



IUPAC Project Summaries

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For complete information on projects see: www.iupac.org/projects

April 2006

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2006-2007 Membership

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www.iupac.org

IUPAC Secretariat
P.O. Box 13757
Research Triangle Park, NC 27709-3757, USA
Tel: +1 919 485 8700
Fax: +1 919 485 8706
E-mail: secretariat@iupac.org

I PHYSICAL AND BIOPHYSICAL CHEMISTRY DIVISION

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 H₂O and H₂S. However, now it is well known that both H₂O and H₂S form a hydrogen bonded (H₂X)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.

Title: *A database of water transitions from experiment and theory*

Number: 2004-035-1-100

Objective:

Critical compilation, experimental determination and validation, and theoretical verification and extension of accurate frequency, energy level, line intensity, line width, and pressure effect spectral parameters of water and all of its major isotopologues.

Description:

The full characterization of the spectrum of water vapor from the microwave to the near ultraviolet is a prerequisite for modeling and understanding of many fields in chemistry, physics and engineering, including (1) atmospheric modeling, with emphasis on the definitive understanding of global warming (water vapor is responsible for about 70 % of the known atmospheric absorption of sunlight and the majority of the greenhouse effect), (2) communication-related fields using the Earth's atmosphere, such as satellites and telecommunication, (3) astronomy, such as that of cool stars (where hot water is a major constituent), (3) water lasers and masers, widespread in outer space, (5) study of comets, based on fluorescence spectroscopy, and (6) combustion research, such as rocket exhausts, forest fires, and turbine engines (hot steam is a major product of most combustion processes).

The present collaborative effort is aimed at devising and constructing a database comprising, eventually, the complete linelist of all major isotopologues of water for studies at all temperatures.

Title : *Establishing recommended data on thermodynamic properties of hydration for selected organic solutes*

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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.

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.

Title : *Developments and applications in solubility*

Number: 2005-016-1-100

Objective:

Solubility is a basic phenomenon underlying most industrial processes. The objective of this project is to prepare a book that will bring together recent developments in solubility studies that have a bearing on industrial applications, especially that rigorous work which is underpinned by thermodynamic considerations.

Description:

The book will highlight important areas of new research involving theory, techniques, results, modeling, simulation and industrial applications related to solubility. It will include chapters on super critical fluids, data banks, "green chemicals", molten salts, liquid-liquid phase equilibria, nanotechnology, industrial solutions including cryogenic solutions, predictions, simulations and molecular modeling, gases in polymers, metallurgical and hydrometallurgical processes, food, pharmaceutical and cosmetics industry and separation processes.

Title : *Solubility and thermodynamic properties related to environmental issues*

Number: 2005-048-2-100

Objective:

The objective is to bring together recent developments in SOLUBILITY studies which have a bearing on ENVIRONMENTAL ISSUES. This, we believe, could lead to new ways of thinking and solving problems related to environmental issues and pollution. The focus is on the importance of the basic property - SOLUBILITY - in understanding environmental pollution and hence overcoming pollution problems.

Description:

The book will highlight important areas of new research related to solubility and its applications to environmental issues. There will be 25 chapters, focusing on areas such as: predicting and modeling of environmental pollutants from basic thermodynamics considerations and properties such as solubility; designing remediation and cleaner industrial processes based on basic thermodynamic properties; predicting and measuring the uptake of pollutants and new industrial chemicals in humans and in animals; solubility together with environmental issues related to, health science, mining, pesticides, soil chemistry, supercritical and phase equilibria separation processes, gasoline additives, ionic liquids in industry, corrosion control, surfactants, green synthesis, surface adsorption and biodegradable plastic films.

Solubility is a basic phenomenon which determines the level of most pollution problems, both environmental and industrial. No book exists which focuses on recent work highlighting the importance of solubility and thermodynamic properties to environmental issues.

Projects recently completed or near completion:

New Edition of Experimental Thermodynamics Vol II

Quantities, terminology and symbols in photothermal and related spectroscopies

Recommendation for the use of AFM in the direct measurements of colloidal forces

Measurement and interpretation of electrokinetic phenomena

Chemical thermodynamics in industry

Evaluated kinetic data for combustion modeling

Revision of "Quantities, Units and Symbols in Physical Chemistry" and the Appendices (3rd edition)

Thermochemistry of chemical reactions: nomenclature, symbols and experimental methods for bond energies

Spectroscopy under extreme conditions of temperature and pressure

Critical compilation of vapour liquid critical properties

II INORGANIC CHEMISTRY DIVISION

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.

Title: *Calibration of organic and inorganic oxygen-bearing isotopic reference materials*

Number: 2005-022-1-200

Objective:

The purpose of this project is to assess the relative amounts of oxygen isotopes in internationally distributed organic and inorganic isotopic reference materials and publish "consensus" values and uncertainties for these materials.

Description:

During the past three decades, the determination of the relative amounts of stable isotopes of the light elements (H, C, N, O, and S) has dramatically increased because of expanded use in hydrology, environmental studies, microbiology, forensic investigations, atmospheric investigations, oceanography, etc. In the last 10 years, determination of the relative amounts of the isotopes of oxygen in organic and inorganic solids has increased because of developments in instrumentation. In the last 5 years, several new oxygen isotopic reference materials have been prepared. However, the values of the relative amounts of oxygen isotopes in these new materials and in older materials are not well known. Thus, the problem arises that two isotope laboratories analyzing the same sample may not report the same result within analytical uncertainty because they do not know what values to accept for internationally distributed oxygen isotopic reference materials.

The purpose of this work is to bring together expert analytical laboratories (Jena, Reston, Leipzig, Canberra, and Zurich) to measure the relative amounts of oxygen isotopes in isotopic reference materials. This highly coordinated analytical effort will include inorganic materials, organic materials, atmospheric oxygen, and two water reference materials-the scale for expressing relative amounts of oxygen isotopes in natural materials is anchored by the two isotopic reference materials VSMOW water and SLAP water. Strict analytical protocols will be designed and followed by all laboratories.

Title: *Evaluated published isotope ratio data (2005-2007)*

Number: 2005-027-1-200

Objective:

Evaluate isotope ratio publications between 2005 and early 2007, to determine "best isotope ratio measurements" for compilation and publication in a 2009 TICE, recommend "new" standard atomic weights, and publish "Atomic Weights of the Elements 2007" in *Pure and Applied Chemistry*, which will also include a table of relative atomic masses and half-lives of selected radionuclides.

Description:

The aim of the task group is to evaluate isotope ratio publications between early-2005 and early 2007. The evaluated data will be incorporated into the CIAAW* Table of Isotopic Composition of the elements (TICE) and Table of Standard Atomic Weights. This project is an interim step in the evaluation of isotopic data production for the next proposed publication of TICE in 2009.

The Subcommittee on Isotopic Abundance Measurements (SIAM) recognizes that there are a number of elements that need particular attention and for which significant publications are expected. These include Zn, Ca, Mg, and Si: for which two, significantly different, high precision publications have recently been assessed by IUPAC, is in the process of being resolved and will require evaluation.

The task group will evaluate recently published isotope ratios and resulting atomic-weights. Detailed discussions and calculations will be carried out on any chemical element for which new isotope ratio information exists.

Projects recently completed or near completion:

Nomenclature of inorganic chemistry - Revised 'Red Book' - part I

III ORGANIC AND BIOMOLECULAR CHEMISTRY DIVISION

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.

Title: *"Global Climate Change" - Translation and Dissemination of a monograph for Secondary Schools*

Number: 2005-015-1-300

Objective:

- To translate a monograph on "Global Climate Change", from Italian into English, Spanish and Portuguese.
- To provide a total of 2000 copies of this monograph, translated into these three languages, for initial dissemination and evaluation by relevant secondary school authorities, professional science teaching bodies and secondary teachers in Australia, Spain, Portugal and other selected countries.
- To demonstrate the central role of chemistry in the treatment of issues of global importance and particularly the contribution that green chemistry can make.
- To determine the future potential demand for this monograph in secondary schools.

Description:

A monograph on "Global Climate Change" written in Italian, has been produced by the Italian Consorzio Interuniversitario Nazionale "La Chimica per L'Ambiente" (INCA; ISBN: 88-88214-12-7) and distributed to Italian secondary schools. This monograph or booklet, constitutes one of the early chapters from a senior secondary textbook on "Introduction to Green Chemistry" which will be produced by INCA as part of its Green Chemistry Series. The monograph is gaining considerable popularity in Italy, leading to its adoption by many science teachers as a resource for the curriculum. The booklet also has the unique feature of introducing green chemistry to secondary school students. It stresses the central role of chemistry in understanding the Global Climate Change issue.

This booklet can serve as a significant and popular resource for secondary schools in other parts of the world; however, it needs to be reproduced in other languages. In the first instance, it is proposed to translate the booklet into English, Portuguese and Spanish. This will allow a significant number of countries to be covered, including parts of Europe, the UK, Australia and New Zealand, South Africa, as well as most of the countries in the North and South American continents.

Title: *Development of methodologies and protocols for documentation, evaluation of safety and efficacy and standardization of herbal medicine*

Number: 2005-034-1-300

Objective:

Development of methodologies and protocols for the

1. Documentation of traditional knowledge of medicine using existing information & databases and by collecting new information from traditional healers
2. Scientific evaluation of efficacy, toxicity & dose form of herbal/traditional medicine
3. Standardization of raw materials, intermediates and final product of herbal medicine

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 safe and effective herbal medicines in a standardized way is essential. So also is the necessity to document and preserve the traditional medical knowledge which is disappearing. With the above background the necessity of establishing a Multidisciplinary International Research Centre on Herbal Medicine was felt.

Title: *Strategic Planning for a new East Asian Network for Organic Chemistry*

Number: 2005-039-2-300

Objective:

To establish a new collaborative East Asian Network, closely linked to IUPAC, in order to build and foster a sustainable program of high-quality organic chemistry research, education and chemistry-based applications. especially in less developed Asian countries.

Description:

Background - It has been estimated that 30% of the research done in the field of organic chemistry in the world is being produced in Asia. While this statistic is encouraging, a careful inspection shows that productive research is presently concentrated in a few countries in the region, and is by no means a common phenomenon across all countries in Asia. Previous cooperative networks (such as the Network for the Chemistry of Biologically Important Natural Products, and the UNESCO Network for Natural Products) have either ceased to operate entirely or are languishing through lack of funding. There is now an opportunity - and indeed a responsibility - for IUPAC to take the initiative in this matter, and plan the establishment of a new Network. Such an initiative would complement a major program being undertaken by the Japan Society for the Promotion of Science (JSPS).

Title : *Chemistry for Biology - an inventory of interdivisional and interdisciplinary activities within IUPAC in the field of biological chemistry*

Number: 2005-042-1-300

Objective:

Biological Chemistry is a rapidly developing multi-disciplinary area with strong links to molecular and mechanistic topics. The objective is to make a feasibility study and an inventory of current and planned IUPAC activities in the area and also to suggest and initiate new activities.

Description:

Biological Chemistry is a multi-disciplinary area with strong links to fundamental molecular and mechanistic topics. These topics are essential for the progress in the field. IUPAC shall be visible and shall have a central role in efforts to support strong links between chemistry and biology. The medicinal area and, to some extent, also the agricultural area have, already brought these two basic sciences together and have a lot of experience of multi-disciplinary research and development. However, IUPAC, with its Divisions, is mainly based on basic chemistry and its applications. Focus has been on fundamental chemistry and on its industrial applications, which has been successful and shall always be the fundament of IUPAC. However, new scientific areas of multi-disciplinary nature are approaching and there is a need to include these within the work of IUPAC. Biological Chemistry is such a topic.

Projects recently completed or near completion:

Post-genomic chemistry

Chemical actinometry

Green Chemistry in Latin America

Green chemistry in Russia

Workshop for formulation of plans for the establishment of a "Center of Natural Products Research (CNPR)"

Development of guidelines for the transmission of information on organic synthesis (Abbreviation guidelines and glossary of terms for protecting groups in synthesis)

IV POLYMER DIVISION

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: *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: *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: *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.

Title: *Microstructure and properties of thermotropic liquid crystalline polymer blends and composites*

Number: 2004-044-2-400

Objective:

To evaluate the microstructure-property correlation of thermotropic liquid crystalline polymer blends and composites

Description:

The synthesis and modification of thermotropic liquid crystalline polymers (TLCP) for different final applications are currently hot topics of industrial as well as academic research. The copolymerization of different comonomers leads to polymers with different liquid crystalline characteristics, melting temperatures, rheological behavior. The incorporation of some comonomers is applied to reduce the processing temperature but still keep the liquid crystalline characteristics. TLCPs having different chemical structure are processed to different end-use forms of products by injection molding, extrusion, stretching, blowing and spinning. TLCPs are currently produced by Solvay, Eastman, Ticona, Polyplastics, DuPont, Mitsubishi, Sumitomo, and Unitika, and are commercialized as glass fiber-filled, glass beads-filled, glass flakes-filled, silica-filled grades for injection-molded parts, and tubes, films, bottles and fibers in IT, automobile, chemical, medical and hi-tech industries. The microstructure of commercialized TLCP blends and composites is closely related to their processing conditions. The relation between the rheological properties and the resultant microstructure of these blends and composites should be well established. The aim of this research is to evaluate microstructure-property relation of the commercialized TLCP blends and composites (e.g. glass fiber-filled grades) by the rheological measurement (dynamic and steady rheology), morphology observation (SEM, WAXD) and property evaluation (mechanical tests).

Title: *Efficiency and reproducibility of temperature rising elution fractionation (TREF)*

Number: 2005-009-3-400

Objective:

The aims of this project are (1) to fractionate a given number of Polyethylene (PE) test samples with regard to their composition using a given experimental procedure, (2) to compare the quantity and chemical composition of the obtained fractions in the partner laboratories, (3) to compare the results with regard to influence of the instrumental setup and reproducibility and (4) to establish suitable conditions for the compositional fractionation of polyethylene. Finally conclusions shall be drawn with regard to the comparability of the results and the robustness of TREF procedures in daily routine.

Description:

TREF is a technique which fractionates semicrystalline polyolefins from solution according to composition and microstructure. The technique has been invented in the late 1970s. In TREF the polymer is dissolved in a suitable solvent at elevated temperatures. Subsequently the solution is slowly cooled down to crystallize the sample. In the third step the sample is eluted by fresh solvent at successively rising temperatures. The fractions are collected and analyzed after workup. The instrumental setup and experimental parameters which are used vary between the different laboratories. Crystallization and elution can be carried out either in a column which is packed with a porous support or in a reactor without packing. As there was no commercial instrumentation available until the late 90s the equipment which is used is in most cases in-house constructed. The steps of crystallization and elution are influenced by the concentration of the polymer, the dimensions of the reactor, the type of support used and the cooling rate. However there are no guidelines about these parameters and little information is available in the literature. Therefore the results from different laboratories are difficult to compare. Due to the pivotal importance of TREF for the compositional fractionation of polyethylene it is highly important to compare the results between different laboratories. TREF is used in various countries, ranging from industrialized nations to developing countries.

Title: *Repeatability and reproducibility of sample preparation and analysis in high-temperature SEC*

Number: 2005-011-3-400

Objective:

Standardization of the experimental conditions for the HT-SEC analysis of polyolefins. The particular emphasis shall be on the sample preparation with regard to dissolution temperature and time, the sample measurement with regard to column temperature and the column set, and with regard to the detection technique (RI, ELSD, Visco, LS). Although there is an ASTM method for the analysis of polyolefins by HT-SEC (ASTM D 6474), procedures for sample preparation are not addressed adequately. The application of different detectors in HT-GPC is not addressed at all.

Description:

Round robin tests on standard HDPE, standard PP, standard LLDPE, ultrahigh-MW PE

1. step: measurements according to existing procedures in the different labs
2. step: standardization of measurement and detection
3. step: standardization of sample preparation

Title: *Accuracy and reproducibility of functionality type analysis of poly(ethylene oxide) homo and copolymers by LC-CC*

Number: 2005-021-3-400

Objective:

The aims of this project are

1. to establish critical LC conditions for poly(ethylene glycol) using a given experimental procedure,
2. to compare the critical eluents compositions in the partner laboratories,
3. to separate and quantify a given number of PEO test samples with regard to functionality type distribution, and
4. to compare the results with regard to accuracy and reproducibility. Finally, conclusions shall be withdrawn on the robustness of LC-CC procedures in daily routine.

Description:

A range of poly ethylene glycols (PEG) having different molar masses will be characterized by liquid chromatographic methods. We will mainly focus on the liquid chromatography at the critical point of adsorption (LC-CC) Using these technique polymers can be separated selectively with regard to chemical composition or functionality, as has been shown for macromonomers, random and block copolymers, and polymer blends. Since the method becomes widely used it is necessary to find and establish standard procedures and to study the accuracy and reproducibility.

Data will be accumulated from different labs in an academic and industrial environment. A further key will be to study the sensitivity of the different experimental conditions applied in the different labs. An ambiguous target will be the characterization of "real world samples" e.g. PEG's having different endgroups.

Title: *Micro-structural, melt processing and mechanical properties of compatibilised PA 6/ABS-blends*

Number: 2005-023-2-400

Objective:

Investigation of the influence of compatibilisation of PA6/ABS blends on melt processing, micro-structure and mechanical properties and their mutual interactions.

Description:

Blending of polymers is a technologically important procedure in polymer processing and a powerful tool in order to improve the end use properties of polymeric materials. The understanding of relevant micro-structural mechanisms during melt processing and of deformation on morphology in the solid state is essential in order to optimise the blending of polymers with respect to processability and performance. For example, it is often necessary to prepare a two phase polymer blend with a co-continuous morphology during extrusion. Therefore it is crucial to understand quantitatively the deformation of the phases and the processes leading to the break-up or the coalescence of micro-structures during mixing. Compatibilisation of the constituents generally improves the mechanical properties of the blend. In this context, the degree of compatibilisation, the mobility of the compatibiliser at the interface and in the bulk and its influence on interfacial tension and coalescence of droplets are important properties, which determine the final blend morphology and the mechanical performance. In the past, the relevant physical phenomena in complex multiphase blends (e.g., the industrially important PA 6/ABS blends) have only been partially explored. Especially, melt elongational properties, their influence on morphology and melt stability during processing were not the focus of previous studies.

Title: *Short course in polymer characterization - POLYCHAR 14*

Number: 2006-003-1-400

Objective:

Provide knowledge on techniques of Polymer Characterization, particularly so for participants from third world countries. At the same time prepare the participants for understanding lectures and presentations during the following 14th Annual POLYCHAR World Forum on Advanced Materials (Polymer Applications & Theory).

Description:

The Short Course will be held by well-known experts in their field and will promote students, in particular newcomers in the field of Polymer Science, to participate in the Conference with a much better understanding, it offers an overview over the most important techniques of polymer characterization and introduction into recent developments. The course lecturers are available for the students throughout the days of the following Conference for further engrossing of the lectures.

Projects recently completed or near completion:

Terminology related to multiphase polymer composites and blends

Molecular characterization of polyamides 6, 11 and 12

Round Robin test on the molecular characterization of epoxy resins by liquid chromatography

Definitions of terms relating to reactions of polymers and functional polymers

Conducting polymer colloids and nanofilms

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

Annual course on polymer characterization

Melt rheology and concomitant morphology in polyblends and polyalloys

V ANALYTICAL CHEMISTRY DIVISION

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 address 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.

Title: *IUPAC Stability Constants Database - completion of data collection up to 2006*

Number: 2005-014-1-500

Objective:

1. To bring the literature coverage in the IUPAC Stability Constants Database up-to-date to 2006, to be accomplished by 2008 (3.5 years). Coverage is currently complete to the end of 2002 for 26 mainstream journals, to 2001 for 11 journals, 2000 for 9 journals.
2. To establish a team of experts to supervise data entry and oversee quality control (all currently done at one university) and establish a succession of experts to continue this work beyond the current project.

Description:

Data compilation for SC-Database involves literature search, evaluation, data entry using the program SCEnter, and quality control checks on entered data. The data are then sent to the data coordinator, Academic Software (AS), for conflation of master files.

Data compilation was a voluntary effort (Commission V.6) until the mid-90's but this was unable to keep pace with publications. In 2000 a Division V project was funded by the Project Committee to "Complete data collection up to 2000+". This project, completed in April 2005,- captured data for 47 journals, ca 1995-2001,- captured some 1000 "missed" references (1970-95),- corrected many errors transferred from the book volumes (1900-1973)- completed compilation for 8 additional or new journals (environmental, engineering and biochemical) bringing the total to 55 journals.

SC-Database is used as the principal source of literature data for the steady stream of "Critical evaluations of stability constants" that are published by Division V. For this reason also, it is necessary to keep the database up-to-date.

Although such evaluations come within the scope of Division V and its Solubility and Solution Equilibrium Data sub-committee, the relevance of the database is much wider, particularly to aspects of inorganic chemistry, physical chemistry and environmental chemistry. Division V is investigating ways of encouraging a more inter-Divisional ownership of the database.

Title: *Glossary of terms related to solubility - updates and revisions to the Orange Book*

Number: 2005-017-1-500

Objective:

This project will produce a set of Recommendations for publication in *PAC* and replace the existing Section 3.2.5 of the Compendium of Analytical Nomenclature (the Orange Book). The new text in glossary format will cover terminology related to the solubility of gases in liquids, liquids in liquids and solids in liquids.

Description:

Clear and consistent use of agreed-upon terminology and nomenclature is essential for unambiguous scientific communication. For many years IUPAC has carefully prepared recommendations for terminology and nomenclature related to the various branches of chemistry. These recommendations are disseminated to the international community of chemists and users of chemical information, by publication in *Pure and Applied Chemistry (PAC)* and as a series of monographs collectively known as the "color books" including the Compendium of Analytical Nomenclature (the Orange Book, itself a collection of recommendations previously published in *PAC*). In recent years the color books have begun a migration to the world wide web where their content is readily accessible to a broader audience than was possible for the bound volumes. The existing section of the Orange Book that treats solubility equilibria (3.2.5) is quite brief and limited to the aqueous solubility of ionic substances. This project will revise, expand and update this section with a comprehensive treatment of terminology related to solubility including the solubility of gases in liquids, liquids in liquids, and solids in liquids.

Projects recently completed or near completion:

Determination of trace elements bound to soil and sediment fractions

Electrochemical detection in flowing media: Classification and recommendation

Guidelines for calibration in analytical chemistry. Part 2: multicomponent calibration

Electroanalysis with piezo-electric devices

Non-selective sensors arrays ("Electronic Nose", "Electronic Tongue") chemical analysis: classification and characterization

Ionic strength corrections for stability constants

IUPAC stability constants database - completion of data collection up to 2000+

Assessment of uncertainty associated with soil sampling in agricultural, semi-natural, urban and contaminated environments (SOILSAMP)

Analytical electromigration techniques

Critical evaluation of the state of the art of the analysis of light elements in thin films

Solubility of volatile and gaseous fluorides in all solvents

Critical evaluation of stability constants of metal complexes of complexones for biomedical and environmental applications

Compilation of K_0 and related data for NAA in the form of electronic database

IA and IIA azoles, cyanates, cyanides and thiocyanates

VI CHEMISTRY AND THE ENVIRONMENT DIVISION

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.

Title: *Establishment of guidelines for the validation of qualitative and semi-quantitative (screening) methods by collaborative trial: a harmonized protocol*

Number: 2005-024-2-600

Objective:

Establishment of an internationally harmonized protocol (guidelines) for the organisation and interpretation of collaborative trials for the validation of qualitative methods.

Description:

The organization of collaborative trials for the validation of analytical methods requires many important aspects to be taken into account, including the preparation of suitable test materials and the selection of an appropriate protocol for the organisation and interpretation of data from suitable collaborative trials. The protocol should be available as internationally agreed Guidelines. The Guidelines need to provide information as to be required number of participating laboratories, characteristics of the test materials to be used in the study and details on the statistical treatment of the results. It is now important for an objective assessment to be made on whether a method, once validated, is fit-for purpose and information on how this to be achieved should also be given in the Guidelines. Most quantitative analytical methods, when adopted and published as an International Standard, are now required to be validated according to the international harmonized protocol.

Projects recently completed or near completion:

Mycotoxin methods for developing countries - aflatoxins in paprika, corn, pistachios, peanuts, and figs

Local and regional contribution to air pollution in Asian developing countries

Local radiation balance: the influence of aerosol

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

VII CHEMISTRY AND HUMAN HEALTH DIVISION

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 drug target 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.

Title: *Distance learning in toxicology: Effective teaching through technology*

Number: 2005-013-1-700

Objective:

The objective of this symposium is to present/clarify issues surrounding development/delivery of online courses in toxicology. Instruction in the development of these courses and several examples of robust programs involving distance learning around the world will be presented. Discussions relating to cost, effectiveness, and overall quality of distance learning in toxicology will be incorporated into the symposium.

Description:

A symposium about distance learning in toxicology is proposed in which speakers from around the globe will be discussing their efforts in this arena. This symposium will be presented at the Society of Toxicology (SOT) annual meeting in San Diego, CA March 5-9, 2006. This symposium is important because undoubtedly, distance learning has come of age. Moreover, online courses in toxicology specifically stand to benefit many individuals studying the effects of chemicals on humans, animals, and the environment.

Title: *Plants as sources for nutraceuticals in Latin America*

Number: 2005-031-2-700

Objective:

Establish the importance of Nutraceuticals in health care in developing societies, with food shortage. Economic opportunity of the Nutraceuticals vs. molecules of natural origin in Latin America. Possibilities of research, development and innovation in Nutraceuticals in Latin America. Possibilities of industrialization and patents of Nutraceuticals in Latin America.

Nutraceuticals: a) Functional foods that have potentially disease - preventing and health promoting properties (American Nutraceuticals Association; b) Healthy foods or food ingredients that provide health benefits beyond the traditional nutrients it contains (American Dietetic Association).

Description:

Collect data in Latin American countries. Identification plants, especially those which are natives of the continent, which are used in Latin American societies as Nutraceuticals. Estimate clinical security, related to the consumption of Nutraceuticals used in Latin America as well as for exportation. Consider the possibility of patents and industrialization of Nutraceuticals that are native of the Latin American countries.

Title: *Review of stand alone drugs*

Number: 2005-032-2-700

Objective:

The project will study drugs having no structural and pharmacological analogues. In several cases it is not possible to improve an existing drug with the help of analogues. The "Stand Alone Drugs" will be studied among the most frequently used drugs (e.g. Top 500 drugs). The project will afford a review article on them.

Description:

Acetylsalicylic acid is one of the oldest small molecule drugs, which is at the same time a "Stand Alone Drug" having a specific property as an irreversible inhibitor of COX-1 enzyme. Several efforts tried to improve acetylsalicylic acid with

the help of analogue-based research. These efforts remained unsuccessful. The same is true in several other Stand Alone Drugs, such as diltiazem (L-type calcium antagonist), levodopa (dopamine pro-drug) etc.

Analogue-based Drug Discovery (ABDD) has been the most successful direction in drug research. An IUPAC project studied this field and a book was published in January 2006 on this topic as a result of the IUPAC project. This successful approach of the drugs research has, however, limitations. To the limitations of the ABDD belong the "Stand Alone Drugs", whose analogue-based modifications did not afford new drugs.

The aim of the project "Review of Stand Alone Drugs" will identify these drugs among the most frequently used drugs (e.g. Top 500 drugs) and their role on medicinal chemistry will be studied. Identification of Stand Alone Drugs will help the orientation among the drugs, because stand alone drugs and analogues represent the two main fields among the drugs. Drugs without known mechanism of action are out of the scope of this study.

Title: *Prototype analysis of glossary terms to establish biological context by text data mining*

Number: 2005-049-1-700

Objective:

To extend the usefulness and applicability of the glossaries, it would be worthwhile to explore methods for identifying the various contexts in which the terms appear in the scientific literature.

Description:

A prototype project using a text data mining tool, LexiMine, from LexiQuest, an SPSS company, will evaluate the ability to automatically, objectively and exhaustively analyze downloaded journal articles in terms of their syntactical construction. This analysis will generate a concept map of all concepts within the analyzed articles and this will be compared with the list of terms from the glossaries to establish their presence within the literature, their interactions and relationships, both among themselves and with other concepts, and show the link to the original citation in the text. In this manner it will be possible to identify and evaluate the glossary terms for their contextual extensions of their definitions. This can be used to either develop a parallel and complementary glossary that may be published directly or as a web-enabled product, or to augment the existing glossaries and compendium.

Title: *Prototype analysis of molecular biomarkers in cancer*

Number: 2005-050-1-700

Objective:

Molecular Biomarkers have become a major focus of disease management and drug development, particularly in oncology. This prototypic study will identify the existing biomarkers in breast cancer and classify them in terms of disease progression and also as to their clinical vs. research use.

Description:

Biomarkers are typically used to establish presence or absence of disease, genetic risk and endpoints for clinical trials. The Human Genome Project has identified a large number of potential targets for drug development, but without the necessary validation for implementation in drug discovery programs. Our perspective of disease has evolved from simply the difference between non-disease and disease states as we recognize the progression from non-disease, potential genetic risk, diagnosis, disease staging, disease stratification, therapeutic selection, recurrence and outcome as elements of disease progression. There is a need to understand the relationship between biomarkers and their association with these components of disease to optimize their utility in both research and clinical settings. In addition, many biomarkers have been noted in research environments without entering the formal FDA approval process to enable clinical application. We believe that this level of definition and clarification would be useful for the drug and diagnostic industries and healthcare, in general, and would like to use biomarkers in breast cancer as a prototype to show the potential value of such an undertaking.

Projects recently completed or near completion:

Glossary for toxicokinetics of chemicals

Post-genomic chemistry

Properties and units in medical molecular biology

Analogue-based drug discovery

VIII CHEMICAL NOMENCLATURE AND STRUCTURE REPRESENTATION DIVISION

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.

Projects recently completed or near completion:

Nomenclature of inorganic chemistry - Revised 'Red Book' - part I

IUPAC International chemical identifier (InChI)

Fullerene nomenclature - part II

CHEMRAWN

No projects listed since 2003.

Projects recently completed or near completion:

CHEMRAWN XV - Chemistry for Water

CHEMRAWN XVI - Innovation in the chemical industry: the way from pure to applied chemistry

COMMITTEE ON CHEMISTRY EDUCATION (CCE)

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.

Title : *Micro-scale chemistry for student laboratories in India*

Number: 2005-002-2-050

Objective:

Micro-scale approach has been widely accepted on ground of economy, safety, saving of time, ease of experimentation and so on. Unfortunately its acceptance for student laboratories in the developing world is not as widespread as it should be. This project aims at consolidating the beginning made in India for micro-scale kit design and for teacher training.

Description:

The well-known micro-scale expert from Sweden, Christer Gruvberg, conducted eight demo Workshops in March-April, 2004 for a hands-on demonstration of the efficacy of the micro-scale approach for school laboratories. This led to the formulation of a strategy for training teacher and also to the design of a local kit being marketed by a local entrepreneur.

This project will consolidate and expand the scope of the ongoing work through partnership with Industry for large-scale kit production and for design of a 'home-kit', and partnership -- under CCE auspices -- with international experts for designing a micro-scale program for South Asia.

Title : *e-Quiz for promoting chemical education*

Number: 2005-003-2-050

Objective:

Conducting a quality Quiz is an effective way of canalizing student interest in chemistry beyond the confines of syllabi. This expectation has been borne out through an exploratory exercise held during 2003-2004 in which nearly 5000 students participated from over 40 schools in Delhi, Mumbai, Kanpur and Kota (near Jaipur).

Description:

Background - A Chemistry Quiz titled RASAYANIKA ('Chemistry' is called 'Rasayan' in Sanskrit) was conducted in Delhi in 2003 under the auspices of the JK Foundation for Human Development (JKFGD) - a part of the JK Organization which is one of the most prestigious Industrial Houses in India. The Indian Quiz is an adaptation of the pioneering work carried out by Dr. Charles Fogliani under the auspices of the Royal Australian Chemical Institute. (The Australian National Chemistry Quiz is being conducted by Dr. Fogliani in the Australasian region since the 1980s.) RASAYANIKA is designed to improve the awareness of the role that Chemistry plays in everyday life in a developing country like India. The highly enthusiastic response from students and teachers in 2003 led to the idea of conducting the Quiz outside Delhi in 2004.

It is now felt that it will be useful to go on-line to reach a wider audience and to professionalize the assessment tools and techniques so that RASAYANIKA becomes a catalyst for improving student interest in Chemistry. To enable the participation of schools where Chemistry is not taught in English, the on-line version will also be accessible in local languages where necessary.

The objective is to design the on-line version of the exploratory trials conducted in 2003 and 2004. This will enable students to take part from all over India in 2005-06 and pave the way for a regional extension of the Quiz.

Title : *Multiple use of chemicals and professional code of conduct*

Number: 2005-028-1-050

Objective:

To facilitate the community of chemists and chemical engineers to learn about the key provisions and requirements of the Chemical Weapons Convention (CWC), in order to integrate issues related to CWC and its implementation into chemistry teaching, and to promote codes of ethical and professional conduct of chemists and chemical engineers.

Description:

The CWC and the role of chemists was the subject of a joint meeting of IUPAC and the Organisation for the Prohibition of Chemical Weapons held in Oxford (UK) from 9-12 July 2005. Two recommendations of the meeting were (i) the need for chemists to develop their own codes-of-conduct, and (ii) for the development of educational material which describes the CWC and the obligations it places on the 160 member states who are signatories.

This project will address the first recommendation, i.e. the need for chemists to develop their own codes-of-conduct. A conference on **Chemical Education and Responsible Stewardship** will be organized at the D.Mendeleev University of Chemical Technology of Russia, Moscow, Russia from 30 Oct to 1 Nov 2005. The goal of the conference is to discuss problems and share the experience on themes such as social responsibility of chemists and chemical aspects of industrial and life safety.

Title : *Educational material for raising awareness of the Chemical Weapons Convention and the multiple uses of chemicals*

Number: 2005-029-1-050

Objective:

To develop educational material for IUPAC chemists and chemistry teachers about the Chemical Weapons Convention (CWC). The material will start with the beneficial use of chemicals, and raise awareness about the possible misuses of chemicals, including the production of chemical weapons. Students will be encouraged to develop their own codes-of-conduct.

Description:

The CWC and the role of chemists was the subject of a joint meeting of IUPAC and the Organisation for the Prohibition of Chemical Weapons held in Oxford (UK) from 9-12 July 2005. Two recommendations of the meeting were (i) the need for chemists to develop their own codes-of-conduct, and (ii) for the development of educational material which describes the CWC and the obligations it places on the 160 member states who are signatories. It was felt important to place the CWC in the context of the beneficial uses and misuses of chemicals, and raise awareness of multiple uses of the same substances.

Chemists played a formative role in the development of chemical warfare (CW) and the CWC aims to prevent any recurrence of this activity. But very few chemists know much about the CWC and what it covers, and few chemistry students realize that beneficial substances can be misused to produce chemical weapons. Educational material will fill this gap and help get the message across to those in a position to harm the convention but, more importantly, to encourage the peaceful uses of chemistry, which are legion.

Title : *New directions in teaching, learning and evaluation of chemical sciences at tertiary level in Sri Lanka*

Number: 2005-030-1-050

Objective:

To replace the currently practicing knowledge based education in Chemical Sciences at tertiary level with modern methods by empowering academics with relevant knowledge and skills. Focus will be on novel teaching, learning and evaluation methods with an emphasis on curriculum development, new assessment methods and evaluation tools.

Description:

The science education process in Sri Lanka has faced a serious problem in the recent years. Higher education is available only for about 6% of the applicants each year due to lack of state university facilities. From state universities,

the major producer of science graduates in the country, only about 45% complete the degree whilst others opt for low paid jobs prior to completion of the degree (N.B. The job insecurity after graduation being the major reason). Despite the low number of science graduates produced by state universities the unemployment rate of science graduates is as high as 50%. The reason for this, as envisaged by the developing industrial sector in the country, is the poor quality of graduates lacking relevant skills such as innovativeness, intellectual skills, independent working ability, decision making ability etc. Unemployed graduates' frustration is causing problem in the country.

The root cause for low quality graduates, has been identified as due to traditional teaching methods still largely practiced in SL. In turn, regrettably, there has been no opportunity for university academics to educate or improve themselves on novel teaching methods. No attempt has ever been made to address this issue by the higher education sector of SL.

Projects recently completed or near completion:

Chemical education and sustainable development

DIDAC worldwide

Chemistry's contributions to humanity - A feasibility study

Frontiers of chemical sciences: research and education in middle eastern countries

Flying chemists program - 2005 visit to India

COMMITTEE ON CHEMISTRY AND INDUSTRY

Title: *IUPAC-UNESCO-UNIDO Safety Training Program: A Fellowship Program for Safety and Environmental Protection in Chemical, Biotechnological and Pharmaceutical Production*

Number: 022/11/93 [This is an ongoing project]

Remarks: Interaction with UNESCO and UNIDO; involvement with IUPAC Company Associates throughout the developed world.

Objective:

The IUPAC-UNESCO-UNIDO Safety Training Program allows safety experts from developing countries to learn 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.

Each scientist or engineer accepted into the Safety Training Program is assigned to an IUPAC Company Associate in an industrialized country. The period of training is typically one to three weeks. Accommodation, subsistence and travel expenses are provided for all trainees.

Successful candidates are professional scientists and engineers who are currently:

1. Involved at a supervisory or managerial level in chemical companies, government institutions or scientific institutions;
2. Engaged in aspects of safety and environmental protection in chemical, pharmaceutical, or biotechnological production or in the teaching of these fields;
3. Have the ability to influence safety practices in their places of employment and elsewhere within their home country.

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 Mitsui 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 date 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.

Title: *Occupational Health and Safety Assessment in East Africa*

Number: 2005-046-1-022

Objective:

To enable industrialists and other stakeholders in East Africa to appreciate the purpose of an occupational health and safety (OH&S) management system; explain the legislative framework relevant to such an OH&S management system; and explore the purpose and intent of Occupational Health and Safety Assessment Series (OHSAS) 18001 and 18002. To reach that objective, a 3-day conference will be organized in Nairobi, Kenya, on 27-29 September 2006.

Description:

Whereas developed country industrialists take OH&S issues very seriously, their counterparts in the developing world do not always do so. This is largely due to lack of awareness, non-enforcement of relevant safety laws and regulations, and a lack of a systematic structure that guides the establishment of sound OH&S management systems. The end result has been an uncoordinated approach to safety issues, a development that exposes workers to high levels of risks. There is therefore an urgent need for developing country industrialists and key stakeholders to be exposed to OHSAS specifications that give requirements for an OH&S management system and enables organizations to control their full range of risks. This OHSAS specification is applicable to any organization that wishes to establish an OH&S management system so as to eliminate or minimize risks to employees and other parties; implement, maintain and continually improve on its OH&S management system; assure itself of its conformance with its stated OH&S policy; demonstrate such conformance to others; seek certification of its OH&S management system and make a self declaration of conformance with OHSAS specifications. This fits in with the objectives of the IUPAC/COCI Health and Safety Fellowship program. If health and safety experts from the East African Region are exposed to OHSAS specifications, they will be able to guide industrialists in the setting up of comprehensive occupational health and safety programs.

Projects recently completed or near completion:

Identification of Projects of Interest to the Chemical Industry

IUPAC-UNESCO-UNIDO Safety Training Program Workshop, Beijing, China (40th IUPAC Congress, Aug 2005)