RECENT ACTIVITIES OF IUPAC DIVISIONS

September 2006

Produced by the Committee on Chemistry and Industry (COCI)
**Recent Books**

- Chemical Thermodynamics for Industry - Letcher, T.M. - Royal Society of Chemistry, 2004

**Glossaries**

- Glossary of terms in photocatalysis and radiation catalysis
- Glossary of terms used in photochemistry (3rd version)

**Projects Near Completion or in Press**

- Revision of "Quantities, Units and Symbols in Physical Chemistry” and the Appendices (3rd edition)
- Thermochemistry of chemical reactions: nomenclature, symbols and experimental methods for bond energies
- Spectroscopy under extreme conditions of temperature and pressure
- Critical compilation of vapour liquid critical properties
- XML-based IUPAC Standard for experimental, predicted, and critically evaluated thermodynamic property data storage and capture (ThermoML)
- Temperature scanning micro(calorimetry)

**Selected Current Projects**

- Evaluation kinetic data in atmospheric chemistry
- Standard potentials of radicals
- Electrochemical impedance spectroscopy – terminology, nomenclature and data exchange formats
- NMR chemical shifts: updated conventions*
- Ionic liquids database
- Selected free radicals and critical intermediates: thermodynamic properties from theory and experiment
- Thermodynamics and non-equilibrium criteria for development and application of supplemented phase diagrams
- Heat capacity of liquids: critical review and recommended values for liquids with data published between 2000 and 2004
- Categorizing hydrogen bonding and other intermolecular interactions
- A database of water transitions from experiment and theory
- Establishing recommended data on thermodynamic properties of hydration for selected organic solutes
- Developments and applications in solubility
- Solubility and thermodynamic properties related to environmental issues

**Recent and Forthcoming Conferences**

- Chemical Thermodynamics, 30 July - 4 August 2006, Boulder, CO, USA
- Solution Chemistry, 16-20 July 2007, Perth, Australia

**Awards**

- Rossini Lectureship Award and 4 IACT Doctorate Awards (sponsored by Elsevier) presented at the IUPAC International Conference on Chemical Thermodynamics, Boulder, CO, USA, August 2006
RECENT ACTIVITIES OF DIVISION II – INORGANIC CHEMISTRY

RECENT BOOKS

KEY RESPONSIBILITY
Division II is responsible for the Commission on Isotopic Abundances and Atomic Weights, which keeps data up to date and confirms the names of new elements.

PROJECTS NEAR COMPLETION OR IN PRESS
High-temperature mass spectrometry: Instrumental techniques, ionization cross-sections, pressure measurements, and thermodynamic data (IUPAC Technical Report), Pure Appl. Chem. 77(4), 683-737, 2005
Name and symbol of the element with atomic number 111 (IUPAC Recommendations 2004), Pure Appl. Chem. 76(12), 2101-2103 (2004)
Name and symbol of element of atomic number 110 (IUPAC Recommendations 2003), Pure Appl. Chem. 75(10), 1613-1615 (2003)

SELECTED CURRENT PROJECTS
Isotopic compositions of selected elements
Determination of atomic weights using new analytical techniques
Classification, terminology and nomenclature of borophosphates
Towards defining materials chemistry
Calibration of organic and inorganic oxygen-bearing isotopic reference materials
Evaluated published isotope ratio data (2005-2007)

RECENT AND FORTHCOMING CONFERENCES
Coordination Chemistry, 13-18 Aug 2006, Cape Town, South Africa
Organometallic Chemistry, 2-6 Aug 2007, Nara, Japan
Phosphorus Chemistry, 15-21 Apr 2007, Xiamen, China
Transactinide Elements, 23-28 Sep 2007, Davos, Switzerland
Within Division III there are sub-committees that focus on:
- Organic synthesis
- Biomolecular chemistry
- Green chemistry
- Photochemistry
- Structural and mechanistic chemistry
- Biotechnology.

**RECENT BOOKS**

- Green chemistry in Russia, Tundo, P. and Lunin, V.V., INCA, 2004 [ISBN 5-211-05001-0]

**PROJECTS NEAR COMPLETION OR IN PRESS**


**SELECTED CURRENT PROJECTS**

- Green chemistry in the Arab region
- Reference methods, standards and applications of photoluminescence
- "Global Climate Change" - Translation and dissemination of a monograph for secondary schools
- Development of methodologies and protocols for documentation, evaluation of safety and efficacy and standardization of herbal medicine
- Strategic Planning for a new East Asian Network for Organic Chemistry
- Chemistry for Biology - an inventory of interdivisional and interdisciplinary activities within IUPAC in the field of biological chemistry

**RECENT AND FORTHCOMING CONFERENCES**

- Chemical Biology, 9-13 Sep 2006, Antalya, Turkey
- Green Chemistry, 10-15 Sep 2006, Dresden, Germany
- Pesticide Chemistry, 6-11 Aug 2006, Kobe, Japan
- Novel Aromatic Compounds, 22-27 July 2007, Awaji City, Japan
- Organometallic Chemistry, 2-6 Aug 2007, Nara, Japan
- Biotechnology, Oct 2008, Dalian, China

**THE THIEME-IUPAC PRIZE IN SYNTHETIC ORGANIC CHEMISTRY**

The Thieme-IUPAC Prize is awarded every two years on the occasion of IUPAC’s International Conference on Organic Synthesis (ICOS) to a scientist under 40 years of age, whose research has had a major impact on the field of synthetic organic chemistry. The Prize is sponsored jointly by Georg Thieme Verlag, IUPAC, and the Editors of Synthesis, Synlett, Science of Synthesis, and Houben-Weyl.
RECENT ACTIVITIES OF DIVISION IV – POLYMER

PUBLICATIONS
Macromolecular Symposia is published by WILEY-VCH, and presents contributions in the field of macromolecular chemistry and physics from selected international meetings, including those of IUPAC, the European Polymer Federation (EPF), the American Chemical Society (ACS) and the Society of Polymer Science, Japan (SPSJ).

Recent Volumes have been:
- Advanced Polymers, Composites and Technologies
- Molecular Mobility and Order in Polymer
- Macromolecule-Metal Complexes
- Fillers, Filled Polymers and Polymer Blends
- Polymers for Africa

RECENT REPORTS

SELECTED CURRENT PROJECTS
- Efficiency and reproducibility of temperature rising elution fractionation (TREF)
- Repeatability and reproducibility of sample preparation and analysis in high-temperature SEC
- Accuracy and reproducibility of functionality type analysis of poly(ethylene oxide) homo and copolymers by LC-CC
- Micro-structural, melt processing and mechanical properties of compatibilised PA 6/ABS -blends
- Short course in polymer characterization
- Definitions of terms relating to individual macromolecules, their assemblies, and dilute polymer solutions
- Guide to macromolecular terminology and nomenclature
- Terminology for self-assembly and aggregation of polymers
- Recommendations on the abbreviated terms of polymers
- Towards defining materials chemistry

RECENT AND FORTHCOMING SPONSORED CONFERENCES
- 14th World Forum on Advanced Materials, 17-21 April 2006, Nara City, Japan
- World Polymer Congress 2006, 16-21 July 2006, Rio de Janeiro, Brazil
- International Symposium on Radical Polymerisation: Kinetics and Mechanism, 3-9 September 2006, Il Ciocco, Italy
- Advanced Polymers for Emerging Technologies, 11-12 October 2006, Busan, Korea
- IUPAC Polymer Conference on Mission and Challenges of Polymer Science and Technology, 10-14 June 2007, New York, US

SAMSUNG – IUPAC YOUNG POLYMER SCIENTIST AWARD
In 2003 the Samsung General Chemicals Co. (presently the Samsung Total Petrochemical Co. Ltd.) of South Korea donated USD 125,000 to the Polymer Division in order to help IUPAC stimulate polymer education and research in the world. According to the agreement between the IUPAC Polymer Division and Samsung, only the interest earned from this endowment may be used for the following four areas:
1. Samsung–IUPAC Young Polymer Scientist Award
2. Travel Grant for Students from Economically Disadvantaged Countries
3. Support of the WPC Organizing Committee
BOOKS AVAILABLE ON THE IUPAC WEB SITE
Compendium of Analytical Nomenclature (http://www.iupac.org/publications/analytical_compendium/)

PROJECTS NEAR COMPLETION OR IN PRESS
Revision in the international harmonised protocol for the proficiency testing of (chemical) analytical laboratories
Recommendations for NMR measurements of high pK values and equilibrium constants in strongly basic solutions
Interdisciplinary harmonised approach to metrological traceability of chemical measurement results
Mutual solubility of hydrocarbons and water Uncertainty estimation and figures of merit for multivariate calibration

SELECTED CURRENT PROJECTS
Comparable pH measurements by metrological traceability
Guidelines for potentiometric measurements in suspensions
Standardization of analytical approaches and analytical capacity-building in Africa
IUPAC stability constants database - completion of data collection up to 2006
Glossary of terms related to solubility - updates and revisions to the Orange Book
Trace elements analysis: role of grain size distribution in solid reference materials
Determination of selenomethionine in selenized yeast supplements
Adjustment, estimation and uses of equilibrium reaction constants in aqueous solution
Selection and use of proficiency testing schemes for limited number of participants
Establishment of guidelines for the validation of qualitative and semi-quantitative (screening) methods by collaborative trial: a harmonized protocol
Mutual solubility of alcohols and water (update of SDS Vol 15)
Transition and 12 to 14 main group metals, lanthanide, actinide and ammonium halates

RECENT AND FORTHCOMING CONFERENCES
Combining and reporting analytical results, 6-8 March 2006 - International APAT - IUPAC Workshop on the role of (metrological) traceability and (measurement) uncertainty for comparing analytical results, Roma, Italy.
International Congress on Analytical Sciences, 25-30 June 2006, Moscow, Russia

ANALYTICAL CHEMISTRY DIVISION TASK GROUPS
The Analytical Chemistry Division has a number of task groups dealing with:
- Communication
- Critical evaluations of data
- Quality assurance
- Electronic Resources/ Terminology
- Emerging analytical communities
- Emerging analytical issues
RECENT ACTIVITIES OF DIVISION VI – CHEMISTRY AND THE ENVIRONMENT

BOOKS AVAILABLE ON THE IUPAC WEB SITE
Green chemistry in Russia, Tundo, P. and Lunin, V.V., INCA, 2004 [ISBN 5-211-05001-0]

PROJECTS RECENTLY COMPLETED OR IN PRESS

SELECTED CURRENT PROJECTS
Air pollution models in environmental management and assessment
Biophysico-chemical processes of heavy metals and metalloids in soil environments
Remediation technologies for the removal of arsenic from water and wastewater
Development of simplified methods and tools for ecological risk assessment of pesticides
Environmental colloids: behaviour, structure and characterisation
Establishment of guidelines for the validation of quantitative and semi-quantitative (screening) methods by collaborative trial: a harmonised protocol
Impact of transgenic crops on use of agrochemicals and the environment

RECENT AND FORTHCOMING CONFERENCES
11th IUPAC International Congress of Pesticide Chemistry, 6-11 August 2006, Kobe, Japan
Environmental Best Practices, 7-10 Aug 2006, Olsztyn, Poland
XIIth IUPAC International Symposium on Mycotoxins and Phytotoxins, 21-26 May 2007, Istanbul, Turkey

CHEMISTRY AND THE ENVIRONMENT DIVISION’S SUB-COMMITTEES
The Chemistry and the Environment Division has the following sub-committees:

- Food chemistry
- Biophysico-chemical processes in environmental systems
- Chemistry of environmental compartments (soil, water, air)
- Crop protection chemistry
RECENT ACTIVITIES OF DIVISION VII – CHEMISTRY AND HUMAN HEALTH

BOOKS
Fundamental Toxicology for Chemists (1996)
Drug Metabolism: Databases and High Throughput Testing During Drug Design and Development (1999)
Analogue-based Drug Discovery (2005)

GLOSSARIES
Glossary of Terms in Quantities and Units in Clinical Chemistry (1996)
Glossary of Terms Used in Computational Drug Design (1997)
Glossary of Terms Used in Medicinal Chemistry (1998)
Glossary of Terms Used in Combinatorial Chemistry (1999)
Glossary of Terms Used in Toxicokinetics (2004)
Glossary of Terms Used in Pharmaceutical Technology
Glossary of Terms Used in Pharmaceutical Process Chemistry
Glossary of Drug Metabolism Terms
Glossary of Terms Used in Toxicology

OTHER RECENT PUBLICATIONS
Essential Toxicology – Educational Modules in PDF Format on IUPAC Website
Properties and Units in the Clinical Laboratory Sciences (2004)
Impact of Qualitative Analysis in Laboratory Medicine (2005)
Postgenomic Chemistry (2005)
Surveys of Research and Training in Medicinal Chemistry
United States
Europe
Japan
India, Pakistan and Sri Lanka
Explanatory Dictionary of Concepts in Toxicology

SELECTED CURRENT PROJECTS
Medicinal Chemistry and Drug Development
Human Drug Metabolism Database
Chemical and Pharmacological Aspects of Natural Products with Medicinal and Nutritive Value
Compendium of Terms Associated with Drug Discovery and Development
Glossary of Terms Used in Biomolecular Screening
Practical Studies for Medicinal Chemistry – An Integrating Approach for Developing Countries
Plants as Sources for Nutraceuticals in Latin America
Prototype Analysis of Molecular Biomarkers in Cancer

Toxicology and Risk Assessment
Quantifying the Effects of Compound Combinations
Educational Material for Teaching Toxicology
Training of School Children on Pesticides and Health
Distance Learning in Toxicology: Effective Teaching through Technology

NPU/Clinical Chemistry
Recommendations for the Use of Nanotechnology in Clinical Laboratories
Concepts and Structure for Requests in Clinical Laboratories
Global Use of the C-NPU Concept System for Properties in Toxicology
Internationally Agreed Terminology for Observations in Scientific Communication
Imunochemistry of Metal Sensitization

THE IUPAC RICHTER PRIZE IN MEDICINAL CHEMISTRY
Acknowledges the key role that medicinal chemistry plays toward improving human health. Awarded every two years to an internationally recognized scientist whose accomplishments demonstrate an outstanding level of contribution to the practice of medicinal chemistry or drug discovery.
The Division is responsible for maintaining and developing standard systems for designating chemical structures, including both conventional nomenclature and computer-based systems. This responsibility is to be fulfilled by:

1. Identifying the needs of the user community.
2. Generating projects arising from those needs.
3. Identifying project leaders and task groups to carry out the work.
4. Administering approved projects financially, monitoring their progress, and approving resulting recommendations for review by established IUPAC procedures.
5. Identifying new sources of expertise and enabling their involvement in projects.
6. As far as possible, ensuring that nomenclature systems projects and the resulting recommendations are compatible with each other, with established IUPAC recommendations, and with computer-based systems for manipulating chemical names and structures.

The Division has an Advisory Subcommittee of about 40 people, charged with advising the Division Committee on the needs of the community, and developing project proposals.

**RECENT REPORTS**


**SELECTED CURRENT PROJECTS**

- Extension of IUPAC rules for stereo descriptors to include coordination numbers 7-12
- Source-based nomenclature of single-strand organic polymers
- Graphical representation standards for chemical structure diagrams
- Nomenclature of cyclic peptides
- IUPAC International Chemical Identifier (InChI): promotion and extension
- Nomenclature of phosphorus-containing compounds of biochemical importance

**RECENT AND FORTHCOMING CONFERENCES**

- XML in Chemistry and IUPAC Chemical Identifiers, 12-14 November 2003, NIST, Gaithersburg, USA
- CAS/IUPAC Conference on Chemical Identifiers and XML for Chemistry, 1 July 2002, Columbus, USA

**BOOKS AVAILABLE ON THE IUPAC WEB SITE**