



# IUPAC PROJECT SUMMARIES

The following summaries represent projects, since 2002, for each of the 8 Divisions of IUPAC:

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June 2004

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# I PHYSICAL AND BIOPHYSICAL CHEMISTRY DIVISION

**Title:** *Thermodynamics of ionic liquids, ionic liquid mixtures, and the development of standardized systems*

**Number:** 2002-005-1-100

**Objective :**

1. To initiate systematic studies of thermodynamic and thermophysical properties of Ionic Liquids (IL) based on the needs of industrial chemical processes.
2. To establish a reference system of IL's and IL and liquid mixtures with reliable stability and purity and well defined thermodynamic properties.
3. To define guidelines which research activities and future cooperation should be directed to.

**Description:**

Ionic liquids represent a new class of liquid solvents having the character of molten salts. Recently synthesised compounds are moisture, air and temperature stable. A large number of ionic combinations are possible for designing special properties. IL's have gained large interest during the last few years. They have no detectable vapor pressure and therefore exhibit an ideal system of solvents for new homogeneous catalytic reactions and other chemical production processes with respect to a "green chemistry". An increasing number of successful applications are described in the literature. The utilization of IL's in industrial chemistry requires a systematic study of their thermodynamic and thermophysical properties, which are of considerable interest for chemical process design.

**Title:** *Chemical thermodynamics in industry*

**Number:** 2002-063-1-100

**Objective :**

To bring to the attention of a wide audience, the pivotal role that Chemical Thermodynamics plays in the Chemical Industry of the 21st century.

**Description:**

A book is being written for chemical engineers and industrial chemists, those funding chemical research, and research students and general chemists.

**Title:** *Recommended values of the viscosity of molten iron and aluminium*

**Number:** 2003-005-1-100

**Objective :**

The widely different data obtained for the viscosity of molten iron and aluminium will be critically reviewed via an inter-laboratory comparison and recommended values will be proposed.

**Description:**

Wide ranges of values of viscosity of both molten iron and aluminium 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 used to convert the measurements to viscosity.

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 aluminium and iron need to be critically reviewed and recommended values suggested. This may result in the need for an inter-laboratory comparison.

**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, 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

**Task Group**

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 utilisation 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 modelling. Thermochemical kinetic estimations sometimes provide 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 optimised 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. 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.

## II INORGANIC CHEMISTRY DIVISION

**Title:** *A new comprehensive report on the isotopic compositions of the elements for global user communities*

**Number:** 2002-049-2-200

**Objective:**

To design, compile and produce a new comprehensive report on the Isotopic Compositions of the Elements, containing updated data and in a format suitable for the 21st Century.

**Description:**

In the past, the Commission on Isotopic Abundances and Atomic Weights (CAWIA) has produced several tables of the isotopic compositions of the elements (e.g. the most recent published in 1997) with isotopic data representing the best available measurements and representative materials. The aim of this project is to update and drastically upgrade this information, which has not been done in 7 years. Apart from the upgrading (incorporating new information obtained since 1997), the data handling procedures for the future table should also be modified to achieve recommended isotopic compositions that are fully in line with standard atomic weights. This is not always the case today.

**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. 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:** *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- $\sigma$  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.

### III ORGANIC & BIOMOLECULAR CHEMISTRY DIVISION

**Title:** *Chemical actinometry*

**Number:** 2002-008-1-300

**Objective :**

Updating the document on "Chemical Actinometry" published in *Pure Appl. Chem.* 61(2), 187-210, 1989 and extending its coverage to solid-state systems and to near-UV radiation.

**Description:**

The document on "Chemical Actinometry" has been very well received by the photochemical community. The original publication in 1989 has been referred to 72 times according to the WEB of Science. There is a need to extend the coverage to the solid state, expand the gas phase systems and cover in more detail the near-UV radiation region, in view of the renewed interest on research in this area, due to environmental reasons. A search of the literature from 1989 to 2000 reveals that a series of publications in the field have appeared in these areas. A critical assessment of the actinometers should also be included.

**Title:** *Glossary of terms used in photochemistry (3rd version)*

**Number:** 2002-024-1-300

**Objective :**

Updating and expanding the "Glossary of Terms used in Photochemistry " published in *Pure Appl. Chem.* 1996, **68**, 2223.

**Description:**

The "Glossary of Terms used in Photochemistry" as published in 1996 (which already included ca. 500 terms) needs updating since errors have been detected with respect to definitions in the Green Book "Quantities, Units and Symbols in Physical Chemistry", published by the Physical Chemistry Division. In addition, terms related to the use of polarized light in photoinduced reactions should be included. By their very nature Glossaries need frequent updating to keep abreast of new terms and procedures arising from technological developments.

**Title:** *South East Asian, and neighbouring countries, Green Chemistry Network*

**Number:** 2002-028-1-300

**Objective :**

To develop a South East Asia and Neighbouring Countries Green Chemistry Network for the purposes of facilitating greater collaboration in research and education in Green Chemistry throughout the region.

**Description:**

The 'S.E. Asia and Neighbouring Countries Green Chemistry Network' would be a body designed to actively promote the development of Green Chemistry, at both a research and educational level. The network, which would be held together by strands of student exchange, would be designed to foster the development of greater collaboration between complementary research efforts in neighbouring countries, with the goal of providing local industries with better access to developments at the forefront of Green Chem research in the context of each nation's current state of industrialisation.

**Title:** *An IUPAC coordinated web page on Green/Sustainable Chemistry*

**Number:** 2002-029-1-300

**Objective :**

The objective is to provide on the IUPAC web site an additional web page that provides a central reference point on Green Chemistry, with links to all relevant sites worldwide.

**Description:**

Green/Sustainable Chemistry is now one of the most important means for relating chemistry to social needs. Many organisations have already made progress in this area. IUPAC itself has also constituted an Inter-Divisional Sub-Committee on Green Chemistry. IUPAC has been asked to establish a web page on its web site, and to oversee and maintain it. Such a web page would share information with other relevant organisations, and have links to them. Such organisations might include UNIDO, EU, WHO, FAO, FECS, FACS and UNESCO.

**Title:** *Fighting microbial resistance through development of new antimicrobial agents, directed against new specific targets*

**Number:** 2002-030-1-300

**Objective :**

Increasing resistance of microorganisms against available antimicrobial agents is of major concern amongst scientists and clinicians worldwide. In general, it is observed that pathogenic viruses, bacteria, fungi and protozoa are more and more

difficult to treat with the existing drugs. Notorious examples are Tuberculosis, Malaria, and AIDS. The objective of the project is to combine international scientific expertise in order to develop new antimicrobial drugs, based on new specific targets.

**Description:**

Resistance of microorganisms is the result of normal evolutionary processes of natural selection that cannot be stopped and in the best cases can be delayed.

Development of new antiprotozoal, antibacterial and antiviral drugs can only be effective if different experts worldwide combine their expertise to tackle the immense problems of humanity in the near future. For this purpose, interactions between (micro)biologists, synthetic and medicinal chemists are essential.

**Title: *Green Chemistry in Latin America***

**Number:** 2002-064-1-300

**Objective :**

The project is aimed at increasing the awareness and attracting the interest of university students in Latin America universities towards the Green/Sustainable Chemistry activities, by highlighting their general roles and simultaneously presenting already on-going activities in Latin America. The aim of this Project is the production of a book like "Green Chemistry in Africa".

**Description:**

The book will be specifically designed for university students, with particular attention for students in Latin America universities and will be written in Spanish. The book plans to highlight the relevance of Green/Sustainable Chemistry in general, and to underline its potential relevance for developing countries.

The inclusion of a section on Green Chemistry education has the additional objective of linking research activities to the preparation of future specialists, by generating channels for a fast and effective dissemination of information. The project may be a pilot initiative for future green-chemistry activities in Latin America by IUPAC and related associations (scientific collaborations, networking, etc.).

**Title: *Green chemistry in Russia***

**Number:** 2003-026-1-300

**Objective :**

This project is aimed at increasing the awareness and interest of university students in Russian and Former USSR universities and other educational institutes and industrial chemists towards the Green/Sustainable Chemistry activities, by highlighting their general significance and presenting already on-going activities in different regions of Russia. The aim of project is to produce and disseminate a book like "Green Chemistry in Africa" and "Green Chemistry in Latin America".

**Description:**

The book will be designed for university students and for industrial chemists and will be written in Russian. This makes it possible to disseminate the book not only in Russia, but also in Former USSR republics, such as Belorussia, Ukraine, Kazakhstan and Uzbekistan. The book plans to underline the relevance of Green/Sustainable chemistry in general, and to elucidate its potential importance for Russia and other Former USSR countries.

**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 the project is to produce and disseminate a book like "Green Chemistry in Africa" and "Green Chemistry in Latin America" and "Green Chemistry in Russia".

**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 "Centre 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:**

*Background* - Herbal/traditional medicines have been playing an important role in the primary health care of the people around the world, specifically in the developing countries. In order to keep pace with the modern medicines, the production of herbal medicines in a standardised way is essential. The World Health Organization has stressed 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. The present project is submitted for moving forward in fulfilling the following main objectives:

- a) To carry out systematic and proper documentation of the existing available knowledge of traditional and folkloric medicines;
- b) Screening of existing herbal/traditional medicines and other preparations for their efficacy, toxicity (if any) and dose forms;
- c) To make formulations of herbal/traditional medicines in a proper scientific way;
- d) To coordinate research and development activities for developing drugs from natural sources and to augment facilities for such research activities;
- e) To provide service to herbal medicine producers for the manufacture of safe and quality products.

**Title:** *Toward a core organic chemistry curriculum for Latin American universities*

**Number:** 2002-010-1-050

**Objective :**

- 1) Propose general recommendations for up-to-date university curricula in organic chemistry, without interfering with instructors' freedom.
- 2) Contribute to the public understanding of chemistry by introducing fundamental concepts showing the involving of organic chemistry in most aspects of common life.
- 3) Facilitate communication, transferability of courses and exchange of students, as well as insertion of the graduates in transnational industries. The task group initially worked with a worldwide scope, the current presentation is limited to the Latin American universities as a more manageable first approach. If this project is successful, it might be extended to other developing countries and/or regions.

**Description:**

IUPAC is in a unique position to facilitate the international education of chemistry students. We propose to develop recommendations for curricula in organic chemistry, including a set of required and recommended topics to be covered at each educational level in the University. The project will also focus on the ways that education in developing countries could be aided. This will assure students of receiving an interchangeable preparation and will guarantee the adequacy of a student's preparation. Our goal is to ensure that students reach an acceptable level of knowledge by the end of their course of studies, without undue gaps.

**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, magnetic susceptibility corrections, and conventions for shielding tensors.

**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 [endorsed by IUPAC in the 1970s] 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 [ $^1\text{H}$ ] resonance of tetramethylsilane [TMS] in a 1 percent solution in  $\text{CDCl}_3$ . Since its publication only a year ago, this recommendation has been well received by the international NMR community; has been widely disseminated by publication in NMR journals and presentations at NMR conferences, as detailed below; and has been publicised by one of the three major NMR equipment manufacturers.

## IV MACROMOLECULAR DIVISION

**Title:** *Structure and properties of polyester elastomers composed of poly(butylene terephthalate) and poly(caprolactone)*

**Number:** 2002-052-1-400

**Objective:**

To evaluate the relationship among the chemical structure, the higher-order structure, and the mechanical and rheological properties of the elastomers.

**Description:**

The idea of thermoplastic elastomers brought a big innovation to the rubber industry as well as the field of the polymer science. The rubber materials, which have no need of vulcanization and are easy to be recycled, have attracted the technological and academic interests for these years. The mechanical performance of the thermoplastic elastomers is strongly affected by the higher-order structure of hard segments of the chains. The aim of this project is to make clear the structure-properties relation of polyester-type elastomers categorized in engineering elastomers, composed of poly(butylene terephthalate) as the hard segment and poly(caprolactone) or poly(tetramethyleneglycol) as the soft segment.

**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.

The first objective of this project is to develop a standard file format for storage of measurement data enabling a simplified data exchange. A subsequent objective will be the implementation of the file format in the software of the participating manufacturers and to convince further manufacturers to join.

**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. 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.

**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, 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 to:

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:** *Polymerization processes and polymers in dispersed systems*

**Number:** 2002-017-1-400

**Objective:**

Many researchers involved in studies on polymers in dispersed systems came to the conclusion that a concerted and broad-based effort is now needed to prepare and define properly the comprehensive list of terms and definitions essential to describe, unambiguously, new, dispersed polymerization processes and products. At the same time, definitions of many of the older processes and products already existing in books and papers have to be clarified. A thorough, internationally based feasibility study has shown that more than 200 terms need to be considered and that more than 50 are indispensable.

**Description:**

During the last decade, new types of polymerizations in dispersed systems have been invented and polymer particles with new kinds of properties and structures have been synthesized. Consequently, a large group of industrially important polymerization processes is now carried out in dispersed systems. Also, polymers in dispersed systems are used in diverse areas, such as the paint industry, microelectronics, medicine, cosmetics and biotechnology. Due to their complicated compositions and structures, the same name is often used, in scientific journals and at conferences, for different processes or products and, conversely, different names are used for the same process or product. In many instances, lack of clarity leads to confusion and to difficulties in proper scientific and technological understanding.

**Title:** *Critically evaluated propagation rate coefficients for free-radical polymerizations: acrylic acid alkyl esters*

**Number:** 2002-023-1-400

**Objective:**

Critical evaluation of propagation rate coefficients for free-radical polymerization of alkyl acrylic acid esters with this  $k_p$  data being derived from pulsed-laser initiated polymerizations in conjunction with polymer molecular weight analysis by size-exclusion chromatography.

**Description:**

First-principles modelling of free-radical polymerizations remain an important objective for polymer science and industry, in order to efficiently introduce process modifications and new products. The lack of reliable rate coefficients remains a major impediment in reaching this goal. For measurement of individual propagation rate coefficients,  $k_p$ , the IUPAC Working Party on "Modelling of Polymerisation Kinetics and Processes" recommended pulsed-laser initiated polymerization (PLP) in conjunction with size-exclusion chromatography (SEC) as the method of choice. This technique has been successfully used to determine reliable propagation rate coefficients for several monomers. After having established benchmark value data of  $k_p$  for styrene and a series of methacrylates in three previous publications of the IUPAC Working Party (fourth manuscript in preparation), the intention of the present project is to collate reliable  $k_p$  data for alkyl acrylates. The knowledge of kinetic data for these monomers is of great importance, as they are frequently used in technical polymerisations, e.g. in the coatings and adhesives industries.

**Title:** *Short course in polymer characterization - POLYCHAR 12*

**Number:** 2003-021-2-400

**Objective:**

Provide knowledge on techniques of Polymer Characterization, particularly so for participants from third world countries. POLYCHAR is derived from Polymer Characterization

**Description:**

There will be tutorial lectures by leading world experts on techniques of Polymer Characterization. Topics include: Thermogravimetry; Differential Scanning Calorimetry including StepScan and Thermally Modulated Calorimetry; Thermal Mechanical Analysis; pVT-Measurements; Dynamic-Mechanical Analysis; Mechanical Testing including Quasi-static and Transient Techniques; Tribology including Friction, Scratch Testing and Surface Tension Determination; Electron Microscopy; Interface Characterization; Electrical Properties of Polymers; Polymer Spectroscopy.

**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 will be 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 36 years in educating young scientists from emerging countries offers up-to-date facilities for postgraduate training in polymer science. The number of participants in each of the six runs held so far varied between 5 and 13, depending on the funds available. 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. The results of the research are published in international technical journals. The cumulative results of the eight runs of the Course at the end of 2003 were: "62 participants, 51 papers in international journals published and 69 communications at international meetings."

**Title:** *Terminology for radical polymerizations with minimal termination - the so-called "living" and/or "controlled" radical polymerization*

**Number:** 2002-006-2-400

**Objective:**

To provide recommendations for nomenclature and terminology in relation to modern (1994-) techniques of radical polymerisation, variously described in the literature as, e.g., "living" and/or "controlled".

**Description:**

There has been an explosion of renewed interest in radical polymerisation during the last nine to ten years, stemming largely from the discovery of new polymerization techniques, which provide products with novel molecular architecture, composition, and molar-mass distribution. This burst of activity has given rise to a diverse and uncoordinated terminology. The use of inappropriate terms, and the lack of uniformity of practice, constitutes severe impediments to intelligible communication and effective literature searching, with consequent potential to retard the development of this important field.

**Title:** *Glossary of class names of polymers based on their chemical structure and molecular architecture*

**Number:** 2002-014-1-400

**Objective:**

To elaborate the IUPAC document in which commonly used class names of polymers based on molecular structure features will be summarised, classified and divided to categories according to their semantic origin and their definitions will be given.

**Description:**

The document deals with macromolecular terminology, which is typical and unique field of activity of the IUPAC organisation. The document will comprise about 130 entries.

**Title:** *Conducting polymer colloids and nanofilms*

**Number:** 2002-019-1-400

**Objective:**

The design of processible forms of conducting polymers. Preparation of water-borne polyaniline colloids and *in situ* polymerized films of submicrometre thickness.

**Description:**

The development of processible forms of conducting polymers by the formation of colloids and thin nanofilms is proposed. The colloids are produced during the oxidation of aniline with ammonium peroxydisulfate in acidic aqueous medium in the presence of a suitable polymeric stabilizer. The polyaniline films grow *in situ* under similar reaction conditions virtually on any surface (or interface). The various macroscopic and microscopic substrates coated with conducting-polymer overlayer find uses in analytical chemistry, separation science, organic catalysis, conducting composite materials and in the development of microelectronics. Especially the nanofilms are of interest because of the brush-like ordering of polymer chains in them. The project proposes to follow the same preparative protocol in various laboratories and to compare the properties of the resulting materials on international level. For the colloidal forms, the particle size and polydispersity determined by dynamic light scattering will be the main criterion. The films will be compared with respect to their thickness by using optical absorption measurements after calibration.

**Title:** *Strategic study of world polymer science*

**Number:** 2002-057-1-400

**Objective:**

Systematic overview and analysis of the trends in contemporary polymer science and technology around the world in relation to MMD's future activities, strategies, and missions, via a statistical approach based on "World Polymer Organizations", an MMD-approved directory of polymer science organizations, which is to be updated and expanded in this project for the statistical trends analysis and to be internationally distributed with a summary report.

**Description:**

It is certainly of utmost importance for MMD to hold an objective, systematic, and updated view of the trends in polymer science and technology in the world, so as to soundly perceive its missions and challenges and thereby to formulate its future strategies and activities as an organization that is to guide and help world polymer community. This Project is intended to provide MMD and polymer community with updated information and primary statistical analysis about the world polymer organizations, their activities, and scientific/technological trends therein.

## V ANALYTICAL CHEMISTRY DIVISION

**Title:** *Recent advances in electroanalytical techniques: characterization, classification and terminology*

**Number:** 2002-002-2-500

**Objective:**

Revision and updating of an old IUPAC document on classification, characterization and nomenclature of electroanalytical techniques. The product will be a unified computer readable compilation to facilitate the future updating of the Orange Book and relevant terms in the Gold Book.

**Description:**

An old IUPAC technical report: "Classification and Nomenclature of Electroanalytical Techniques (Rules Approved 1975)" has not been updated for over two decades. Accordingly, the material based on this document embodied in Chapter 8 of the IUPAC "Orange Book" is out of date. During this period, several electroanalytical techniques lost their importance while new techniques have been developed and have found widespread use. Therefore, there is a clear need for a modern and updated document concerning the characterization, classification and recommendation of the relevant terminology for the new currently used electroanalytical techniques.

**Title:** *Performance evaluation criteria for preparation and measurement of macro and microfabricated ion-selective electrodes*

**Number:** 2002-003-2-500

**Objective:**

During the past several years, the application of microfabrication technologies of practical microsensor devices has entered the field of biology and medicine and is beginning to serve as the driving force for discoveries in cell biology, neurobiology, pharmacology, and tissue engineering. In parallel, the methodology of ionophore based liquid membrane ISEs has now entered the arena of trace analysis and precision science due to the latest updated and upgraded R/D of this method. This circumstance has made it necessary to also upgrade and update the evaluation criteria for the preparation and measurements of ISEs, primarily microfabricated ISEs and potentiometric cells. This is in fact the purpose of this project.

**Description:**

There are more or less generally accepted evaluation criteria for ISEs. In this new document, we will deal with the specialities of macro- and microfabricated ISE sensors; standard procedures for the microfabricated devices are much more critical compared to macroelectrodes. In addition, some evaluation criteria for the micro reference electrodes are of the same importance.

**Title:** *Optical spectrochemical analysis using waveguides and optical fibers*

**Number:** 2002-009-2-500 (previous 540/15/95)

**Objective:**

Nomenclature, symbols, units and their usage in spectrochemical analysis XXI; this document is concerned with fundamentals of guided radiation in waveguides and fibres, and classifies their effects with respect to analyte, properties of receptors, matrix effects, and assay types.

**Description:**

This document deals with the fundamentals and the application of guided radiation in waveguides or fibre optics and its interaction with sensitive layers coated to these optical devices. Besides these sensitive layers being chemical or biochemical receptors, interactions on analyte concentration, matrix effects and different assays types are discussed. These waveguides are used for radiation transport and in addition found widespread application in evanescent field techniques with direct or indirect detection via a marker substance. The various methods to interrogate the properties of radiation or waveguides by interaction with the sensitive layer are dealt with in this document also. It cannot cover bioanalytical test schemes, optical detection methods in absorbance or luminescence.

**Title:** *Definitions and fields of application of the terms robust and rugged and the characteristics or qualities of robustness and ruggedness in analytical chemistry*

**Number:** 2002-058-1-500

**Objective:**

To develop precise and unequivocal definitions of the terms robust and rugged and the related characteristics/qualities of robustness and ruggedness to be applied to avoid confusion in the various areas of analytical chemistry. Also, to examine the possible quantitative implications and expression of the above terms and characteristics.

**Description:**

There is considerable confusion in the scientific and textbook literature as to the use of the terms *robust* and *rugged* and the associated characteristics/qualities of *robustness* and *ruggedness*. Many authors use the terms and the associated characteristics as if they were synonymous; others use only one term and characteristic, namely *robust/rugged* or *rugged/ruggedness*, whilst a few distinguish their use. Some restrict the field of application to *robust/robustness* to statistical methods of data evaluation and *rugged/ruggedness* to experimental design. The use of *robust* in connection with statistical tests is supported by some professional statisticians and by current word usage as given in the recent "New Shorter Oxford English Dictionary", but which however gives one of the several meanings of *rugged*, as *robust* based on American literature usage.

**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 labelled compounds and radiopharmaceuticals to be used in radiodiagnostics, metabolic radiotherapy, radioimmunotherapy.

**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.

## VI CHEMISTRY AND THE ENVIRONMENT DIVISION

**Title:** *Fats, Oils and Oilseeds Analysis and Production - an International Workshop*

**Number:** 2002-011-2-600

**Objective :**

To hold a workshop on Fats, Oils and Oilseeds Analysis and production in Tunisia, in order to disseminate IUPAC's activities, to present recent advances in lipid chemistry and show links between IUPAC and international organizations such as Codex Alimentarius, ISO, AOCS, ASA and FOSFA.

**Description:**

North Africa (Morocco, Tunisia, Algeria) has been for many years a major oil producer and has a large agroindustry, centred on producing and processing vegetable oils. Apart from that, North Africa is also an important source for numerous native oils with potential food or industrial applications. The proposed workshop represents the first one sponsored by IUPAC in North Africa in this area. Thus, it will be a tremendous opportunity to spread IUPAC's work to all professionals related to the chemistry and processing of animal and vegetable fats and oils, as well as to chemistry students who may pursue a career in research and/or to work in the oils industry.

**Title:** *Determination of trace elements in oils and fats by inductively coupled plasma optical emission spectroscopy (ICP-OES) - evaluation of a method by collaborative study*

**Number:** 2002-013-2-600

**Objective :**

To collect precision data through international collaborative study for a universal method for the measurement of trace elements in fats and oils using inductively coupled plasma optical emission spectrometry, and to provide the supplementary data necessary to support an international standard method for the fats and oils industry.

**Description:**

Trace element contamination of food grade fats and oils is regulated by Codex Alimentarius and national standards. The levels of certain elements pose a problem for the processing industry. Atomic absorption spectrometry has been a common technique applied to the measurement of trace element content. The expense involved in instrument maintenance, the requirements for sample handling and the poor reproducibility of the results when tested on a random sample, suggests that a more reliable technique is required. ICP-OES is a popular alternative method for trace element determination. It allows for the direct aspiration of solvent diluted fats and oils and gives results without the prior ashing step. At this time there is no international standard method using ICP-OES for trace elements. A study is proposed which would measure trace elements in oil using ISO 5725 and IUPAC harmonized guidelines. Laboratories affiliated with AOCS and FOSFA International, and also those proposed by ISO/TC 34/SC 11 from locations around the world will be invited to participate.

**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. A recent report by Pontolillo and Eganhouse (U.S. Geological Survey Water-Resources Investigations Report 01-4201) indicates that the literature concerning these properties is fragmented and tends to perpetuate erroneous values.

We propose an exhaustive compilation and critical evaluation of these four properties including manufacturer data, which may not have appeared in the primary literature.



**Title:** *Crop protection chemistry in Latin America: Harmonized approaches for environmental assessment and regulation*

**Number:** 2003-013-1-600

**Objective and Description:**

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 are 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 harmonised 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:** *Bio-physical chemistry of fractal structures and processes in environmental systems*

**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".

**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 mg/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.

**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.

**Title:** *Air pollution models in environmental management and assessment*

**Number:** 2003-058-1-600

**Objective and Description:**

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 will 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:** *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 characterising 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 characterisation.

## VII CHEMISTRY AND HUMAN HEALTH

**Title:** *Compendium of terms associated with drug discovery and development*

**Number:** 2002-001-1-700

**Objective:**

Publish as a book, a compilation of the glossaries pertinent to chemistry and drug development, which have been published in *Pure and Applied Chemistry* (PAC) during the past decade i.e. since 1992. This would be a handy reference work for chemists and associated technical people in drug development.

**Description:**

The following appropriate nine glossaries have been published in PAC since 1992. To these may be added two glossaries which are currently under active construction i.e. Glossaries of Terms in Pharmaceutical Process Chemistry and in Pharmaceutical Technology:

Glossary of terms used in combinatorial chemistry

Glossary on drug metabolism terms

Glossary of terms used in medicinal chemistry

Glossary of terms used in computational drug design

Glossary of terms used in bioinorganic chemistry

Nomenclature in laboratory robotics and automation

Glossary of bioanalytical nomenclature. I: General terminology, body fluids, enzymology, immunology

Glossary for chemists of terms used in toxicology

Glossary for chemists of terms used in biotechnology

It is proposed that each glossary will constitute a separate chapter according to subject matter. In each chapter, the terms will be listed alphabetically and references listed at the end (of each chapter). Where the same term occurs in two (or more) different glossaries, the versions will either be compared and modified to a common definition or cross-referenced.

**Title:** *Analogue-based drug discovery*

**Number:** 2002-051-1-700

**Objective:**

To publish a book on "Analogue-based Drug Discovery". It should serve as a reference book for medicinal chemists, and afford an easily usable overview on drugs, drug classification and analogue types.

**Description:**

The book will illustrate the considerable success that has been achieved in the development of new drugs based on the leads provided by established drugs. Such new drugs are often considered deprecatingly as "me-too" products. However, the book will demonstrate that it is part of the very important process whereby drug action is optimised for a given therapeutic effect.

**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.

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 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 meet 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 and Description:**

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. IUPAC has long recognised this fact and in 1993 published a Glossary for Chemists of Terms Used in Toxicology as an IUPAC Recommendation. This Glossary has received wide recognition as authoritative and, in particular, has been adopted by the U.S. National Institutes of Health as the glossary for its TOXNET website. This website is now being updated and the Task Group Chairman has been asked if the existing IUPAC Glossary is being revised and brought up to date. This is clearly necessary since toxicology has developed considerably in the 11 years since the glossary was published.

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. It is proposed to seek input widely and to co-operate with the U.S. National Institutes of Health National Library of Medicine so that the revised glossary can link effectively into their Toxnet system and be hyperlinked to the educational resource Tox Tutor on their website. This will help to ensure wide use of the Glossary. Acceptance of this Glossary as a global tool to serve chemists and others will have an impact on a number of scientific fields and help to maintain a good image of both IUPAC and of chemistry in society generally.

**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. 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.

## VIII CHEMICAL NOMENCLATURE AND STRUCTURE REPRESENTATION DIVISION

**Title:** *Nomenclature of rotaxanes*

**Number:** 2002-007-1-800

**Objective:**

Establishment of standards for nomenclature of rotaxanes and catenanes.

**Description:**

There are currently no standards for nomenclature of rotaxanes and catenanes. During the last 15 years, the scientific community has shown increasing interest in these two fields of small molecules. Standardisation of nomenclature in this field is highly desirable and long overdue.

**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 Red Book extend only as far as coordination number 6. Hey-Hawkins and Sommer have recently described 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:**

Hey-Hawkins and Sommer have recently described a procedure for assigning stereo descriptors to 7-coordinate complexes that can be regarded as capped octahedra. This relies on the established nomenclature processes of defining a principal axis (through the capping position and the central atom), assigning the ligand positions to a series of planes perpendicular to the principal axis and then numbering the ligand positions in sequence, starting at the "highest" plane. The chirality is then assigned on the basis of the numbering sequence. Currently the Red Books only deal with coordination numbers up to 6, plus pentagonal bipyramidal structures, so that the increasing numbers of complexes with higher coordination number cannot be treated by established rules.

The project aims to present a unified treatment for higher coordination numbers.

**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:**

When the structure-based nomenclature of polymers was first published (1976), the commission of macromolecular nomenclature expected that the system would be soon widely used, but this was not the case and the source-based names, of which only ca.20 were allowed as exceptions in the Appendix of the document, still prevail over structure-based. Though the structure-based nomenclature is very systematic and logical so as to give only one name for one polymer, it often results in very complex or very long names contrary. This is one of the reasons why structure-based names are not so popular. Another reason for the preference for source-based names is their direct relation to monomer names and to the historical trivial names. Very recently the commission officially admitted for the first time the general use of the source-based nomenclature for homopolymers in the "Generic" document (2001) saying, "The commission has now decided to recommend source-based nomenclature as an alternative official nomenclature for homopolymers". However, because the source-based nomenclature has been treated as a second ranked nomenclature for a long time, no scrutiny has been made on it and many problems have been left unsolved. It is desirable to minimize such shortcomings while keeping the practicality of the source-based nomenclature.

**Title:** *Graphical representation standards for chemical structure diagrams*

**Number:** 2003-045-3-800

**Objective:**

To extend IUPACs leadership in the development of standard nomenclature and terminology in chemistry into the domain of chemical structure diagrams, and to provide a single, comprehensive set of guidelines for creating chemical structure diagrams in printed and in electronic media.

**Description:**

Although some existing IUPAC nomenclature recommendations already discuss some aspects of chemical structure diagrams, they do so only tangentially. Even if they were to be collected in one location, these existing recommendations on chemical

structure diagrams are incomplete, and do not discuss many basic issues. As a result, many organizations have formulated their own guidelines for creating chemical structure diagrams; however, none of those guidelines is comprehensive. Provision of a single, comprehensive set of guidelines for creating chemical structure diagrams would be a significant benefit to the chemistry community.