

Report to Council (January 2006 - June 2007)
IUPAC Analytical Chemistry Division (V)
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I. Highlights and executive Summary

- The Division is continuing to maintain and to extend a portfolio of good projects.
- A contestable project selection process for funding (two rounds per year) is working satisfactorily.
- The Division supports actively the maintenance and updating of two key IUPAC publications, *The Compendium of Analytical Terminology (Orange Book)* and the *IUPAC Stability Constant Database (SCDB)*.
- A consultative team is working with Academic Software to ensure the on-going maintenance of *SCDB* when Academic Software relinquishes this role in the near future. This currently involves a generic IUPAC arrangement with FIZ-Chemie (Berlin) to take over the management of the IUPAC website and its eventual management of a web version of *SCDB*.
- The Division has selected a small number of priorities for the biennium and is focusing its energy on these. To cultivate a spirit of “collective responsibility” it has restructured in six Teams each of which has responsibility for one priority area.
- Communication within the Division and with other officers of the Union is maintained through the newsletter “Teamwork”. Project progress reports are in the public domain since they are appended to the webpage devoted to each project.
- The Division has been coordinating two series of articles for CI on the topics of “Emerging needs of developing countries” (series completed) and “Tools of the Trade”.
- The Division is building bridges (a) with chemists in “developing countries”, (b) with sister organizations that have field experience in developing countries (IAEA, UNIDO, IOCD), (c) with other unions and expert bodies (IUPAP, BIPM).

II. Report of Activities since January 2006 (organised by the goals of the IUPAC strategic plan)

II.1. Addressing global issues in analytical chemistry sciences

This item addresses the IUPAC goal to provide leadership as a worldwide scientific organisation that objectively addresses global issues involving the chemical sciences.

Project initiation and management

The ACD has confirmed the six core activities for the biennium: (i) communication, (ii) critical evaluation of data, (iii) quality assurance, (iv) electronic resources/terminology, (v) emerging analytical communities, and (vi) emerging analytical issues. Each of these activities has been assigned a team of 4-6 members (TM + AM + NR) with the priority task of project initiation and management in the relevant areas. Each team has a collective responsibility and is encouraged to:

- Determine the scope of its responsibility and activities;
- Develop a strategy for effective communication between and by its members;
- Identify activities that advance the goals of IUPAC in its designated area;
- Achieve at least one significant output each year (e.g. letters to Editors; an IUPAC or ACD presentation at a conference; an article for CI; a Project Proposal; etc.);
- Accept responsibility for leading Division activities in its designated area;
- Facilitate a ‘roll-over’ of its activities at the end of the current biennium.

Communication

The role and responsibility of the ACD members is to increase the visibility of the ACD to the outside world and to promote the IUPAC project oriented approach. The Division maintains communication with all its members, and officers of other Divisions and Operational committees, through its newsletter Teamwork <http://www.iupac.org/divisions/V/Teamwork/>, edited by the Division VP.

The Division interacts with all Task Groups on an eight-monthly basis via a Project reporting system. The reports are read by all Division members and are reviewed at Division (or Division Officers’) meetings. They provide an “early warning system” for any projects that are struggling, alert the Division to the need for reviewers and allow re-assessment of dissemination plans as the projects near completion. These reports are appended to the respective Project pages on the IUPAC website, so that project progress is in the public domain.

Global issues

One global issue being addressed is the measurement of pH, through the project: *Comparable pH measurements by metrological traceability. Part I: Water quality monitoring and assessment; Part II: Clinical and biochemical matrices*. This project sees a continuation of work by the “pH task group” [*Measurement of pH. Definition, Standards and Procedures. 2002*] and it has the financial and professional backing of three Divisions and COCI. Another global issue addressed is the concept of ‘fair trade’. Fair trade can only arise between nations when all have adequate and quality-assured laboratories and their methodology meets the current requirements for metrological traceability. These issues are particularly relevant to the less developed nations. These concepts were the basis of a successful joint project proposal with IOCD which includes two Division V members, titled: “*Standardisation of analytical approaches and analytical capacity building in Africa*”. This project involves a melding of IUPAC technical expertise with IOCD appreciation of geopolitical issues in developing countries.

II.2. Providing tools for international standardisation

This item addresses the IUPAC goal to facilitate advancement of research in the chemical sciences through the tools that it provides for international standardisation and scientific discussion.

The Analytical Chemistry Division actively pursues these goals through its program of critical evaluations of data, the establishment of guidelines for Quality Assurance in chemical methods and associated sampling, and by the updating of analytical terminology and making it readily available via the web.

(a) *The Orange Book: http://www.iupac.org/publications/analytical_compendium/*

The route for updating terminology in the OB is via formal publication in PAC. Examples of issues being currently addressed through projects are: Glossary of Terms related to Solubility; Revision of terminology in separation science; Terminology, quantities and units concerning production and applications of radionuclides in radiopharmaceutical and radioanalytical chemistry; Internationally agreed terminology for observations in scientific communications; Standard definitions of terms relating to mass spectrometry. The text will be progressively converted to ICTNS-accepted format; it will also be aligned with the Gold book version, so that there is only one version of terminology within the IUPAC database.

(b) *The IUPAC Stability Constants Database (SCDB)*

This is the most comprehensive compilation of stability constants available, covering the years 1877 to 2004+. 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.

Division V has in place a Project to continue the evaluation, collection and entry of data through to 2008. To minimise risk the data collection team will be expanded from one site to involve experts in up to four countries (currently two).

The future of SCDB was the subject of a Division V presentation to the Bureau meeting in 2004. 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. This company has now signalled 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.

(c) *Recommendations concerning quality assurance*

The Working Party on Harmonisation of Quality Assurance continues to produce publications that are of value to chemists in analytical laboratories; e.g. Revision of the IUPAC/ISO/AOAC protocol for proficiency testing; Harmonised guidelines for single-laboratory validation of methods of analysis; and Terminology for soil sampling. The WPHQA will make a major presentation at the GA on “Metrological Traceability of Measurement Results in Chemistry”

(d) *Critical evaluation of solubility and solution equilibrium data*

The Division's Solubility and Solution Equilibrium Data sub-committee (SSED) has an active portfolio of projects. They embrace the critical evaluation of solubility data related to (a) mobility of metals in the environment, (b) industrial processes, and (c) human health. The outputs appear as review papers (Solubility Data Series) in the Journal of Physical and Chemical Reference Data and are thence transferred to the NIST-IUPAC Solubility Database: <http://srdata.nist.gov/solubility/>, or are published as book volumes, such as, e.g. *Biomineralization – Medical Aspects of Solubility*, E. Königsberger and L-C. Königsberger (eds.), John Wiley & Sons, Chichester, England, 2006. Significant “umbrella” projects include a 25-chapter book volume on “*Solubility for industry*” and “*Chemical speciation of environmentally significant heavy metals with inorganic ligands*”.

(e) Tools of the Trade

The Division's Communications Team has worked with Dr Meyers to organise a new series of articles for CI that emphasises the advancement of research in the chemical sciences through the tools that IUPAC provides. This series commenced in September and features articles from several Divisions and OCs.

II.3. Assisting chemical industry

This point reflects the IUPAC goal to assist chemistry-related industry in its contribution to sustainable development, wealth creation, and improvement of the quality of life.

Chemistry-related industry is served by the active program of critical evaluations of solubility data and of solution equilibrium data, and by the continuance of data compilation (and subsequent evaluation) for the IUPAC Stability Constant Database. The current projects on pH (*Comparable pH measurements by metrological traceability*) and metrological traceability (*Metrological Traceability of Measurement Results in Chemistry*) are highly relevant to industry. The SSED were joint organisers of the 12th International Symposium on Solubility Phenomena (Freiberg, 2006) at which there was significant emphasis on industrial issues and involvement of industrial chemists.

II.4. Fostering communication among scientific organisations

This point reflects the IUPAC goal to foster communication among individual chemists and scientific organisations, with special emphasis on the needs of chemists in developing countries.

Analytical Chemistry in developing countries. “Emerging needs in developing countries” is one of the Division's priority areas and is the responsibility of one Team “Emerging Analytical Communities”. The Division is fortunate in having several members with established professional links with Africa (Jan-Åke Jönsson, Walter Lund and Roger Smith). Nelson Torto (Botswana) serves the ACD as a Provisional Member representing the IUPAC Associate Organisation, SEANAC. To increase awareness of the needs of developing countries the Division arranged a series of articles for Chemistry International. These articles on Emerging issues in developing countries commenced in the March 2005 issue. The Division is significantly involved in the project with IOCD: “Standardisation of analytical approaches and analytical capacity building in Africa”. The division seeks actively to assure the representativeness of emerging analytical countries at the associate or titular member level and generate links to countries not represented by a NAO.

Building bridges with other organisations. The ACD is formally represented in the following organizations: EURACHEM, the Inter Agency Meeting (IAM), the International Committee on Weights and Measures/Consultative Committee for Amount of Substance - Metrology in Chemistry (CIPM/CCQM), the International Committee on Weight and Measures/Joint Committee for Guides in

Metrology (CIPM/JCGM), the International Organization for Standardization - Committee on Reference Materials (ISO REMCO), and Co-operation on International Traceability in Analytical Chemistry (CITAC).

The IWP HQA organised, together with the Italian Environmental Protection Agency (APAT), which also hosted the event, an international workshop on Combining and Reporting Analytical Results - The Role of (metrological) Traceability and (measurement) Uncertainty for Comparing Analytical Results. The Workshop was sponsored by the Centre for Materials Development, Italy, the International Atomic Energy Agency (IAEA), the Consultative Committee for Amount of Substance - Metrology in Chemistry (CCQM), the International Bureau of Weights and Measures (BIPM), the Co-operation on International Traceability in Analytical Chemistry (CITAC), the ISO Committee on Reference Materials (ISO REMCO) and UNIDO. It reflected a very good co-operation of the WPQA and ACD with listed organizations. The workshop was attended by 120 participants from 35 countries. The workshop can be considered as confirmation of the new dynamics set in motion by the joint ACD – IAEA- WPQA meeting in Vienna and opening towards IUPAC and UNIDO. Proceedings of the workshop were published by the Royal Society of Chemistry as a special series book.

The Division is actively involved (3 out of 6 TG members) in an inter-Union project “*Recommendations for Isotope Data in Geosciences*” (RIDIG) which draws on complementary expertise present in IUGS and IUPAC.

Improving communication. Dissemination of project outcomes is a crucial issue for improving the impact of our work in the chemistry community. This is overseen by the “Communications” team. Owing to efficient collaboration with Dr. Meyers, the WEB page is better attuned to the perception of those who are not familiar with the IUPAC system and processes. Improved lines of communication between TG chairs and the Division have been facilitated by the establishment of an 8-monthly Project reporting system in which the TGC responds to questions re progress, milestones, difficulties, opportunities for further work, etc. These progress reports are appended to the respective project pages. The Division has been pro-active in recommendations for improved IUPAC representation at conferences. It considers that there is scope for enhanced involvement of IUPAC representatives at IUPAC-sponsored conferences. This could be aided if conference organisers were required to discuss the nomination of an IUPAC representative with the relevant Division ahead of submitting the AIS.

II.5. Broadening national membership base

This item addressed the IUPAC goal to broaden its national membership base and will seek the maximum feasible diversity in membership of IUPAC bodies in terms of geography, gender and age.

Division V has in place a strategy, which is communicated to the Nominations’ Committee, to ensure the widest possible geographic representation. The Division actively sought participation of N. Torto as a Provisional Member representing the ANO, SEANAC. Within its own structures, the Division works to ensure **active** involvement of all AM, TM and NR.

III. Challenges and solutions

The principal challenges to the ACD include:

- a) The breadth of its portfolio. The Division is aware of its limited resources and has identified a manageable number of priorities for the biennium (*cf.* II.1)
- b) The need to extend the base of recruitment of new projects and task group chairmen from outside IUPAC. The Division initiated a system of mini-symposia to bring in external expertise. A

workshop on Future opportunities and challenges for the ACD Division was organised at the GA in Beijing.

- c) The generation of members' collective responsibility for the goals of the Division, the needs of countries not represented, and the long-range goals of IUPAC. The Division is answering this challenge by having formed Teams, each with collective responsibility for one priority area. The Division finds important to maintain active communication among members through the newsletter, Teamwork.
- d) Maintaining momentum through the biennium and with the change of biennia. The team system and maintenance of extensive Division records and archives (WEB site, Teamwork) are expected to facilitate the smooth roll-over with the change of biennia.
- e) Effort focused on the needs of developing countries and on links with other agencies (*cf.* II.4)

IV. TABULAR MATERIAL

IV.1. Publications 2006 – 2007

Chemical speciation of environmentally significant metals with inorganic ligands Part 2: The Cu^{2+} - OH^- , Cl^- , CO_3^{2-} , SO_4^{2-} , and PO_4^{3-} systems (IUPAC Technical Report)

Pure Appl. Chem. 79(5), 895-950, 2007

Guidelines for potentiometric measurements in suspensions Part B. Guidelines for practical pH measurements in soil suspensions (IUPAC Recommendations 2006)

Pure Appl. Chem. 79(1), 81-86, 2007

Guidelines for potentiometric measurements in suspensions Part A. The suspension effect (IUPAC Technical Report)

Pure Appl. Chem. 79(1), 67-79, 2007

The International Harmonized Protocol for the proficiency testing of analytical chemistry laboratories (IUPAC Technical Report)

Pure Appl. Chem. 78(1), 145-196, 2006

Guidelines for NMR measurements for determination of high and low pKa values (IUPAC Technical Report)

Pure Appl. Chem. 78(3), 663-675, 2006

Uncertainty estimation and figures of merit for multivariate calibration (IUPAC Technical Report)

Pure Appl. Chem. 78(3), 633-661, 2006

The International Harmonized Protocol for the proficiency testing of analytical chemistry laboratories (IUPAC Technical Report)

Pure Appl. Chem. 78(1), 145-196, 2006

Parts 9-12 in IUPAC-NIST Solubility Data Series 81, Hydrocarbons with Water and Seawater – Revised and Updated, A. Mącznyński, Volume Editor, 2006

C_{10} Hydrocarbons with Water, *J. Phys. Chem. Ref. Data*, Vol. 35 (1), pp. 93-151, 2006

C_{11} and C_{12} Hydrocarbons with Water, *J. Phys. Chem. Ref. Data*, Vol. 35 (1), pp. 153-203, 2006

C₁₃–C₃₆ Hydrocarbons with Water, *J. Phys. Chem. Ref. Data*, Vol. 35 (2), pp. 687-784, 2006
 C₅–C₂₆ Hydrocarbons with Seawater, *J. Phys. Chem. Ref. Data*, Vol. 35 (2), pp. 785-838, 2006

Book: T. M. Letcher (ed.), *Thermodynamics, Solubility and Environmental Issues*, Elsevier, Amsterdam, 2007.

IV. 2. Current portfolio of projects

a) Recent projects (started after Jan 1st, 2006)

2006-010-1-500 - Adjustment, estimation and uses of equilibrium reaction constants in aqueous solution

2006-022-1-500 - Spectrochemical Analysis - Conversion of Orange Book Chapter 10 to Glossary Format

2006-037-1-500 - Metal-focussed -omics: guidelines for terminology and critical evaluation of analytical approaches

2006-032-1-500 - Solubility data related to industrial processes. Mutual solubility of ethers and ketones with water (**SSED project**)

2006-033-1-500 - Solubility data related to industrial processes. Rare earth metal chlorides (Sc, Y, lanthanoids) in water and aqueous systems (**SSED project**)

2006-034-1-500 - Solubility data related to industrial processes. The solubility of oxygen in all solvents (**SSED project**)

2006-016-1-200 - Recommendations for isotope data in geosciences (**Interdivisional**)

2006-039-2-600 - Extraction and fractionation methods for exposure assessment related to trace metals, metalloids and hazardous organic compounds in terrestrial environments (**Interdivisional**)

b) Other projects

1999-050-1-500 - Chemical speciation of environmentally significant heavy metals and inorganic ligands

2001-041-2-500 - Recommendation on the use of countercurrent chromatography in analytical chemistry

2001-072-1-500 - Low activation materials for fusion technology: State and prospects

2002-002-2-500 - Recent advances in electroanalytical techniques: characterization, classification and terminology

2002-003-2-500 - Performance evaluation criteria for preparation and measurement of macro and microfabricated ion-selective electrodes

2002-009-2-500 - Optical spectrochemical analysis using waveguides and optical fibers; Series on Nomenclature, Symbols, and Units in Spectrochemical Analysis

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

2003-015-2-500 - Terminology, quantities and units concerning production and applications of radionuclides in radiopharmaceutical and radioanalytical chemistry

2005-014-1-500 - IUPAC stability constants database - completion of data collection up to 2006

2005-017-1-500 - Glossary of terms related to solubility - updates and revisions to the Orange Book

2005-035-2-500 - Trace elements analysis: role of grain size distribution in solid reference materials

2005-041-2-500 - Determination of selenomethionine in selenized yeast supplements

Interdivisional Working Party on Harmonization of Quality Assurance (IWPQA) projects

2001-010-3-500 - Metrological traceability of measurement results in chemistry

2005-019-2-500 - Selection and use of proficiency testing schemes for limited number of participants

2005-024-2-600 - Establishment of guidelines for the validation of qualitative and semi-quantitative (screening) methods by collaborative trial: a harmonized protocol*

Subcommittee on Solubility and Equilibrium Data (SSED) projects

2002-025-1-500 - Solubility data of compounds relevant to mobility of metals in the environment. Inorganic actinide compounds

2002-031-1-500 - Solubility data of compounds relevant to mobility of metals in the environment. Alkaline earth metal carbonates

2002-032-1-500 - Solubility data of compounds relevant to mobility of metals in the environment. Metal carbonates

2002-035-1-500 - Solubility data of compounds relevant to human health. Solubility of substances related to urolithiasis

2002-036-1-500 - Solubility data of compounds relevant to human health. Solubility of hydroxybenzoic acids and hydroxybenzoates

2002-037-1-500 - Solubility data of compounds relevant to human health. Solubility of halogenated aromatic hydrocarbons

2002-043-1-500 - Solubility data related to industrial processes. Carbon dioxide and the lower alkanes at pressures above 2 bar: methane to butane

2002-044-1-500 - Solubility data related to industrial processes. Carbon dioxide in aqueous non-electrolyte solutions

2002-045-1-500 - Solubility data related to industrial processes. Solids and liquids in supercritical carbon dioxide

2002-050-1-500 - Solubility data related to industrial processes. Acetonitrile: ternary and other multicomponent systems

2005-006-1-500: Mutual solubility of alcohols and water (update of SDS Vol 15)

2005-033-1-500 - Transition and 12 to 14 main group metals, lanthanide, actinide and ammonium halates

Division participation in interdivisional projects

2003-060-2-400 - Terminology on separation of macromolecules

2003-056-2-500 - Standard definitions of terms relating to mass spectrometry

2004-021-1-300 - Reference methods, standards and applications of photoluminescence

2004-023-1-700 - Internationally agreed terminology for observations in scientific communication

2004-005-2-500 - Comparable pH measurements by metrological traceability

2004-017-1-500 - Standardization of analytical approaches and analytical capacity-building in Africa

IV3. Division representation at conferences

- International Congress on Analytical Sciences (ICAS 2006), Moscow, Russia, June 2006

- 12th International Symposium on Solubility Phenomena and Related Equilibrium Processes, Freiberg, Germany, July, 2006

- International Symposium on Metallomics, Nagoya, November 2007