



IUPAC PROJECT SUMMARIES

The following summaries represent projects, since 2005, for each of the 8 Divisions and Operational Standing Committees:

I	PHYSICAL AND BIOPHYSICAL CHEMISTRY DIVISION	4
II	INORGANIC CHEMISTRY DIVISION	6
III	ORGANIC AND BIOMOLECULAR CHEMISTRY DIVISION	8
IV	POLYMER DIVISION	10
V	ANALYTICAL CHEMISTRY DIVISION	14
VI	CHEMISTRY AND ENVIRONMENTAL HEALTH DIVISION	16
VII	CHEMISTRY AND HUMAN HEALTH DIVISION	20
VIII	CHEMICAL NOMENCLATURE AND STRUCTURE REPRESENTATION DIVISION	23
	CHEMRAWN COMMITTEE	24
	COMMITTEE ON CHEMISTRY EDUCATION	25
	COMMITTEE ON CHEMISTRY AND INDUSTRY	27

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

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2006-2007 Membership

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I PHYSICAL AND BIOPHYSICAL CHEMISTRY DIVISION

Title: Liquid intrusion and alternative methods for the characterization of macroporous solids

Number: 2006-021-2-100

Objective:

To analyse the various liquid intrusion techniques available today to assess the pore-size of materials (with special attention to the pores above 50 nm width), together with other alternatives, in order to provide (i) a critical and comparative appraisal and (ii) an appreciation about the ways which should be favoured and developed to solve the issue described hereafter.

Description:

The principal method used today to analyse the macropore range (i.e. above 50 nm width) is indeed the mercury intrusion method, where the handling of mercury, the inevitable spills and the need to recycle the mercury polluted by the sample do raise a health and environmental problem. Both the improvement of the mercury intrusion approach and its replacement by other methods raise technical issues.

The aim of this project is to provide a first step towards satisfactory answers, by listing, examining and evaluating all trials already made in the field. These include the intrusion of safer liquids (other molten metals, water, organics...) and also the extension of the analysis of capillary condensation data up to the macropore range where, for technical reasons it was, until recently, considered inapplicable. In any case, the need of improvement and/or of alternative methods is urgent. By clarifying the situation, this project should help selecting and developing the most promising approaches. The issue concerns most scientists and industrialists working with porous materials (catalysts, pharmaceuticals, building materials, stones of ancient monuments to be restored or protected, adsorbents for chromatography, liquid purification or gas separation ...) and it needs an evaluation accepted and used by all persons involved all over the world.

Title: Recommendations for nomenclature and databases for biochemical thermodynamics

Number: 2006-023-3-100

Objective:

To revise IUPAC Recommendations for Nomenclature and Tables in Biochemical Thermodynamics 1994*. Update these recommendations and increase their usefulness by providing more about computers and databases that have been developed since 1994. Describe the connection between the thermodynamics of enzyme-catalyzed reactions and the kinetics of enzyme-catalyzed reactions that is provided by Haldane relations.

Description:

The concept of a transformed Gibbs energy G' that provides the criterion for spontaneous change and equilibrium at a specified pH was developed in 1992 (Alberty, *Biophys.* 42, 117-131 and 43, 239-254), and so it is quite remarkable that the IUPAC Recommendations were published in *Pure Appl. Chem.* 66, 1641-1666 (1994). They were reprinted in *Eur. J. Biochem.* 240, 1-14 (1996). A lot has happened in the field since 1994, especially the use of computers and the publication of articles and putting databases on the web.

Title: Wet surface vibrational spectroscopy experiments

Number: 2006-050-3-100

Objective:

To promote the application of wet surface vibrational spectroscopies (ATRIRS, SEIRAS, SERS) to problems in interfacial chemistry by selecting, testing, and disseminating to universities a collection of experiments suitable for undergraduate teaching laboratories and able to be performed with inexpensive equipment.

Description:

Undergraduate experiments in interfacial chemistry are presently dominated by measurements of macroscopic quantities such as surface tension and amount adsorbed when increasingly spectroscopic and microscopic data are presented in the corresponding lectures. IUPAC can take a lead in encouraging a more modern molecular approach to interfacial physical chemistry through international collaboration of leading expertise to compile and test a series of appealing experiments which can be readily carried out in undergraduate laboratories with relatively inexpensive equipment.

This project brings together leading physical chemists in the fields of attenuated total reflection infrared spectroscopy (ATRIRS), surface enhanced infrared spectroscopy (SEIRAS), and surface enhanced Raman spectroscopy (SERS), to select practicable experiments which can be carried out in teaching situations throughout the world. Both SERS and SEIRAS employ finely divided metal surfaces while the ATRIRS particle film approach can be applied to any solid. All of the chosen surface spectroscopies are applicable to solid/aqueous interfaces that are of considerable interest in studies of natural and technological systems. Examples include the study of adsorbed electrode intermediates and the investigation of adsorbed collectors used as flotation agents for mineral extraction.

Title: Guidelines for modulated-temperature differential scanning calorimetry (MTDSC)

Number: 2007-002-1-100

Objective:

Recommendations on methods of operation and guidelines on standardized ways of selecting the different parameters of modulation in the use of modulated-temperature differential scanning calorimeters; including the multi frequency temperature pulses technique.

Description:

Modulated-temperature differential scanning thermal analysis techniques are widely used in many fields. Particularly in pharmaceutical, food and polymer studies where first order transitions, glass transitions and polymorphism are key issues. All sorts of relaxation phenomena as well as coupled thermal and kinetic contributions can advantageously be investigated and selectively studied with such techniques. Produced commercially by a number of companies, sophisticated instruments are used by individuals without the required level of knowledge and expertise necessary to extract the correct information from well established procedures. The project should bring a consistent set of recommendations to be internationally approved for the use of modulated-temperature calorimetry.

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 Isotope 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.

Title: Recommendations for isotope data in geosciences

Number: 2006-016-1-200

Objective:

Update and harmonize recommendations on half-lives and isotopic compositions.

Description:

The inter-Union project with the International Union of Geological Sciences (IUGS) strives to provide an authoritative recommendation based on a critical re-evaluation of data on half-lives and decay schemes of long-lived radioactive nuclides used by the geological and planetary science communities. A specific goal of the project is to reconcile current inconsistencies between values used in geological and planetary sciences on the one hand, and those used in the nuclear physics and chemistry communities on the other.

The project will draw on complementary expertise present in IUGS and IUPAC. Previous work by IUGS (Working Group "Decay constants in geochronology") and IUPAC (Commissions II.1 "Isotopic abundance" and V.7 "Radiochemistry and Nuclear Techniques") will be included, harmonized, and updated. IUGS-IUPAC interaction will be tightened.

Title: Assessment of fundamental understanding of isotopic abundances and atomic weights of the chemical elements

Number: 2006-025-1-200

Objective:

Review fundamental issues and concerns that have been raised by members of the Commission on Isotopic Abundances and Atomic Weights (CIAAW). Discuss the issues and present the recommendations to CIAAW on the solution to the problems that will help to provide a future direction for the work of CIAAW on isotopic abundances and atomic weights of the chemical elements.

Description:

During the 20th century, the CIAAW evaluated the atomic weights, isotopic abundances and their variations and made recommendations to a general chemical community. This project will evaluate a number of questions that have arisen.

Title: Priority claims for the discovery of elements with atomic number greater than 111

Number: 2006-046-1-200

Objective: The IUPAC/IUPAP Joint Working Party is charged with examining the priority claims for the discovery of elements with atomic number greater than 111.

Description:

The procedures to be followed in assigning priorities and the subsequent naming process will be the same as those used for the recently named elements darmstadtium and roentgenium with atomic numbers 110 and 111, respectively.

In brief, the submissions received will be examined by a IUPAC/IUPAP Joint Working Party of experts the membership of which is approved by the Presidents of IUPAC and of the International Union of Pure and Applied Physics (IUPAP). The JWP will issue its findings in the form of a report and the successful claimants will then be invited to propose a name for any element for the discovery of which they have been given priority.

III ORGANIC AND BIOMOLECULAR CHEMISTRY DIVISION

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.

IV POLYMER DIVISION

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, in (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: *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.

Number: 2005-043-2-400

Title: Terminology for self-assembly and aggregation of polymers

Objective:

With nanoscience and nanotechnology underpinning and lending focus to many of the developments in modern functional materials, aggregation and self-assembly in polymers is of growing importance. This project is aimed at proposing a list of terms and definitions to be accepted and respected by chemists and others working as materials scientists within academia and industry.

Description:

The physical and chemical properties of aggregated polymers and polymer molecules that spontaneously assemble into ordered structures are more often determined by these macroscopic structures than by the individual polymer molecules from which they are built. Typically, molecules that have assembled into micelles might act as hosts to smaller molecules that are held in place by solvation effects at the micellar core, whilst those that have assembled into vesicles (walled, cell-like structures) can physically encapsulate guest species. Neither of these situations can be attributed to the polymer chain structures except insofar as they might determine the nature of the aggregation or assembly. Self-assembly in liquid crystalline polymers and block copolymers is equally complex and important. An extended terminology is required to describe these macroscopic systems, as already evidenced by the impossibility of writing these introductory sentences without resorting to the use of two such terms. Some terms will be of relatively recent introduction. Other, older terms will be in common usage by physical chemists and some by materials scientists, and perhaps more familiar to such specialists than to polymer scientists. Many of the terms might also be totally unfamiliar to scientists whose background is not rooted in chemistry or material sciences. It is therefore necessary to identify terms specific to aggregation and self-assembly of polymers, and to harmonize and enforce their use by the people active in the field.

Title: Recommendations on the abbreviated terms of polymers

Number: 2006-004-1-400

Objective:

To provide recommendations or guidelines regarding the use of abbreviations and abbreviated terms for the names of polymers and polymeric materials.

Description:

Abbreviated terms for polymers are very important to avoid repetition of lengthy polymer names, not only for the authors of articles, but also for the readers and the editors of journals. Industrial people use a well-established ISO list of abbreviated terms, but it contains only about a hundred items (116 in ISO 1043-1, the third edition in 2001), selected on the basis of the scale of production mainly. On the other hand, the academic journals in the polymer field treat several hundreds of polymers annually, including new polymers, some with complicated structures. Thus, it is almost impossible to derive a systematic and unique abbreviated term from a polymer name while maintaining one-to-one correspondence between the two (as observed in the ISO list) in order to make the abbreviation self-standing.

In the present project, which aims at the use of abbreviated terms in academic journals, it will be suggested to authors that in the first instance they use their own abbreviated terms and define them when they appear for the first time in their articles.

Title: Terminology for conducting, electroactive and field-responsive polymers

Number: 2006-028-1-400

Objective:

With the awarding of the 2000 Nobel Prize in chemistry for work on semiconducting polymers and the recent advances in the realm of organic electronics for displays, solar cells and other applications, the entire field of electroactive polymers is of growing importance. This project is aimed at proposing a list of terms and definitions to be accepted and respected by chemists and others working as materials scientists within academia and industry.

Description:

The physical and chemical properties of electroactive and field responsive polymers and polymer molecules are being increasingly investigated for scientific study, technology development and commercialization by diverse scientific communities. In view of the rapid development and steadily increasing number of applications of polymers as active functional materials in a construction of integrated circuits and electronic and optoelectronic devices such as diodes, light-emitting diodes, switches, photovoltaic cells, analytical sensors, storage batteries, etc., a need for effective and clear communication among chemistry, polymer physics and materials communities is of increasing importance. Chemical acronyms for the polymers being used, terms for their properties and tools for characterization are diverse and used with inconsistency. It is the aim of this project to provide chemists, physicists and materials scientists with a useful glossary that can facilitate this interdisciplinary communication and help to understand the rationale lying behind the terms and definitions originating from various fields of science and technology.

Title: Glossary of thermal and thermomechanical properties of polymers

Number: 2006-041-1-400

Objective:

To identify the most important terms concerning thermal effects properties of relevance for polymers and to give recommendations of unequivocal definitions of these terms.

Description:

In literature and practical use it is obvious that there is a significant lack of a collection and unequivocal definitions of such terms in the field of polymer science. Some terms are even used in entirely different contexts or with different meanings to those intended. This project shall give definitions of terms related to thermal and thermomechanical properties of polymeric bulk materials.

The terms which have been selected for the preliminary list are those met in the conventional thermal (calorimetric) and thermomechanical (static or dynamic) characterization of polymeric materials. The project will be based to some extent on earlier reports related to nomenclature and terminology of thermal analysis published by the International Confederation for Thermal Analysis and Calorimetry.

Title: International tutorial in polymer characterization - 15th POLYCHAR short course

Number: 2006-042-1-400

Objective:

International, interactive tutorial for students from developing countries in modern techniques of polymer characterization.

Description:

This Educational Project in Polymer Science is in particular suited for students from developing and "third world" countries to up-date their knowledge and skills in polymer characterization by interactive oral courses presented (1 day) by distinguished scientists. Since this annual course is moving to a new place in each year this tutorial is not restricted to one country or just one geographical area.

Since the tutorial takes place in the days before an important IUPAC-sponsored Conference (World Forum on Advanced Materials-POLYCHAR 15), the tutorial has also proven to be a good opportunity to prepare the students for their participation in the following conference, where many of them is given the chance to present their scientific work (IUPAC Student Poster Award). With the tutorial being an independent event, the chronological proximity and order have been proven to be of great advantage for the success of the Tutorial. With topics in different fields of polymer characterization, the focus is shifted each year slightly. The tutorial takes advantage of the fact that the course lecturers are participants of the following POLYCHAR World Forum and are available for the students for a whole week.

V ANALYTICAL CHEMISTRY DIVISION

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.

Title: *Trace elements analysis: role of grain size distribution in solid reference materials*

Number: 2005-035-2-500

Objective:

Generally, solid reference materials (RM) of the same matrix from different producers can present different particles size distributions and this could affect the homogeneity of the material and the minimum representative sample required for trace elements analysis. The final aim of the proposed project is to develop a guide to be used by reference materials producers and by the analytical community to select the most appropriate particle size distribution of a considered reference material to fit the analytical needs.

Description:

The existing guidelines for Reference Material (RM) producers do not report any indication for the selection of the most appropriate particle size distribution during the production of these materials. In the case of solid RM, particle size distribution plays a vital role on the homogeneity of the material and on the minimum representative sample required for trace element analysis. Generally, RMs of the same matrix but from different producers show different particle size distributions. For soil and sediment RMs, particle size distribution can vary from <120 μm to <20 μm . From one side,

finer particles can increase the homogeneity of the material (between and within bottle homogeneity) but from the other side, the RM obtained can be different, in terms of grain size, by the real samples routinely analyzed in the laboratories (e.g. contaminated soil analysis commonly is carried out on samples particle size < 2 mm. The project will bring together the results of experimental work that is being funded by different participants.

Title: Determination of selenomethionine in selenized yeast supplements

Number: 2005-041-2-500

Objective:

To provide the analytical, nutrition- and health- science community with clear guidelines on the determination of selenomethionine (the most abundant Se species) in yeast and yeast-based products.

Description:

Consumption of Se enriched food and feed supplements has increased dramatically as a result of the numerous health benefits reported, including protection of cells against the effects of free radicals, the normal functioning of the immune system and thyroid gland as well as protection against various forms of cancers. Yeast based supplements have emerged as an acknowledged means of alleviating selenium nutrient deficiencies, but it is evident from earlier studies that they are inconsistent in their makeup relative to label indications. Production of yeast-supplements, both animal and human, is a rapidly growing industry. IUPAC had already addressed the methodology of selenium speciation in biological materials in a report (*Pure Appl. Chem.*, Vol. 72, No. 3, pp. 447-461, 2000). The report had a decent impact on the research community having obtained over 60 citations (Source: ISI).

The purpose of this project is to examine critically the existing methodology published in peer reviewed journals, and issue recommendations on the determination of this extremely important nutritional supplement. The task group is composed of scientists having a considerable experience in the field and a record of collaborations with different industrial companies interested in this issue. The work is going to be carried out in close collaboration with the potential stakeholders: the four major companies on the market: Alltech, Lallemand, Lesaffre and PharmaNord.

Title: Adjustment, estimation and uses of equilibrium reaction constants in aqueous solution

Number: 2006-010-1-500

Objective:

To prepare (and improve) programs to treat quantitatively the dependence of activity coefficients (and hence equilibrium constants) on ionic strength and on the presence of dissolved gases. To explore and test computer-based ways of displaying these effects graphically and the influence they will have on species distribution curves.

Description:

A previous IUPAC project has produced a suite of programs to study quantitatively the influence of ionic strength changes on equilibrium constants, with particular emphasis on using Specific Interaction Theory (SIT). In this project we propose to extend this work in the following ways:

- To apply Pitzer parameters in a more general way to equilibria of environmental and industrial importance. Particular importance will be given to sea water and mixed fluids.
- To extend and improve a database of published SIT and Pitzer-related parameters. This database may be accessed by all relevant programs in the suite and may be edited by the user.
- Currently the package allows calculations on the effects of dissolved O₂. This will be extended to cover other environmentally important gases (e.g. air, H₂, N₂, rare gases, N₂O, CH₄, and other paraffins)
- To explore and test ways of displaying graphically the relationship between ionic strength and temperature with activity coefficients, lg K^o and lg K;
- To explore and test ways of displaying graphically the effects of errors on the relationships studied above.
- To calculate, and demonstrate graphically, the effect of errors on species distribution curves.
- To prepare a database of reliable literature values of the dependence of stability constants on temperature.

Title: Spectrochemical Analysis - Conversion of Orange Book Chapter 10 to Glossary Format

Number: 2006-022-1-500

Objective:

Chapter 10 of the Orange Book is a narrative style compilation of many Spectrochemical Analysis Committee terminology documents, all also written in narrative style. These definitions need to be converted to glossary style. Many terms in Chapter 10 are also included in the Gold Book and in Chapter 11 of the Orange Book in glossary format. These terms need to be rectified with the narrative style usage in Chapter 10 to achieve a complete glossary format spectrochemical analysis terminology appropriate for XML conversion.

Description:

There is an extensive list of spectrochemical analysis terms in the latest print version and the present on-line version of the Orange Book (IUPAC Compendium of Analytical Terminology). Most of these terms are contained in Chapter 10, which is in narrative format for historical reasons. The early Commission V.4 (Spectrochemical Analysis) documents adopted narrative style rather than glossary format to enable simultaneous definitions and usages to be achieved.

Chapter 11 contains a number of the same terms, but in glossary format. The Gold Book also contains a number of the same terms, in glossary format.

The goal of this project is to rectify the definitions of terms presented in both OB chapters 10 and 11, as well as those already in the Gold Book, and convert terms unique to OB chapter 10 from narrative to glossary format.

New terminology entries are not a goal of this project. Updated definitions of terms already included will be.

Title: Metal-focussed -omics: guidelines for terminology and critical evaluation of analytical approaches

Number: 2006-037-1-500

Objective:

The objectives of the project are (1) the definition of terms related to analytical chemistry of interactions of metals with biomolecules in environmental, nutrition and life-sciences, such as e.g. metallome, metalloproteome, and the corresponding -omics, (2) a critical evaluation of analytical techniques suitable for metallomics, and validity and pertinence of data obtained.

Description:

Bioinorganic analytical chemistry is a rapidly developing discipline at the interface of trace element analysis and analytical biochemistry which targets the detection, quantitation, identification and characterization of complexes of metals (metalloids) with molecules of natural origin (biomolecules) by hyphenated (coupled) techniques. The advances of trace element analysis in life sciences resulted in proliferation of new terms related to the description of metal-interactions with biomolecules. Examples of these terms include: metallome, ionome, metalloproteome, metallogenome, metallometabolome, heteroatom-tagged proteome, single element proteomes (ex. selenoproteome) and the corresponding -omics. The terms are being coined by various disciplines and the lack of communication among them results in the growing confusion. All terms are very recent and have not been considered in the Guidelines for Terms Related to Chemical Speciation Analysis.

The project targets the speciation analysis community organised around the European Virtual Institute of Speciation Analysis, structural genomic consortia, clinical biochemistry, medicine and health sciences communities (characterization of metal-related diseases and related areas, heteroatom-containing species as new clinical biomarkers), nutrition and metabolic sciences (molecular targets of metal binding for essential nutrients and toxic metals), and environmental toxicology (toxic metals in life-sciences and their environmental effects). It should be of interest to regulatory bodies answering the question on what valid information can be obtained in quantitative and routine way in the metal-related -omics areas.

VI CHEMISTRY AND THE ENVIRONMENT DIVISION

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.

Title: *Evaluation of food and feed safety implications of (altered) residues of pesticides applied on transgenic (GM) crops*

Number: 2006-015-3-600

Objective:

The primary objectives of this project are:

1. Update of past and future trends in GM Crops Production
2. Definition/determination of the characteristics of specific agrochemical residues
3. Evaluation of the health impact of (altered) agrochemical residues in edible crops, and
4. Assessment of regulatory measures and food and feed safety requirements

Description:

The world wide area cultivated with GM crops has increased continuously over the last ten years, amounting to 90 million hectares in 2005, which, by comparison, equal the total areas of California, Nevada, and Utah. Most of these crops are grown in the United States, Argentina, Brazil, Canada, China, Australia, South Africa, and India. These crops usually have been modified with either or both of two traits, *i.e.* herbicide resistance and insect resistance. While these traits are of agronomic and environmental importance, some experimental crops also possess traits geared towards consumer needs (*e.g.* high protein contents), which may in some cases also be combined with other agronomic traits. Moreover, crops with agronomic traits may find new applications, such as in the control of parasitic weeds that are sensitive towards herbicides applied to herbicide-resistant crops or insect-resistant crops with lowered mycotoxin contaminations caused by less insect infestation and less concomitant mould infection.

The project will provide a greater attention to these global trends and especially on the MRLs to be set for residues of the pertinent pesticides applied on GM crops and commodities destined for the international trade. Accordingly, the project is to update the information gathered during the previous project, and to expand on the levels of residues of agrochemicals in GM crops, as well as the estimated exposure of humans and animals to these residues, and the MRLs to be set for the pertinent pesticides in these crops, touching on the issues of socio-economic importance, including international harmonization of regulatory thresholds and consumer concerns. In a broader sense, these data will be considered with regard to potential risks and benefits of GM crops compared to conventional crops.

Title: *Crop Protection Chemistry in Asia: Harmonized Approaches for Safety Evaluation, Regulation, and Protection of Trade*

Number: 2006-017-2-600

Objective:

Crop protection chemistry is at a critical juncture in Asia. Large populations are supported by intensive agriculture, and there is a resulting need for reliance on agrochemicals and biotechnology for crop protection purposes. In addition to local consumption, export of agricultural products is also a major source of income for some countries within the region, with Japan and the U.S. being two of the most important export destinations. The scientific study, evaluation, and regulation of crop protection chemistry are rapidly developing in Asia, particularly with respect to product quality, risk assessment, and food residues. There is a growing desire on the part of scientists, regulators, and industry leaders in the region to consider and adopt international approaches to meet Asian crop protection chemistry needs. Some of the impetus driving this interest is the increased participation in world trade that has occurred during the past decade, which has brought new challenges to the agricultural exporting countries in the region. In the development and adoption of new approaches for crop protection chemistry, there is a need to consider lessons learned in other regions and to adapt

for local use the various harmonized approaches which are now available. These include international recommendations and standards from such international bodies as OECD, FAO, and Codex as well as the recommendations of recently completed and ongoing IUPAC projects.

The primary objectives of this project are to:

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

Description:

The first phase of the project will be to evaluate the current situation and state-of-the art with respect to Objective 1. An interdisciplinary working group, comprising experts from academia, government, and industry, will be created to facilitate this effort. Major emphasis will be placed on issues related to product quality, environmental and human safety assessment, and residues in food.

The second phase of the project will be a workshop focused on Objective 2 which will be held in China during October 2007 to bring together the diverse regional stakeholders in crop protection chemistry from the research and regulatory communities. Co-sponsorship for this activity has already been arranged with China Agricultural University, Beijing Pesticide Society, and the Agrochemicals Division of the American Chemical Society and additional sponsorships will be sought from the China Ministry of Agriculture, CropLife China, and CropLife Asia. The workshop will include presentations, posters, panel discussions, and hands-on demonstrations.

The third phase of the project will be compilation of a set of recommendations related to Objective 3 and will occur during 2008. This will be accomplished via the project working group, augmented with additional experts identified during the workshop. Conclusions and recommendations will be published in both hard copy and electronic format (web-based). It is anticipated that one or more additional IUPAC project proposals may emerge.

Title: Extraction and fractionation methods for exposure assessment related to trace metals, metalloids and hazardous organic compounds in terrestrial environments

Number: 2006-039-2-600

Objective:

- Critical evaluation of traditional single and sequential extraction schemes as well as novel flow-through fractionation methods for the assessment of environmental exposure related to trace elements (heavy metals, metalloids) and persistent organic pollutants in soils, sediments, compost, and sewage sludge
- Establishment of a series of recommendations for accurate and comprehensive studies on the current or potential mobility/ bioavailability of hazardous compounds in solid phase-soil solution systems

Description:

Accumulation of heavy metals, arsenic, and organic pollutants (e.g. polycyclic aromatic hydrocarbons, polyhalogenated species and pharmaceutical residues) in different compartments of the biosphere, and their possible mobilization under environmentally changing conditions cause adverse health effects. Correct exposure analysis concerned with soils, sediments, and sewage sludges as sinks for trace elements (TE) and persistent organic pollutants is extremely important for environmental management and risk assessment.

The aim of this proposal is to review at a fundamental level the progress made by different authors and institutions (e.g. in the framework of EC Standards, Measurement and Testing Programme) and then provide a series of recommendations on the use of batchwise and flow-through leaching/extraction methods for appropriate exposure analysis of TE and organic pollutants in contaminated soils, sediments, and sludges of different type and origin. It is of particular importance to demonstrate that similar methodologies have a great potential for the exposure assessment of both organic and inorganic contaminants.

Title: Environmental Risk Assessments for the Registration of Pesticides used in Rice Paddy Fields

Number: 2006-044-2-600

Objective:

1. To provide a state-of-the-art review of environmental risk assessment approaches for pesticide use in paddy rice agriculture.
2. To exchange views from different areas of the world on this topic so as to identify research needs and recommend a set of best practices for future assessments.

Description:

Background - In China and many countries in the South East Asian area rice is an important crop. Although the management of growing rice may be different in different parts of the world also many similarities may be accounted for, like partly inundation of the rice crop (paddy fields), application of plant protection products (PPP) and the registration process to allow the application of PPP in the rice growing countries. Registration of PPPs applied in rice may follow a decision of the government and may be based on a risk assessment process. Risk assessment may be involved for several aspects like humans, the environment, the applicators or the workers. The proposal in this project

will focus on the environmental risk assessment for pesticides applied in paddy rice fields. Sometimes the environmental risk assessment process is absent and in other countries the risk assessment may be carried out in different ways. Knowledge of the risk assessment process as carried out in other countries may stimulate countries to actively be involved in the registration of pesticides.

In bringing across differences in rice management systems as well as differences in risk assessment procedures all parties may be able to learn from each other and apply newly developed methods in the specific procedures for registration of pesticides applied in paddy rice fields in their own countries.

Title: Combination of chemical analytical measurements and remote sensing techniques for coastal water monitoring. The cases of Eastern Mediterranean and Black Sea

Number: 2006-049-2-600

Objective:

The objectives of this project are, to record the state of the art in remote sensing techniques and methods used for marine environment monitoring, to review remote sensing applications in the Eastern Mediterranean and Black Sea region and to assess the potential combination of remote sensing data with in situ and laboratory monitoring.

Description:

Remote sensing techniques have been utilised since 1961 with various types of sensors and applications in environmental and military purposes. Soon enough, the methodologies began to include the monitoring of marine biogeochemical parameters. Remotely sensed airborne or satellite data can provide the necessary spatial perspective to collect information about the sea surface characteristics and water quality on a regional scale. Water quality parameters of interest nowadays include ocean colour and chlorophyll concentration, detection of algal blooms and oil spills and estimation of total suspended solids.

VII CHEMISTRY AND HUMAN HEALTH DIVISION

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: *Glossary of terms used in ecotoxicology*

Number: 2005-047-1-700

Objective:

To facilitate the application of chemistry in ecotoxicology, there is a need for a glossary addressing the terms in ecotoxicology essential for communication between the disciplines. This project will create such a glossary, reflecting IUPAC's concern about the impact of chemicals on health and the environment. It will also complement the previous projects which resulted in glossaries in toxicology and toxicokinetics published in *Pure and Applied Chemistry* which have received wide acceptance and use.

Description:

This glossary will give definitions of terms used in ecotoxicology. It will include terms related to chemical speciation in the environment, sampling, monitoring and environmental analysis, adverse ecological effects of chemicals, ecological biomarkers, and environmental distribution of chemicals.

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.

Title: **Mapping of IFCC-IUPAC laboratory coding system to SNOMED CT (SNOMED CT - Systematized Nomenclature of Medicine Clinical Terms)**

Number: 2006-008-1-700

Objective:

Systematically relating all coded 'properties' in the IFCC-IUPAC coding system for laboratory information to relevant concepts in SNOMED CT clinical terminology.

Description:

In many countries a translation and adaptation of the SNOMED CT clinical terminology is considered, planned, or initiated, for use in national health IT systems and communications. The SNOMED CT core terminology does not support all needs for laboratory information in health care; specific laboratory terminologies exist to serve that purpose. A mapping has been established between concepts in SNOMED CT and the American LOINC laboratory coding system, enabling the laboratory terms to be used in a SNOMED CT context.

The project entails

- establishing a database as a tool for mapping and reporting
- determining rules for systematic mapping
- performing the actual mapping between IFCC-IUPAC properties and SNOMED CT elements - using rule based matching where possible
- identifying concepts used in IFCC-IUPAC terminology, but not yet included in SNOMED CT.
- In order to ensure a close and specific mapping, cooperation with SNOMED International should be established, enabling needed concepts to be established in the SNOMED CT terminology in a planned manner.

Title: **Securing and structural updating of information in the NPU coding system and its environment**

Number: 2006-012-1-700

Objective:

To extract, analyse and preserve less accessible information produced during the first decade of development of the IFCC-IUPAC coding system, and specify the needs for information management in the future. To produce a manual describing how the basic principles of the coding system are implemented in actual coding practise.

Description:

Work under C-NPU defining and coding properties in laboratory science has been going on since the mid-nineties. The database structure designed in the nineties was intended mainly to support the actual coding process (assembly of elements into coded properties), and the production of text files with specific fonts and formatting, intended for paper based publication.

Terminological information about the elements, their sources and their uses in coded properties has been stored, but frequently in an implicit manner, as part of other information elements, rather than explicitly in the database. During almost a decade of coding work, principles and rules for the coding practise have crystallised, but have not been systematically filed. They may be extracted from stored material, like advice to users at laboratories, newsletters retiring 'malformed' codes etc., or they may be present as 'silent information' in the coding environment - i.e. in the minds of the people working with the system.

A review of the information present in the system and its environment is suggested, aiming to analyse and extract implicitly stored data and register 'silent knowledge'. The objective is to preserve the information, to render it accessible for future developers and users, and to specify the needs for structured information management in the future.

Title: An introduction to computer assisted drug design

Number: 2007-006-1-700

Objective:

A book that will provide a broad overview of the useful computational methods in drug design. It is expected that the book will be used for self-study as well as a guide in advanced biochemistry or medicinal chemistry courses.

Description:

The proposed book will be organized along the steps of drug discovery. That is, the first chapters will address the design of screening libraries, the next will address following up high throughput screening hits, and the final chapters will address optimizing a series. Topics will be introduced when first needed, but referenced and expanded as needed for later discussions.

The level of detail in the main body of the book will be conceptual; however, for the more eager reader, additional details will be provided in set-aside boxes. The discussion will not include the details of all the computer programs available for a particular purpose and especially it will not include discussions of how to run the programs. In a similar vein, the citations will generally be to review articles. Every topic will be illustrated with examples.

VIII CHEMICAL NOMENCLATURE AND STRUCTURE REPRESENTATION DIVISION

Title: Nomenclature of phosphorus-containing compounds of biochemical importance

Number: 2006-019-1-800

Objective:

To update and clarify recommendations for naming phosphorus-containing compounds of biochemical importance.

Description:

Existing recommendations have not been revised since 1976. They are obscurely written. Although their tables employ a useful symbolism, the symbols are not defined in the document. Knowledge of many classes of phosphorus-containing compounds, e.g. inositol phosphates, has developed out of recognition since 1976. We believe that it would be helpful to redraft the recommendations (1) more clearly, (2) defining the symbols used, and (3) using as examples compounds that feature widely in biochemistry.

Title: Revision of "Principles of Chemical Nomenclature"

Number: 2006-029-1-800

Objective:

To produce a new version of the original book "Principles of Chemical Nomenclature - A Guide to IUPAC Recommendations", in the light of nomenclature developments since its publication in 1998.

Description:

The IUPAC colour books are currently in a state of revision, especially the inorganic Red Book (published 2005), the organic Blue Book (expected 2007; project 2001-043-1-800), and the macromolecular Purple Book (project 2002-048-1-400). The original book was aimed at pre-University and first-year University students and their teachers, and the new version will have a similar audience. However, it is intended to widen the scope a little, to include more biochemical nomenclature, more organometallic nomenclature, and some treatment of Preferred IUPAC Names (PINs; see both projects 2001-043-1-800 and 2006-038-1-800) and the IUPAC International Chemical Identifier (InChI).

Much of the material and the format of the original version will be retained; this is a revision, not a rewriting.

Title: Preferred IUPAC Names (PINs) for Inorganic Compounds

Number: 2006-038-1-800

Objective:

To develop rules for choosing the Preferred IUPAC Names (PIN) for inorganic compounds, including coordination compounds, organometallic compounds, and compounds that either do not contain carbon, or do contain at least one element from groups 1-12. These rules should result in names that are suitable for use in legal and regulatory documentation.

Description:

The PIN concept has been developed in response to the difficulties that users of nomenclature strike when there is more than one systematic way of naming a compound. This issue is particularly problematic in legal and regulatory applications, where confusion over names could have major health and safety, legal, or financial implications. Rules for choosing PINs for organic molecules have been developed as a major goal of the project for the revision of the Blue Book. That project is nearing completion, and the resulting manuscript is in the IUPAC review process. It is obvious that PINs must also be available for inorganic compounds, but the methods that are typically used to name such compounds are different from those used for organic compounds, and consequently new rules will have to be developed.

A number of critical issues will have to be addressed; these include:

- choice of central atom(s), particularly in polynuclear species;
- clear definition of grammatical rules for the placement of k/h symbols in complicated ligand names;
- selection of retained names, particularly for oxo-acids.

Once these issues have been addressed, the proposals that are developed will be submitted to the IUPAC review process. Further documents will then be prepared that provide detailed guidance for selecting PINs for particular classes of compounds (coordination compounds, organometallic compounds, main group compounds).

CHEMRAWN

Title: CHEMRAWN XVII - Greenhouse Gases: Mitigation and Utilization

Number: 2006-031-1-021

Objective:

Governments struggle with the greenhouse gas (GHG) problem trying to balance this long-term imperative with shorter term needs of the economy and of the emerging nations. Industries seek ways to reduce their emissions but are constrained by the lack of practical technology and of clear government direction. The scientific community is making GHG problem a major area of study.

This conference will bring all three of these groups together, to seek a broad mutual understanding of the current situation and clarity for future directions.

Description:

CHEMRAWN (Chemical Research Applied to World Needs) and the International Conferences on Carbon Dioxide Utilization (ICCDU) will hold a combined conference in Kingston on science and policy related to mitigation and utilization of CO₂ and other greenhouse gases.

The meeting is being held 6 months before the Kyoto-protocol commitment period begins. Signatory governments are committed to meeting their targets within the 2008-2012 time period.

COMMITTEE ON CHEMISTRY EDUCATION (CCE)

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: *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: *The Social Responsibility of Chemists: Responsible Stewardship*

Number: 2006-043-3-050

Objective:

This project is aimed to disseminate new educational means in the field of the chemistry education for sustainable development and education for responsible stewardship, and to promote all aspects of chemistry, not just among the members of the profession, but increasingly to the worldwide community. Chemical education can be effectively used for this purpose because chemistry as a fundamental science and as a scientific basis for a variety of technologies in different branches of industry is deeply involved in the progress of modern civilization.

Description:

An earlier project dealt mainly with the problem of multiple use of chemicals. The disseminated materials included the outlines of two lectures (chemicals with possibilities of multiple use and the OPCW Convention on Chemical Weapons; history of development of codes of conducts for chemists). The audience of the final workshop consisted of chemistry educators and graduate students. The survey made showed the great interest of the audience. The materials are now available at the Green Chemistry Clearing House web-site (in Russian) supported by the Mendeleev University of Chemical Technology of Russia (MUCTR).

This project is aimed at the wider community (including the leading researchers, people from chemical industry and decision makers). As the official environmental monitoring data show, the economic and industrial recovery of Russia and former Soviet republics is resulting now in the deterioration of the quality of the environment, due to old technologies used and little attention paid by the industry and policy decision makers to the rational use of energy and natural resources. The other emerging problem is the danger of chemical and biochemical terrorism. Recently in Russia and other countries of CIS, the cases of explosions (in which students of chemistry departments had been involved)

have been investigated. Urgent measures are to be taken by the chemistry community (scientists, educators and the practitioners).

Title: International Year of Chemistry - Initial strategy planning

Number: 2007-011-1-050

Objective:

To develop for IUPAC a plan to secure the designation by UNESCO of an International Year of Chemistry.

Description:

A number of scientific disciplines have achieved significant benefits through securing designation by UNESCO of an International Year of X. The International Year of Physics was deemed to be a particular success by that community. IUPAC's Bureau has indicated that it would like IUPAC to secure designation by UNESCO of an International Year of Chemistry and has asked the Committee on Chemistry Education to take the lead. Information has been gathered about other International Years and exploratory talks have been held with UNESCO officials. Securing designation requires support from UNESCO centrally, the permanent representatives to UNESCO and national commissions.

COMMITTEE ON CHEMISTRY AND INDUSTRY

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.

Title: *Chemistry in a changing world - new perspectives concerning the IUPAC family*

Number: 2006-030-1-022

Objective:

To organize a Workshop on "Chemistry in a changing world - new perspectives concerning the IUPAC family" to foster communication and discussion about the emerging role of COCI/IUPAC. Thirty representatives of NAOs/chemical societies in the EU-countries (+ Norway and Switzerland) will be invited to participate and to develop a framework for future actions.

Description:

IUPAC occupies a unique and highly esteemed position at the center of the world of chemistry. In recent years an important globalization is taking place in science, industry and society.

This Workshop on "Chemistry in a changing world - new perspectives concerning the IUPAC family" is organized to increase the knowledge among the NAOs/chemicals societies in EU (+ Norway and Switzerland) about the role of COCI/IUPAC and about the changes now taking place. The interaction will provide rare opportunity to learn more about the situation in respective country as concerns chemistry, globalization and IUPAC. It will facilitate and improve dialogues with NAOs in the EU. Received comments will be very useful in generation of new projects and programs and in recruiting new CAs and NAOs. There are new major imperatives for IUPAC to engage more in the debate on chemical environment and the social issues raised.

Although the Workshop for practical reasons is organized within Europe, the subjects to be discussed are global. The Workshop would provide a template for similar workshops in other regions.

Title: *Responsible Application of Chemistry -- An Introduction to Responsible Care*

Number: 2006-047-1-022

Objective:

The objective of this COCI initiative is to create a framework project focusing on the responsible approaches to the application of Chemistry from research through industrial product to the ultimate use and disposal of the products. Responsible Care will be used as a basis for developing an understanding of what responsibilities chemists have in using, handling, and producing and how they should exercise these.

Description:

Responsible Care (RC) is an initiative of the Worldwide Chemical Industry. It started in Canada 20 years ago and is now accepted in 52 countries. The International Council of Chemical Associations, which represents the country associations, adopted the International Charter of Responsible Care in February 2006. This has been signed by 99 companies up to now.

The initiative is well known in the industry, however it is less known, nor understood within the academic and other technical communities. Also, it is not known in many countries where chemicals are not produced but used and in many cases misused.

The results of this initiative will increase the awareness and the application of the ethics of Responsible Care in the institutions related to chemistry around the world, ultimately resulting in safer and environmentally improved ways of developing, making and using chemical products.

Title: IUPAC-UNESCO-UNIDO Safety Training Program Workshop, Turin, Italy

Number: 2006-051-1-022

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 in terms of fellows' home country activities; to learn from invited speakers who are experts in health, safety, and environmental matters; 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 the Safety Training Program 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, safety and environment.

This Workshop is planned as part of activities at the 41st IUPAC Congress under the heading for either Session 1, "Chemistry Protecting the Environment;" Session 2, "Chemistry Protecting Human Health;" or Session 10, "Advances in Chemical Education."

The Workshop will include a panel discussion to identify ideas for improvement and expansion of the scope of the Safety Training Program. The Workshop is intended to span a full day at the Congress, with the presentations and panel discussion preceding the poster presentations for Workshop participants. Posters are also expected to be presented at one of the scheduled Congress poster sessions.