



I U P A C

***RECENT ACTIVITIES
OF
IUPAC DIVISIONS***

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Produced by the Committee on Chemistry and Industry (COCI)



RECENT ACTIVITIES OF DIVISION I – PHYSICAL AND BIOPHYSICAL CHEMISTRY

RECENT BOOKS

Interactions Between Soil Particles and Microorganisms: Impact on the Terrestrial Ecosystem, Vol. 8 - Huang, P.M.; Bollag, J.-M. and Senesi, N. - John Wiley & Sons, 2002
Physicochemical Kinetics and Transport at Biointerfaces, Vol. 9 - Koester, W., and van Leeuwen, H. P. - John Wiley & Sons, 2004
Chemical Thermodynamics for Industry - Letcher, T.M. - Royal Society of Chemistry, 2004
Measurement of the Thermodynamic Properties of Single Phases, Vol. VI - Goodwin, A.; Marsh, K.N. and Wakeham, W.A. Elsevier, 2003
Measurement of the Thermodynamic Properties of Multiple Phases, Vol. VII - Weir, R.D. and de Loos, T.W. - Elsevier, 2005

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
Physical Organic Chemistry, 20-25 Aug 2006, Warsaw, Poland
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

Nomenclature of Inorganic Chemistry - IUPAC Recommendations 2005, Connelly, N.G, Damhus, T., Hartshorn, R.M., and Hutton, A.T., The Royal Society of Chemistry, 2005 [ISBN 0 85404 438 8]

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)

On the claims for discovery of elements 110, 111, 112, 114, 116, and 118 (IUPAC Technical Report), *Pure Appl. Chem.* **75**(10), 1601-1611 (2003)

Atomic weights of the elements 2001 (IUPAC Technical Report), *Pure Appl. Chem.* **75**(8), 1107-1122 (2003)

Atomic weights of the elements. Review 2000 (IUPAC Technical Report), *Pure Appl. Chem.* **75**(6), 683-799 (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



RECENT ACTIVITIES OF DIVISION III – ORGANIC AND BIOMOLECULAR CHEMISTRY

Within Division III there are sub-committees that focus on:

- Organic synthesis
- Biomolecular chemistry
- Green chemistry
- Photochemistry
- Structural and mechanistic chemistry
- Biotechnology.

RECENT BOOKS

Analogue-based Drug Discovery, Fischer, J. and Ganellin, R.C. (Eds.), Wiley-VCH, 2005 [ISBN 3-527-31257-9]
Green Chemistry in Latin America, Tundo, P. and de Rossi, R.H., INCA, 2004 [ISBN 88-88214-16-X]
Green chemistry in Russia, Tundo, P. and Lunin, V.V., INCA, 2004 [ISBN 5-211-05001-0]
Natural Products, Botta, B., ed., Pure and Applied Chemistry 75(2-3), 141-419 (2003), IUPAC, 2003

PROJECTS NEAR COMPLETION OR IN PRESS

Postgenomic chemistry (IUPAC Technical Report), Pure Appl. Chem. 77(9), 1641-1654 (2005)
Chemical actinometry (IUPAC Technical Report), Pure Appl. Chem. 76(12), 2105-2146 (2004)

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

Polyaniline: Thin films and colloidal dispersions (IUPAC Technical Report), Pure Appl. Chem. 77(5), 815-826 (2005)

Chemical structure and physical properties of cyclic olefin copolymers (IUPAC Technical Report), Pure Appl. Chem. 77(5), 801-814 (2005)

Rheological properties and associated structural characteristics of some aromatic polycondensates including liquid-crystalline polyesters and cellulose derivatives (IUPAC Technical Report), Pure Appl. Chem. 76(11), 2027-2049 (2004)

Characterization of polyamides 6, 11, and 12. Determination of molecular weight by size exclusion chromatography (IUPAC Technical Report), Pure Appl. Chem. 76(11), 2009-2025 (2004)

Definition of terms related to polymer blends, composites, and multiphase polymeric materials (IUPAC Recommendations 2004), Pure Appl. Chem. 76(11), 1985-2007 (2004)

Definitions of terms relating to reactions of polymers and to functional polymeric materials (IUPAC Recommendations 2003), Pure Appl. Chem. 76(4), 889-906 (2004)

Rheological and mechanical properties of poly(a-methylstyrene-co-acrylonitrile)/ poly (methylacrylate-co-methyl methacrylate) blends in miscible and phase separated regimes of various morphologies. Part IV: Influence of the morphology on the mechanical properties, Pure Appl. Chem. 76(2), 389-413 (2004)

Critically evaluated rate coefficients for free-radical polymerization 4: Propagation rate coefficients for methacrylates with cyclic ester Groups, Macromol. Chem. Phys. 204, 1138-1150 (2003)

Critically evaluated propagation rate coefficients in free-radical polymerizations: Part III. Methacrylates with cyclic ester groups (IUPAC Technical Report), Pure Appl. Chem. 75(8), 1091-1096 (2003)

Characterization of finite length fibre composites: Part VII. Rheological studies of processed polypropylene-glass composites, Inter. Polymer Processing 18, 20-32 (2003)

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
4. Support of Education-Related Projects.



RECENT ACTIVITIES OF DIVISION V – ANALYTICAL CHEMISTRY

BOOKS AVAILABLE ON THE IUPAC WEB SITE

Compendium of Analytical Nomenclature (http://www.iupac.org/publications/analytical_compendium/)
The IUPAC Stability Constants Database (<http://www.iupac.org/publications/scdb/index.html>)
IUPAC Solubility Data (http://www.iupac.org/publications/ci/2004/2602/ic_solubility.html)

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 Latin America, Tundo, P. and de Rossi, R.H., INCA, 2004 [ISBN 88-88214-16-X]
Green chemistry in Russia, Tundo, P. and Lunin, V.V., INCA, 2004 [ISBN 5-211-05001-0]
Chemicals in the Atmosphere: Solubility, Sources and Reactivity, Fogg, P. and Sangster, J. (Eds.), John Wiley & Sons, 2003 [ISBN: 0-471-98651-8]
Atmospheric Deposition and its Impact on Ecosystems, Van Grieken, R. and Shavah, Y., Universiteit Antwerpen, Belgium, 2002
Green Chemistry in Africa, Tundo, P. and Mammino, L., eds., INCA, 2002 [ISBN 88-88214-07-0]
Green Chemistry Education, Tundo, P. and Patti, T., eds., INCA, 2002 [ISBN 88-88214-00-5]

PROJECTS RECENTLY COMPLETED OR IN PRESS

Aerosols: Connection between regional climate change and air quality (IUPAC Technical Report), Pure Appl. Chem. 76(6), 1241-1253 (2004)
Regulatory limits for pesticide residues in water (IUPAC Technical Report) Pure Appl. Chem. 75(8), 1123-1155 (2003)
Minimum requirements for reporting analytical data for environmental supplies (IUPAC Technical Report), Pure Appl. Chem. 75(8), 1097-1106 (2003)
Significance of impurities in the safety evaluation of crop protection products (IUPAC Technical Report), Pure Appl. Chem. 75(7), 937-973 (2003)
Solute movement in soils with potential rapid by-pass transport (IUPAC Technical Report), Pure Appl. Chem. In press
Endocrine disruptors in the environment (VI.3), Pure Appl. Chem. 75(5), 631-681 (2003)
Glossary of terms related to pesticides (IUPAC Technical Report), Pure Appl. Chem. 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

Medicinal Chemistry for the 21st Century (1992) (1994)
Fundamental Toxicology for Chemists (1996)
Drug Metabolism: Databases and High Throughput Testing During Drug Design and Development (1999)
Handbook of Pharmaceutical Salts: Properties, Selection and Use (2002)
Analogue-based Drug Discovery (2005)
Fundamental Toxicology, 2nd Edition (2006)

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
Natural and Synthetic Substances Related to Human Health (2002-2003)
Mechanisms of Immunosensitisation to Metals (2004)
Properties and Units in the Clinical Laboratory Sciences (2004)
Impact of Qualitative Analysis in Laboratory Medicine (2005)
Postgenomic Chemistry (2005)
Guidelines for Terminology for Microtechnology in Clinical Laboratories (2006)
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
Immunochemistry 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.



RECENT ACTIVITIES OF DIVISION VIII – CHEMICAL NOMENCLATURE AND STRUCTURE REPRESENTATION DIVISION

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

Nomenclature of Inorganic Chemistry - IUPAC Recommendations 2005, Connelly, N.G, Damhus, T., Hartshorn, R.M., and Hutton, A.T., The Royal Society of Chemistry, 2005 [ISBN 0 85404 438 8]
Numbering of Fullerenes (IUPAC Recommendations 2004), Pure Appl. Chem. 77(5), 843-923 (2005)

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

Nomenclature of Inorganic Chemistry - IUPAC Recommendations 2005, Connelly, N.G, Damhus, T., Hartshorn, R.M., and Hutton, A.T., The Royal Society of Chemistry, 2005 [ISBN 0 85404 438 8]
Compendium of Chemical Terminology - The Gold Book, Spanish edition, Perez, S.S., et al., Editorial Sintesis, 2003 [ISBN 84-7738-955-1]