

## Report of the IUPAC Analytical Chemistry Division (V)

August 2003 – August 2004

Kip Powell, President

### 1. Executive Summary

The Division has an active portfolio of good projects and a steady stream of projects “in preparation”. It has identified a limited number of priority areas for its activities and adopted an approach of “collective responsibility” for these.

#### **Highlights:**

- To facilitate the development of new projects the Division has involved external experts in “mini-symposia” held in conjunction with its GA meeting and its even-year meeting.
- To ensure attention to critical areas it 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 formed seven Teams each of which has responsibility for one priority area. Each Team will identify the outcomes that it wishes to achieve in the biennium.
- To ensure opportunities for participation each NR, AM and TM is assigned to two Teams. The Team structure will facilitate continuity of effort into the next biennium.
- Communication within the Division and with other officers of the union is maintained through the newsletter “*Teamwork*”.
- To assist in communication of IUPAC goals and concerns with member countries the Division is preparing a series of articles for *CI* on the topic of “*Emerging needs of developing countries*”.
- The updating and maintenance of two key IUPAC publications, The Compendium of Analytical Nomenclature (Orange Book) and the IUPAC Stability Constant Database (SCDB), is actively supported by the Division. A consultative team is working with Academic Software to ensure the on-going maintenance of SCDB when AS relinquishes this role in 3 years.
- A contestable funding process is in place (two rounds per year) and is working satisfactorily.
- The Division has made significant moves to build 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).

### 2. Challenges and Solutions

*The principal challenges to the ACD are typical of many IUPAC Divisions:*

- The breadth of its portfolio *vis a vis* the limitations of membership.
- A membership selected for the expertise of individuals, but who must become part of a team.
- The generation of members’ collective responsibility for
  - the goals of the Division
  - the needs of countries not represented
  - the long-range goals of IUPAC
- Maintaining momentum through the biennium and with the change of biennia.

*The principal strategy (solution) adopted by the ACD to address these challenges:*

- Identification of a manageable number of priorities for the biennium. These cover 'Core activities' and 'Emerging issues in analytical chemistry' (see Section 3.1)
- Formation of Teams, each with collective responsibility for one priority area. Each Team
  - consists of AM + NR + TM
  - has responsibility to set and achieve objectives – one significant output per year.
  - has responsibility to ensure a roll-over of activity at the end of the biennium
- Efforts focused on the needs of developing countries and on links with other agencies (Section 3.4).
- Use of mini-symposia to bring in external expertise.
- Maintaining active communication between members, e.g. through the newsletter, *Teamwork*.

### 3. Report on Division activities in relation to IUPAC goals

3.1. *IUPAC will provide leadership as a worldwide scientific organisation that objectively addresses global issues involving the chemical sciences.*

**Setting priorities.** The Division is unable to comprehensively cover all aspects of analytical chemistry. Therefore (a) it has identified priorities that are based on the current needs of the scientific community, and (b) is making use of workshops or 'mini-symposia' to inform the Division members on current issues. The priorities are summarised under the headings 'Core activities' and 'Emerging issues'. The former represent on-going functions of the Division; the latter are more time-dependent and are likely to change to some degree from one biennium to the next:

**Core Activities:**

Communication

Project initiation and management in the areas of:

- Quality Assurance
- Terminology – Orange Book updating
- Critical evaluation of data

**Emerging issues in analytical chemistry:**

- in bioanalytical chemistry
- in process chemistry and nano-chemistry
- in developing countries and scientific communities.

**Core Activities** includes critical evaluation of data, harmonisation of quality assurance methods and maintenance and updating of the Orange Book. It also places a significant emphasis on communication – dissemination, meetings with stakeholders, publications etc. **Emerging issues in analytical chemistry** attempts to keep pace with the evolution of analytical chemistry and to address the needs of chemists in developing countries.

For each priority area a Team of 4-6 has been formed. Each NR is on one Team; most AM and TM are on two Teams. The priorities and Team membership are posted on the web. Each Team has a collective responsibility and has been encouraged to:

- Determine the scope of its responsibility and activities and develop a strategy for effective Team communication and action.
- Develop a strategy for effective two-way communication with appropriate stakeholders.
- Identify activities that advance the goals of IUPAC in its designated area.
- Identify, and facilitate, at least one output that is achievable in year 1 and one in year 2 of the biennium (e.g. letters to Editors; an informal group meeting at a Conference to scope a project idea; an IUPAC presentation at a Conference; an article for *CI*; a vector article for IUPAC or the ACD; an improvement or addition to the ACD website; a new Project Proposal; etc.)

- Inform the Division on opportunities that it identifies for ACD action, including the use of Workshops or Symposia, separate from, or in association with, the GA.
- Accept responsibility for leading ACD activity in its designated area (e.g. assisting Task Groups in development of Project Proposals and in review of completed Projects)
- Facilitate a 'roll-over' of its activities at the end of the current biennium.

The Division is a group of individuals. But by working in Teams we expect to create added value to the sum of efforts of the individuals. Teams will play an important role in sustaining activity between Division meetings. They will provide continuity of experience across biennia.

**Global issues.** One global issue that is being addressed is the concept of '*fair trade*'. Fair Trade can only arise between less developed and more developed nations when the former have adequate and *quality assured laboratories* and their methodology meets the current requirements for *metrological traceability*. These concepts have been the basis of two joint project proposals:

- (a) With IOCD. A project proposal from IOCD, but which includes several Division V members, is titled: "*Standardisation of analytical approaches and analytical capacity building in Africa*". This involves a melding of IUPAC technical expertise with IOCD appreciation of geopolitical issues in developing countries. This project has been successful in obtaining IUPAC funding but still requires major support (\$200,000) from the World Bank and UNESCO.
- (b) With UNIDO and IUPAP. Division V supported the WPQA in preparation of an ICSU proposal on "*Measurement traceability – a fair basis for trade*". This application for funds was not successful but the process of preparing this proposal generated very positive interactions with UNIDO and IUPAP (including participation in a WPQA/Division V workshop) and we are currently looking for ways to capitalise on this relationship.

**Symposia and Workshops.** Mindful of its limited membership and capabilities the Division attempts to capture external expertise to introduce and scope emerging issues or opportunities in analytical chemistry. This has been achieved through mini-symposia held in conjunction with the Division committee meeting at the GA and its even-year meeting. This also places collective responsibility on the Division committee to identify new project opportunities and to encourage formation of Task Groups to address these.

In Ottawa 2003 a mini-symposium on "*New Challenges for Analytical Chemists in Genomics, Proteomics, and Genetically Modified Organisms*" was held. It capitalised on local expertise and on experts attending the Congress meeting. From this event three new projects were identified. To date one has been funded ("*Standard definition of terms related to mass spectrometry*") while those on "*Terminology related to analytical chemistry of metal forms in biological systems: metallomics*" and "*Comparison of the terms: preconcentration/sample preparation as used in GMO analysis and in classical analysis*" have been thoroughly scoped and will soon be assessed as Project Proposals.

In Vienna 2004 a mini-symposium on "Metrological traceability" was held jointly with IAEA staff and the WPQA and attracted speakers from IUPAP, UNIDO, BIPM, IAEA and WPQA. The meeting identified several areas in which IUPAC expertise might be applied. Much was achieved in terms of dialogue and goodwill. We now try to identify possible 'concrete' outcomes from that meeting - IUPAC projects that could be crafted around the ideas and concerns that were shared and will capitalise on the momentum generated. IUPAC will benefit through any projects that link it with agencies that are working much closer to the geopolitical coal-face.

### *3.2. IUPAC will facilitate advancement of research in the chemical sciences through the tools that it provides for international standardisation and scientific discussion*

Division V 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 updating of analytical nomenclature and making it readily available via the web:

- (a) **The Solubility and Solution Equilibrium Data sub-committee (SSED)** has a very active program of projects that embrace the generic topics of critical evaluation of solubility data related to (a) mobility of metals in the environment, (b) to industrial processes, (c) human health. The outputs appear as papers in the Journal of Physical and Chemical Reference Data or as book volumes and are thence transferred to the NIST-IUPAC Solubility Database: <http://srdata.nist.gov/solubility/>. Another project is concerned with Chemical speciation of environmentally significant heavy metals with inorganic ligands.
- (b) **The IUPAC Stability Constants Database (SCDB)** is the most comprehensive compilation of stability constants available. It is the primary source of data for the Critical evaluations of Stability Constants that have been published on a regular basis by Division V. It is a major research tool for those involved in equilibrium modelling of environmental, biological and industrial systems.

In its current form SC-Database represents a 16 year investment of time and expertise by Academic Software (Leslie and Gwyn Pettit). Their generous commitment to IUPAC has been supported by Commission V.6. and currently through a Division V project. SC-Database is a superb record of the published literature and a masterfully crafted software system.

Academic Software wishes to transfer the responsibility for management and maintenance of SC-Database to IUPAC within 3 years.

Division V has formed a consultative team (Folke Ingman, David Moore and Kip Powell) to work with Academic Software and the Executive to effect a successful transition to management by IUPAC or an alternative external systems manager. We note that IUPAC should urgently establish strategies for maintenance, presentation, marketing and management of the database. There is a great risk that it will not be maintained and available to the chemistry community in the future if IUPAC does not act appropriately.

- (c) **The Orange Book**. This is now on-line and searchable.  
([http://www.iupac.org/publications/analytical\\_compendium/](http://www.iupac.org/publications/analytical_compendium/))

The text will be progressively converted to XML format. The result will be that each entry is better linked to other terms and is web-compatible rather than a simple pdf file. The entries will be in ICTNS-accepted format and in common with the Gold book version, so there will be only one version within the IUPAC database.

The route for updating terminology in the OB will be via formal publication in *PAC*. Work is progressing to identify missing topics that needed attention. There are still some problems with equations and formulae.

- (c) **The WPQA** continues to produce publications that are of value to chemists in analytical laboratories; .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*.

### 3.3. IUPAC will 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 evaluation and compilation for the IUPAC Stability Constant Database. The SSED were joint organisers of the 11<sup>th</sup> International Symposium on solubility phenomena (Aviero, 2004) at which there was significant emphasis on industrial issues and involvement of industrial chemists.

The Division is represented in the Task Group for the project: *Chemistry's contributions to humanity*.

*3.4. IUPAC will foster communication among individual chemists and scientific organisations, with special emphasis on the needs of chemists in developing nations.*

*Analytical Chemistry in Developing countries*

The Division seeks to expand activities in this area. It is fortunate in having an active NR from India (Jaya Arunachalam) and in having several members with established professional links with the African continent (Jan-Åke Jönsson, Walter Lund and Roger Smith). Nelson Torto (Botswana), has joined the ACD as a Provisional Member representing the IUPAC Associate Organisation, SEANAC; we will benefit from his contribution. The Division sponsored the attendance of a TM at the inaugural conference of SEANAC in Botswana in 2003. The Division is significantly involved in the project with IOCD: "*Standardisation of analytical approaches and analytical capacity building in Africa*".

One potential difficulty in establishing links with developing countries is that few are members of IUPAC. Is there any effective way that IUPAC can generate an outreach though chemical societies in countries which are currently not NAO?

*Communication*

The Division mini-symposia held in Ottawa and Vienna have assisted with contacts with external organisations and research chemists. The Division has arranged with *CI* to publish a bi-monthly series of short articles on *Emerging needs of developing countries*; these will commence in February. The Division has sought and confirmed 7 contributions to this series.

*Building bridges with other organisations.*

The SSED works actively with NIST in the preparation of critical evaluations for publication in the NIST-IUPAC Solubility Data Series. The joint Division V - WPQA meeting in Vienna showed that many new dynamics can be brought to our activities by discussing and collaborating on focused issues with other organizations, in this case IUPAP, IAEA, UNIDO.

Through the WPQA the Division is represented on the Coordinating Committee on Chemistry and Materials, ISO-Committee on Reference Materials, the International Committee on Weights and Measures, the Consultative Committee for Amount of Substance (BIPM), EURACHEM and CITAC.

*Better Communication.* Dissemination of projects and results is a crucial issue for improving the impact of our work on the chemistry community. This is overseen by the "Communications" team. Improved lines of communication between TG chairs and the Division have been facilitated by the establishment of a 6-monthly Project reporting system in which the TGC responds to questions re progress, milestones, difficulties, and opportunities for further work etc.

The Division is being pro-active in recommendations for improved IUPAC representation at IUPAC-sponsored conferences. It considers that there is scope for improved representation and enhanced involvement of IUPAC representatives at IUPAC-sponsored conferences. This might be aided if conference organisers were required to discuss the nomination of an IUPAC representative with the relevant Division ahead of submitting the AIS. It is all too easy for Conference programs to be 'finalised' ahead of representative appointment, or without reference to IUPAC requirements.

*3.5. IUPAC will utilise its global perspective and network to contribute to the enhancement of chemistry education, the career development of young chemical scientists, and the public appreciation of chemistry.*

The Division has actively participated in the Young Observers scheme. As a result of active contribution to Division goals, the latest attendee, Kermit Murray, has been appointed to the Division committee as an AM. The question of career development for young chemists (in

developing countries) will be raised in one of the proposed articles for *CI*. The Division is represented in the Task Group for the project: *Chemistry's contributions to humanity*.

3.6. 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.

Division V has in place a strategy, which is communicated to the Nominations' Committee, to ensure widest possible geographic representation. The Division actively sought participation of Nelson Torto as a PM representing the ANO, SEANAC.

Within its own structures, the Division works to ensure **active** involvement of all AM, TM and NR.

#### 4. Publications since August 2003:

##### CURRENT PROJECTS

\* Interdivisional project

- 1999-044-2-500 - [Terminology for the description of peak asymmetry in chromatography](#)
- 1999-050-1-500 - [Chemical speciation of environmentally significant heavy metals and inorganic ligands](#)
- 2000-003-1-500 - [Ionic strength corrections for stability constants](#)
- 2000-004-2-500 - [IUPAC stability constants database - completion of data collection up to 2000+](#)
- 2001-041-2-500 - [Recommendation on the use of countercurrent chromatography in analytical chemistry](#)
- 2001-063-1-500 - [Revision of terminology of separation science](#)
- 2001-072-1-500 - [Low activation materials for fusion technology: State and prospects](#)
- 2001-073-1-500 - [Determination of alpha-emitting radionuclides in diet: Review and evaluation of analytical methods for artificial and natural alpha-emitting nuclides in food and human tissue](#)
- 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](#)
- 2003-011-3-600 - [A critical compendium of pesticide physical chemistry data\\*](#)
- 2003-015-2-500 - [Terminology, quantities and units concerning production and applications of radionuclides in radiopharmaceutical and radioanalytical chemistry](#)
- 2003-037-1-500 - [Optical biosensors and bioprobes; Series on Nomenclature, Symbols, and Units in Spectrochemical Analysis](#)
- 2003-056-2-500 - [Standard definitions of terms relating to mass spectrometry\\*](#)
- 2003-060-2-400 - [Terminology on separation of macromolecules\\*](#)
- 2004-017-1-500 - [Standardization of analytical approaches and analytical capacity-building in Africa\\*](#)
- 2004-021-1-300 - [Reference methods, standards and applications of photoluminescence\\*](#)
- 2004-023-1-70 - [Internationally agreed terminology for observations in scientific communications\\*](#)

##### INTERDIVISIONAL WORKING PARTY ON HARMONIZATION OF QUALITY ASSURANCE

- 2000-033-1-500 - [Assessment of uncertainty associated with soil sampling in agricultural, semi-natural, urban and contaminated environments \(SOILSAMP\)](#)
- 2001-010-3-500 - [Metrological traceability of measurement results in chemistry](#)

2003-004-1-500 - [Interdisciplinary harmonised approach to metrological traceability of chemical measurement results](#)

#### **SUBCOMMITTEE ON SOLUBILITY AND EQUILIBRIUM DATA**

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](#)

2002-033-1-500 - [Solubility data related to oceanic salt systems. Part I - Binary systems containing sodium, potassium, and ammonium sulfate](#)

2002-034-1-500 - [Solubility data related to oceanic salt systems. Part II - magnesium chloride-water and calcium chloride-water and their mixtures](#)

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](#)

2002-038-1-500 - [Solubility data of compounds relevant to human health. Antibiotics: peptide antibiotics and macrocyclic lactone antibiotics](#)

2002-042-1-500 - [Solubility data related to industrial processes. Lead sulfate](#)

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](#)

2003-018-1-500 - [Mutual solubility of hydrocarbons and water](#) (update of SDS Vol 37 & 38)

#### **PROJECTS NEAR COMPLETION / IN PRESS**

1999-050-1-500 - [Chemical speciation of environmentally significant heavy metals and inorganic ligands. Part I Mercury.](#)

2001-052-1-500 - [Solubility of volatile and gaseous fluorides in all solvents](#)

2001-085-1-500 - [IA and IIA azoles, cyanates, cyanides and thiocyanates](#)

2003-018-1-500 - [Mutual solubility of hydrocarbons and water](#) (Part 1)

#### **UNDER REVIEW BY ICTNS OR AUTHORS**

550/64/97 - [Non-selective sensors arrays \("Electronic Nose", "Electronic Tongue"\) chemical analysis: classification and characterization](#)

2000-033-1-500 [Terminology in soil sampling](#) (V)

[http://www.iupac.org/reports/provisional/abstract03/faigelj\\_301103.html](http://www.iupac.org/reports/provisional/abstract03/faigelj_301103.html)

2001-055-1-500 - [Critical evaluation of stability constants of metal complexes of complexones for biomedical and environmental applications](#)

2001-075-1-500 - [Compilation of  \$K\_0\$  and related data for NAA in the form of electronic database](#)

2001-038-2-500 - [Recommendations for NMR measurements of high pK values and equilibrium constants in strongly basic solutions](#)

2001-009-1-500 - [Revision in the international harmonised protocol for the proficiency testing of \(chemical\) analytical laboratories](#)

**PUBLISHED REPORTS (2003 - 2004)**

- Alkali and Alkaline Earth Metal Pseudohalides *J. Phys. Chem. Ref. Data*, **2004**(1), 33, 1-176.  
[Ionic strength corrections for stability constants <http://www.iupac.org/projects/2000/2000-003-1-500.html>](http://www.iupac.org/projects/2000/2000-003-1-500.html)
- Chemical speciation of Hg(II) with environmental inorganic ligands. *Australian J.Chem.*, **57**, 1-8 (2004)  
[Guidelines for calibration in analytical chemistry. Part 2: Multicomponent calibration](#) (IUPAC Technical Report)  
*Pure Appl. Chem.* **76**(6), 1215-1225 (2004)  
[Critical evaluation of the state of the art of the analysis of light elements in thin films demonstrated using the examples of SiO<sub>x</sub>N<sub>y</sub> and AlO<sub>x</sub>N<sub>y</sub> films](#) (IUPAC Technical Report)  
*Pure Appl. Chem.* **76**(6), 1161-1213 (2004)  
[Piezoelectric chemical sensors](#) (IUPAC Technical Report)  
*Pure Appl. Chem.* **76**(6), 1139-1160 (2004)  
[Electrochemical detection in liquid flow analytical techniques: Characterization and classification](#) (IUPAC Technical Report)  
*Pure Appl. Chem.* **76**(6), 1119-1138 (2004)  
[Terminology for analytical capillary electromigration techniques](#) (IUPAC Recommendations 2003)  
*Pure Appl. Chem.* **76**(2), 443-451 (2004)  
[Determination of trace elements bound to soil and sediment fractions](#) (IUPAC Technical Report)  
*Pure Appl. Chem.* **76**(2), 415-442 (2004)  
[Critical assessment: Use of supersonic jet spectrometry for complex mixture analysis](#) (IUPAC Technical Report)  
*Pure Appl. Chem.* **75**(7), 975-998 (2003)  
[Critical review of analytical applications of Mössbauer spectroscopy illustrated by mineralogical and geological examples](#) (IUPAC Technical Report)  
*Pure Appl. Chem.* **75**(6), 801-858 (2003)  
[Critical evaluation of stability constants for alpha-hydroxycarboxylic acid complexes with protons and metal ions and the accompanying enthalpy changes. Part II. Aliphatic 2-hydroxycarboxylic acids](#) (IUPAC Technical Report) (V.6)  
*Pure Appl. Chem.* **75**(4), 495-540 (2003)  
[Critical evaluation of the chemical properties of the transactinide elements](#) (IUPAC Technical Report) (V.7)  
*Pure Appl. Chem.* **75**(1), 103-108 (2003)  
[Critical evaluation of stability constants and thermodynamic functions of metal complexes of crown ethers](#) (IUPAC Technical Report) (V.6)  
*Pure Appl. Chem.* **75**(1), 71-102 (2003)

**IUPAC REPRESENTATION AT CONFERENCES**

Colloquium Spectroscopicum Internationale (CSI XXXIII) 7-12.09. 2003 Granada (Spain)

Analytical Forum 2004, 4-8 July 2004, Warsaw (Poland)