



International Union of Pure and Applied Chemistry

Analytical Chemistry Division

Report to Council 2009

(Period covered 2008-2009)

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I Highlights and Executive Summary

- In the current biennium (2008-2009) the core bodies of the Analytical Chemistry Division remain the Division Committee, the Interdivisional Working Party on Harmonization of Quality Assurance ([WPHQA](#)) and the Subcommittee on Solubility and Equilibrium Data ([SSED](#))
- The Division continues to successfully run a number of divisional and interdivisional projects.
- The Division keeps and actively supports its key publication/databases, namely *The Compendium of Analytical Nomenclature - Orange Book*, the *Solubility Database* and the *Stability Constants Database*.
- For the current biennium Division has established focus (interest) groups on Communication, Critical evaluation of data, Electronic resources for IUPAC terminology work, Emerging analytical issues, Metrology, and the Analytical potential of nuclear techniques.
- The Division continues publishing its newsletter *Teamwork*, which serves for communication within the Division and with other IUPAC members and bodies.
- The Division is actively involved in global harmonization and standardization activities, where in current biennium a special emphasis was put to metrology in chemistry.
- The Division actively cooperates with number of international organizations and bodies (e.g. BIPM, CITAC, EURACHEM, IAEA, IAM, IUPAP, UNIDO, etc.)
- Based on a good geographical distribution of its members, and on the above mentioned cooperations, the Division is continuing its efforts in supporting chemists in developing countries and economies.

II Report of activities since January 2008

(Organized by the six Goals of the current IUPAC Strategic Plan.)

Note: Many of the Division activities described below span over more than one point of the IUPAC Strategic Goal.

a) Providing leadership as a worldwide scientific organization that objectively addresses global issues involving the chemical sciences:

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Taking into account limited human resources, the Division can only address a limited number of issues. This is done through interest groups. For the biennium 2008-2009 the following interest groups (formerly tasks groups) were created: *Communication, Critical evaluation of data, Electronic resources, Emerging analytical issues, Metrology and the Analytical potential of nuclear techniques*. Interest groups were established under the new project oriented IUPAC structure. They are expected to reflect the current core interests of the Division and to foster creation of new projects. However, Interest Groups are not aimed to replace any of the Sub-committees or Working Groups and they serve for the biennium when they will be reviewed and terminated or prolonged as appropriate.

The Division continued to publish its newsletter *Teamwork*, as one of the main sources of information within the Division members as well as with other IUPAC Divisions and Committees. Being available on the IUPAC web page <http://old.iupac.org/divisions/V/Teamwork/index.html>, *Teamwork* is also freely available for everybody interested.

b) Facilitating the advancement of research in the chemical sciences through the tools that it provides for international standardization and scientific discussion:

Beside the IUPAC Technical Reports and Recommendations resulting from projects run by the Division (listed in IV.1 and IV.4), the Compendium of Analytical Nomenclature - Orange book, the Solubility Database and the Stability Constants Database, as well as the k_0 -NAA database, remain to be the main Division tools of general interest for analytical chemistry community. However, critical review of [Orange Book](#) coordinated by the Division Secretary revealed a need of complete revision of this document. Revision of the Orange Book is foreseen to be the most important activity for the near future with the involvement of all Division Committee Members. A dedicated one day workshop on Orange Book revision is planned during the IUPAC GA in Glasgow (See also III).

The IUPAC Stability Constant Database (SCDB) is the most comprehensive compilation of stability constants available, covering the years 1877 to 2005. It is the primary source of data for the Critical Evaluations of Stability Constants that are published on a regular basis by Division V. It is a major research tool for those involved in the equilibrium modelling of environmental, biological and industrial systems. The future of SCDB was the subject of a Division V presentation to the Bureau meetings in 2004 and 2007. All aspects of the management of the database — program development, data conflation, advertising, marketing — have for the last 16 years been undertaken on behalf of IUPAC by the developers of the current database, Academic Software. In 2007 this company has indicated that it wishes to transfer the responsibility for management and maintenance of SCDB to IUPAC within about 2 years. Division V formed a consultative team to work with Academic Software to achieve a successful transition of management of SCDB from Academic Software to IUPAC or an alternative external systems manager. Further, the Division was represented by Kip Powell on the Secretary-General's *ad hoc* committee that had as its Terms of Reference: "To explore requirements to achieve a modernized interactive IUPAC web site and an ability for IUPAC to provide large databases of value to chemists". The work of this committee led to the current developing arrangements with FIZ-Chemie. It can be reported now that agreement was reached with the IUPAC Bureau that the database will be frozen as soon as collection of literature data for 2006 is completed. For the future the database will be made available to users through IUPAC as a frozen compilation. Division V is ready to support further work compilations if such a need will be identified in the future.

Regarding [k₀-NAA database](#) contacts were established with the the BIPM Consultative Committee for Ionizing Radiation (CCRI) and the International Atomic Energy Agency (IAEA) regarding future updates and developments. The Division expressed interest for further cooperation and for further hosting this database.

c) Assisting chemistry-related industry in its contribution to sustainable development, wealth creation, and improvement in the quality of life:

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In understanding the role measurement results produced by analytical chemists play in international trade and in helping lowering barriers to trade, the following projects of Analytical Chemistry Division deserve special attention, namely, the *Metrological Traceability of Measurement Results in Chemistry* and the interdivisional project on Comparable pH Measurements by Metrological Traceability. The first project is aimed to establish common understanding of metrological traceability and to describe common concepts as prerequisite for comparability of measurement results, while the second one already utilizes given concepts and applies them to the most frequent chemical measurement – measurement of pH. The third, recently initiated WPHQA project is titled *Investigating out-of-Specification Test Results of Chemical Composition Based on Metrological Concepts*, which is aimed in developing a guide for identification of root causes of out-of-specification (OOS) test results of chemical composition based on metrological concepts. The guide should be helpful for full-scale investigation of OOS test results, already detected according to existing requirements in pharmaceutical and other industries. Another WPHQA project of relevance to industry is *Trace Element Analysis – Role of Particle Size Distribution in Solid Reference Materials*, which is very important for reference materials production in assuring ‘commutability’ of reference materials.

d) Fostering communication among individual chemists and scientific organizations, with special emphasis on the needs of chemists in developing countries.

Members of the Analytical Chemistry Division have been actively involved and have cooperated with the following organizations and bodies: the International Committee on Weights and Measures/Consultative Committee on the Amount of Substance (BIMP/CCQM); the ISO-Committee on Reference Materials (ISO/REMCO); the International Committee on Weights and Measures/Joint Committee for Guides in Metrology (BIPM/JCGM) Working Group 1 and Working Group 2; Inter-Agency Meeting (IAM); the Joint Committee on Traceability in Laboratory Medicine (JCTLM), the Cooperation on International Traceability in Analytical Chemistry (CITAC), etc. One of the most important documents published during this biennium in which Division members were actively involved is the 3rd Edition of the *International vocabulary of metrology — Basic and general concepts and associated terms (VIM)*. IUPAC was together with BIPM, IEC, IFCC, ILAC, ISO, IUPAP and OIML one of eight international organizations, which worked together in producing this document under the coordination of the Working Group 2 of the Joint Committee for Guides in Metrology (JCGM/WG 2).

e) Utilizing global IUPAC perspective and networks to contribute to the enhancement of chemistry education, the career development of young chemical scientists, and the public appreciation of chemistry.

The Analytical Chemistry Division continued to be actively involved in the IOCD project *Standardization of analytical approaches and analytical capacity building in Africa*. Also, as indicated in paragraphs V.5 and V.6, Division members have organized or have been involved in numerous seminars, workshop and conferences in various parts of the world.

f) IUPAC will broaden its national membership base and will seek the maximum feasible diversity in membership of IUPAC bodies in terms of geography, gender, and age

The current and proposed 2010-2011 Division memberships are well balanced regarding geographical distribution, gender and diversity of scientific fields. However, there is still room for improvement regarding involvement of young chemists in projects and other Division activities.

III Other information

In 2008-2009 biennium the WPHQA and SSED have after many years changed their Chair persons. This means that simultaneously with the change of Division Officers all leading positions of the Division have in 2008 been newly occupied.

At the Division last Division Committee meeting in February 2008 in Rome it was confirmed that the Orange Book will remain one of the most important Division products. In this line the Division will focus its efforts on the revision of the complete Orange Book, which should then continuously be updated and

should serve as a source of information for the IUPAC Gold Book. Selection of new Division Members should take this into account in assuring that all fields of analytical chemistry will be properly covered.

IV Tabular material

IV.1 IUPAC Recommendations and Technical Reports 2008-2009

Performance evaluation criteria for preparation and measurement of macro and microfabricated ion-selective electrodes (IUPAC Technical Report)

Pure Appl. Chem., Vol. 80, No. 1, pp. 85–104, 2008.

Glossary of terms related to solubility (IUPAC Recommendations 2008)

Pure Appl. Chem., Vol. 80, No. 2, pp. 233–276, 2008.

Countercurrent chromatography in Analytical chemistry (IUPAC Technical Report)

Pure Appl. Chem., Vol. 81, No. 2, pp. 355–387, 2009.

IV.2 Conference proceedings

30th International Conference on Solution Chemistry (ICSC 30), Perth, Australia, 16–20 July 2007 2008, (E. Königsberger, editor)

Pure Appl. Chem. Vol. 80, No. 6 (dedicated issue)

International Symposium on Metallomics 2007 (ISM 2007), Nagoya, Japan, 28 November–1 December 2007, (H. Haraguchi, editor)

Pure Appl. Chem., Vol. 80, Issue 12, 2008 (dedicated issue)

Challenges to metallomics and analytical chemistry solutions (Sandra Mounicou and Ryszard Lobinski)

Pure Appl. Chem., 2008, Vol. 80, No. 12, pp. 2565-2575, 2008.

IV.3 Books

D. B. Hibbert, *Quality Assurance for the Analytical Chemistry Laboratory*, Oxford University Press, 2007.

IV.4 Current projects

2008-031-1-500: Methods of measurement and evaluation of natural antioxidant capacity/activity

2008-025-1-500: Humic-metal binding constants database

2008-030-1-500: Investigating out-of-specification test results of chemical composition based on metrological concepts

2008-008-1-500: An introduction to the IUPAC-NIST Solubility Data Series: Preparation and use of compilations and evaluations

2008-002-1-500: A glossary of concepts and terms in chemometrics

2007-039-1-024: Extension of ThermoML - the IUPAC standard for thermodynamic data communications

2007-041-1-500: Mechanistic aspects of chemical vapor generation of volatile hydrides for trace element determination

2007-044-1-500: Solubility data related to industrial processes. Solubility in systems with lithium and/or sodium nitrates

2007-047-1-500: Solubility data related to industrial processes. Nitriles C+3: binary and multicomponent systems

2007-046-1-500: Solubility data related to industrial processes. Mutual solubility of esters with water

2007-045-1-500: Solubility data related to industrial processes. Solubility of higher alkynes in liquids

2007-010-2-500: International harmonized protocol for standard preparation, irradiation and measurement for assuring metrological traceable results in neutron activation analysis

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2006-026-1-500: Electrochemical DNA-based biosensors: terms and methodology
2006-039-2-600: Extraction and fractionation methods for exposure assessment related to trace metals, metalloids and hazardous organic compounds in terrestrial environments
2006-037-1-500: Metal-focused -omics: guidelines for terminology and critical evaluation of analytical approaches
2006-034-1-500: The solubility of oxygen in all solvents (update of SDS vol 7. 1981)
2006-033-1-500: Solubility data related to industrial processes. Rare earth metal chlorides (Sc, Y, lanthanoids) in water and aqueous systems
2006-032-1-500: Solubility data related to industrial processes. Mutual solubility of ethers and ketones with water
2006-022-1-500: Spectrochemical Analysis - Conversion of Orange Book Chapter 10 to Glossary Format
2006-016-1-200: Recommendations for isotope data in geosciences
2006-010-1-500: Adjustment, estimation and uses of equilibrium reaction constants in aqueous solution
2005-041-2-500: Determination of selenomethionine in selenized yeast supplements
2005-035-2-500: Trace elements analysis: role of grain size distribution in solid reference materials
2005-048-2-100: Solubility and thermodynamic properties related to environmental issues
2005-033-1-500: Transition and 12 to 14 main group metals, lanthanide, actinide and ammonium halates Series: Solubility Data Series; editor-in-chief: Mark Salomon
2005-024-2-600: Establishment of guidelines for the validation of qualitative and semi-quantitative (screening) methods by collaborative trial: a harmonized protocol
2005-019-2-500: Selection and use of proficiency testing schemes for limited number of participants (chemical analytical laboratories)
2005-017-1-500: Glossary of terms related to solubility - updates and revisions to the Orange Book
2005-014-1-500: IUPAC Stability Constants Database - completion of data collection up to 2006
2004-005-2-500: Comparable pH measurements by metrological traceability
2004-017-1-500: Standardization of analytical approaches and analytical capacity-building in Africa
2003-056-2-500: Standard definitions of terms relating to mass spectrometry
2003-015-2-500: Terminology, quantities and units concerning production and applications of radionuclides in radiopharmaceutical and radioanalytical chemistry
2002-058-1-500: Definitions and fields of application of the terms robust and rugged and the characteristics or qualities of robustness and ruggedness in analytical chemistry
2002-044-1-500: Solubility data related to industrial processes. Carbon dioxide in aqueous non-electrolyte solutions
2002-038-1-500: Solubility data of compounds relevant to human health. Antibiotics: peptide antibiotics and macrocyclic lactone antibiotics
2002-037-1-500: Solubility data of compounds relevant to human health. Solubility of halogenated aromatic hydrocarbons Series: Solubility Data Series; editor-in-chief: Mark Salomon
2002-036-1-500: Solubility data of compounds relevant to human health. Solubility of hydroxybenzoic acids and hydroxybenzoates
2002-035-1-500: Solubility data of compounds relevant to human health. Solubility of substances related to urolithiasis
2002-032-1-500: Solubility data of compounds relevant to mobility of metals in the environment. Metal carbonates (Mn, Fe, Co, Ni, Cu, Zn, Ag, Cd, Hg, Pb)
2002-031-1-500: Solubility data of compounds relevant to mobility of metals in the environment. Alkaline earth metal carbonates
2002-025-1-500: Solubility data of compounds relevant to mobility of metals in the environment. Inorganic actinide compounds
2002-009-2-500: Optical spectrochemical analysis using waveguides and optical fibers
2001-072-1-500: Low activation materials for fusion technology: state and prospects
2001-063-1-500: Revision of terminology of separation science
2001-010-3-500: Metrological traceability of measurement results in chemistry (revised title)
1999-050-1-500: Chemical Speciation of Environmentally Significant Heavy Metals and Inorganic Ligands

IV.5 Conferences/Symposia

The 13th International Symposium on Solubility Phenomena and Related Equilibrium Processes (13th ISSP) was held at Trinity College Dublin, Ireland, from July 27th to 31st, 2008. This was the latest in a successful series of biennial meetings that bring together scientists from diverse areas where solubility and associated equilibria play important roles. The 13th ISSP continued the tradition of multidisciplinary with contributions ranging from theory and modelling, biological systems, industrial processes, environmental chemistry and geochemistry among others.

IV.6 Lectures and seminars

Seminars on the new International Vocabulary of Metrology (VIM 3) were given by P. De Bièvre in: Gaithersburg, USA, National Institute for Standards and Technology, 24 October 2008; Helsinki, Finland, National Institute for Metrology of Finland (MIKES) on 3 February 2009, and Labquality Days on 25 February 2009. Bangkok, National Metrology Institute of Thailand, 24 to 27 March 2009; and Singapore, Health Science Authority, 30 March 2009:

Lectures on the redefinition of the kilogram and the mole were given by P. De Bièvre in: Bangkok, Kasetsart University, 27 March 2009; and Singapore, National University of Singapore, 31 March 2009.

Seminar 'Traceability in Chemistry', 26 February 2008, Rome, Italy
Lecturers: R. Dybkaer, P. De Bièvre, and M. Sega

Lecture on Introduction to IUPAC and other relevant guidance documents was given by A. Fajgelj at the APLAC Workshop on Reference Materials Producers Assessors Training Workshop, Hong Kong. 17 to 19 November 2008.

IV.7 Workshops

IUPAC-SSED Workshop on Metrological Traceability of Solubility Data, 28 February 2008, Rome, Italy
Lecturers: D. B. Hibbert, H. Gamsjäger, M. Costa-Gomez, and D. Knox.

IUPAC-WPHQA Workshop on Trace Element Analysis: Role of Particle Size Distribution in Solid Reference Materials, 29 February 2008, Rome, Italy
Lecturers: M. Belli, A. Sahuquillo, P. de Zorzi, Z. Mester, U. Sansone, and A. Fajgelj

IUPAC Workshop on Metrology, Chinese Academy of Metrology Science (CAMS), Beijing, China, 21 November 2008
Lecturers: A. Fajgelj, B. Hibbert, W. Lund, and Hongmei Li