyalkylene:isoprene and polyalkenylene;isoprene.
3. Issues relevant only to copolymers:
   Discard the "alternative nomenclature"given in the Appendix of the current Copolymer document, to avoid having two nomenclature systems. Avoid many names for a copolymer prepared by polycondensation, in which a same regular copolymer can be prepared from different monomers.

Title: ***Graphical representation standards for chemical structure diagrams***
Number: 2003-045-3-800
Objective:

1. To extend IUPAC's leadership in the development of standard nomenclature and terminology in chemistry into the domain of chemical structure diagrams.
2. To provide a single, comprehensive set of guidelines for creating chemical structure diagrams in printed and in electronic media.
3. To enable IUPAC to serve as the principal, authoritative source for chemical structure representations.

Description:
The project has begun informally with a "scoping exercise" in which some 20 members of the chemistry community were invited to discuss those aspects of creating chemical structure diagrams which are amenable to standardization through IUPAC recommendations. With the ever-increasing importance of electronic publication, this project will consider issues related to the production of chemical structure diagrams both in printed and in electronic media. Where possible, every effort will be made to ensure identical recommendations in all media. The recommendations for the production of chemical structure diagrams will aid in the correct recognition of structural information by the IUPAC/NIST Chemical Identifier algorithm.
In some cases, the current state of chemistry software may preclude the use of the most-preferred styles for chemical structure diagrams. When necessary, this project will also provide practical advice for the production of electronic chemical structure diagrams according to the current state of the art of chemistry software. It is likely that this project will also produce a set of recommendations for enhancements that chemistry software developers may undertake to improve that state of the art.

Title: ***Nomenclature of cyclic peptides***
Number: 2004-024-1-800

Objective:
To extend rule 3AA-19.5 of the *Nomenclature and Symbolism for Amino Acids and Peptides (Recommendations 1983)* to cover all classes of cyclic peptides.

Description:
Cyclic peptides are briefly considered in the *Nomenclature and Symbolism for Amino Acids and Peptides (recommendations 1983)* in part 2 under symbolism. There are no recommendations on naming these peptides. This deficiency will be rectified by the proposed recommendations which will be based on the established procedures for naming peptides.

The recommendations will include rings generated from an acyclic peptide by formation of a peptide or ester bond; by a disulfide link; or by a new carbon-carbon, carbon-nitrogen, nitrogen-oxygen or carbon-sulfur bond (not esters or amides). These new bonds are indicated by the prefix anhydro, cyclo or epoxy, or combinations of them. The inclusion of modified standard amino acids or amino acids not related to standard amino acids will be considered. Any stereochemistry generated by ring formation will be indicated using standard organic conventions.

Title: ***IUPAC International Chemical Identifier (InChI): promotion and extension***
Number: 2004-039-1-800

Objective:

1. To promote its use throughout the chemical information community
2. To extend its applicability to include polymeric structures
3. To explore the need for other extensions, including the ability to handle Markush structures, and to include information on other attributes such as phases and excited states

Description:
Version 1.0 of the Identifier expresses chemical structures in a standard machine-readable format, in terms of atomic connectivity, tautomeric state, isotopes, stereochemistry, and electronic charge. It deals with neutral and ionic well-defined, covalently-bonded organic molecules, and also with inorganic, organometallic and coordination compounds.

We propose to promote actively the use of the algorithm and its associated implementations to developers of commercial chemical software, database compilers and publishers of chemical information, in order to enable sharing of molecular information throughout the worldwide community of chemical scientists.

We propose also to extend the applicability of the Identifier to polymeric structures, and to explore the need for and the practicality of an extension to cover Markush structures.

In addition, we will evaluate the need for inclusion of information on other attributes such as phases and excited states, and take steps to include such information if appropriate.

CHEMRAWN

Title: ***CHEMRAWN XVI - Innovation in the chemical industry: the way from pure to applied chemistry***
Number: 2003-003-1-021
Objective:
A Forum will examine creativity and radical innovation in the chemical industry with the focus on new directions. Today's chemical industry is mature with little payoff from investing in new products, significant process innovation, or fundamental, breakthrough research.
Description:
The forum will have three sessions each with several talks, review of previously submitted papers, and panel discussions:

1. ***Enabling radical innovation***
   Software tools, knowledge management; getting the new ideas and adopting them; market/technology intelligence; computerized methodologies; measuring chemical process efficiency; capturing emerging technologies
2. ***Doing breakthrough research***
   New ways to collaborate in developing innovative products and processes; smart scale-up techniques; instrumentation; what life sciences, and the services sector can teach the chemical industry about research; increasing the odds for success
3. ***Knocking down the barriers to innovation***
   Regulatory support/barriers- internal company practices- lack of talent and resources- killing the good ideas- the game plan for the innovative chemical company.

Title: ***Solving the problem of arsenic contamination in water in Bangladesh***
Number: 2003-050-1-021
Objective:
Hold a workshop-planning meeting at Dhaka University in the first quarter of 2004, to prepare for organization of a larger Regional Workshop in late 2004 or early 2005.
Description:
Naturally occurring arsenic in groundwater contaminates the tube wells in Bangladesh. It is seriously affecting the health of more than 60 million people, as it ultimately leads to a slow and painful death for many. Furthermore, this problem can also affect the water supplies in a number of other countries, such as Argentina, Chile, France, India, and the United States. The problem was described in some detail in the *Chemical and Engineering News* issue of October 21, 2002.

COMMITTEE ON CHEMISTRY EDUCATION (CCE)

Title: ***Young Ambassadors for Chemistry (YAC)***
Number: 2003-055-1-050
Objective:
To enhance Public Understanding of Chemistry through teacher and student school audiences in target transition regions.
The project will be carried out in partnership with a successful global science education programme, to train teachers and provide resources to develop the communication skills of young people and teach them to be young ambassadors for chemistry. It includes an evaluation of the impact of the 'train the trainers' model in increasing public understanding.
Description:
Young Ambassadors for Chemistry (YAC) will be a partnership between *IUPAC's CCE Public Understanding of Chemistry subcommittee* and the Science Across the World Network to facilitate the flow of ideas between chemistry and society. This project will use the 'train the trainer' model to create public interest in chemistry in four transition areas with strong IUPAC CCE representatives: Taiwan, Russia and the Balkans, Argentina, and South Africa.
Science Across the World (SAW) is a successful schools educational programme encouraging communication and shared learning by young people (10-16 years) on important scientific issues of public interest in 90 countries. SAW's web site has an up-to-date database of schools and teachers and established methods for exchanging ideas and information between schools all over the world. As the school is very often at the hub of the community, opinions shared during learning may filter well beyond the student and the classroom. The present project builds on the highly successful collaboration between IUPAC and SAW in a 2003 global poster competition for children, featured on the cover of the Nov/Dec 2003 *Chemistry International*.

Title: ***Public understanding of science: identifying IUPAC's niche***
Number: 2004-047-1-050
Objective:
To propose an appropriate niche for IUPAC and the Committee on Chemistry Education (CCE) in promoting public understanding of science.
Description:
Enhancing the public understanding of science in general and of chemistry in particular is a key element of IUPAC's strategy. There are also a large number of other organizations active in the field, so determining the particular role IUPAC can and should play requires careful analysis. The CCE subcommittee on the Public Understanding of Science Chemistry is charged with providing public understanding through its work to improve chemistry education. The subcommittee wishes to promote the development of an overall IUPAC strategy and to play its own role within that strategy.

Title: ***Flying chemists program - 2005 visit to India***
Number: 2005-004-1-050
Objective:
The one week program for the two visitors will include seminars and discussions with academics, industrial houses and government agencies to identify viable strategies for

- Professional development of in-service and pre-service teachers through the design of an internet-linked strategy which will equip a chemistry teacher with some specific skills needed today to become an effective teacher
- Promoting student interest through a discovery- based approach catalyzed by the skills acquired by teachers participating in the professional development program.

Description:
For this first project under the FCP, Prof. Peter Atkins and Prof. Ram Lamba will make a visit to India in 2005.
The proposed visit in 2005 will focus on

- curriculum development
- development of new assessment tools
- design and implementation of hands-on experiences at all levels of chemistry education
- promote partnerships among universities, universities and industries, and universities, industries and governments
- develop self-learning and self- assessment approaches based on state-of-art technological tools
- create international and intra-national networks for real and virtual partnerships for sharing and monitoring innovative practices
- procurement of seed funds from national, regional and international sources for pilot-testing of the sustainability aspect of a few key innovations.

COMMITTEE ON CHEMISTRY AND INDUSTRY

Title: ***IUPAC-UNESCO-UNIDO Safety Training Program 2004***
Number: 2004-032-1-022
Objective:
Training for two Safety Training Program Fellows at Mitsui Chemical Co., Japan.
Description:
The Safety Training Program allows safety experts from developing countries to learn more about safety and environmental protective measures by visiting and working in plants of IUPAC Company Associates in the industrialized world. IUPAC with the United Nations Educational, Scientific, and Cultural Organization (UNESCO) and the United Nations International Development Organization (UNIDO), have established and maintained the Safety Training Program to promote interactions between developed countries and the developing world to disseminate state-of-the-art knowledge on safety and environmental protection in chemical production. The beneficiaries are expected to use the training in their home countries to improve health and safety.
This environment and safety training will be offered by Mitsui Chemicals Inc. of Japan. The session will take place in in Mitusi facilities between 12 October and 30 October 2004. The course will include lectures, discussions, demonstrations, practical exercise and visits to waste disposal plants.

Title: ***IUPAC-UNESCO-UNIDO Safety Training Program Workshop, Beijing, China***
Number: 2004-031-1-022
Objective:
This Workshop on the Safety Training Program will be used for communication to the public and to IUPAC leadership on recent activities by Fellows of the program in their home countries; to evaluate the effectiveness of the Safety Training Program to data in terms of fellows' home country activities; and to solicit ideas for improvements in the program and for possible expansion to incorporate new Host Companies and new regional trainees.
Description:
The Safety Training Program allows safety experts from developing countries to learn more about safety and environmental protective measures by visiting and working in plants of IUPAC Company Associates in the industrialized world. The International Union of Applied Chemistry (IUPAC) with the United Nations Educational, Scientific, and Cultural Organization (UNESCO) and the United Nations International Development Organization (UNIDO), have established and maintained the Safety Training Program to promote interactions between developed countries and the developing world to disseminate state-of-the-art knowledge on safety and environmental protection in chemical production. The beneficiaries are expected to use the training in their home countries to improve health and safety. This Workshop is planned as part of activities under the heading for Section 8 of the 40th IUPAC Congress, "Innovation in the Chemical and Petrochemical Industries and *Responsible Care* for Society."
Each participant will prepare an oral presentation and poster along with a written paper. A Web page on the IUPAC Web site will be prepared to cover the proceedings and outcomes of the Workshop, where their reports, presentations, and a summary report will be published. The Workshop will include a panel discussion to identify ideas for improvement and expansion of the scope of the Safety Training Program.