

Report of IUPAC Analytical Chemistry Division (V)**August 1999 – May 2001****Folke Ingman, President*****I. Executive Summary***

The Division has had a productive biennium. It has also moved to position itself, in structure and attitude, to make an effective transition from a Commission-based to Task Group-based project system.

1. The new structure for the Division, post 2001, was determined at a meeting of the Executive and all Commission Chairs in May 2000. It ensures continuation of the Division's core business:
 - Quality Assurance,
 - Nomenclature and Techniques,
 - Data Evaluation,
 - Critical Reviews and Guidelines.
2. The eight specific subject areas to be covered by the new Division Committee and its designated TMs are: Electroanalytical chemistry, Environmental analytical chemistry, General Aspects of Analytical Chemistry, Human Health, Nuclear chemistry, Separation methods, Spectrochemical analysis.
3. To effect their timely completion, all projects initiated under the Commission structure are required to be at least at the Commission Review stage before the Brisbane GA. Those unable to meet this deadline have been terminated.
4. During this biennium 19 projects have been published while 4 are 'in press' or with the IDCNS.
5. Seven projects have been approved under the new Project Submission scheme (a total of 16 applications received, with 4 currently under review).
6. Commissions are assembling information to start a Database of Expertise in Analytical Chemistry. This compounding database will be a legacy from the Commissions and will assist successive Division Committees in their search for reviewers and referees, stakeholders and Task Group members and in the formation of Advisory Groups to assist TM.

II. Report on Division Activities, in relation to IUPAC's goals.

Selected outputs from the Division's activities are used to demonstrate its contributions to IUPAC's goals.

1. *Advancement of research in the chemical sciences throughout the world.*

The Division is concerned with Critical Reviews of data that will facilitate both fundamental and applied research. Such activity is indicated by publications from the Commissions on Equilibrium Data and Solubility Data (e.g. '*Critical evaluation of the stability constants of phosphonic acid complexes*'). It is also indicated by current projects such as ('*Critical evaluation and prediction of stability constants of metal complexes of complexones for biomedical and environmental applications*').

It is also concerned with the assembly of Critically Evaluated Databases. Late in 2000 the Division initiated a major project to bring the IUPAC Stability Constant Database up to date to year 2000.

Projects on nomenclature and terminology are of generic value in chemistry. Current, or recent projects deal with terms such as 'Recovery', 'Selectivity', 'Retention parameters in gas chromatography', 'Dimensionality' and 'Chemical speciation and fractionation', as applied in analytical chemistry.

Through the Working Party on Quality Assurance, 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.

2. *Assist chemistry-related industry in its contributions to sustainable development.*

The Division established and has supported the Working Party on pH. The international adoption of a common agreed method for standardisation and measurement of sample pH is a vexed and regionally-sensitive question. Any recommended protocol has the potential for significant financial impact on manufacturers. This inter-divisional Working Party, working in consultation with stakeholders, has produced a Provisional Recommendation ('Definition of pH scales'). This document is on the web and is currently available for comment.

3. *Facilitate the development of effective channels of communication in the international chemistry community.*

A number of current projects have, or will, involve workshops at which significant groups of scientists, including stakeholders, will assist in scoping of the project or in reviewing its initial findings.

A Workshop arranged by the WP on Quality Assurance, held in November 1999, attracted 120 participants from 34 countries: scientists and representatives of agencies, governments, standardisation and accreditation bodies involved in method validation or in acceptance of analytical methods for legislative purposes. From this meeting, a joint project with FAO, IAEA and AOAC Int. evolved: '*Preparation and harmonisation of internationally harmonised guidelines for in-house method validation*'. Its objectives are to provide both general and specific guidelines on methods for determination of pesticide and veterinary drug residues and trace organic contaminants in food.

The project on 'Solubility Phenomena – Application for Environmental Improvement' will use a Workshop to identify appropriate international bodies for collaboration and sponsorship, to identify specific environmental issues and the means of outreach to environmental specialists.

4. *Contribute towards the enhancement of education in chemistry and to the public understanding of chemistry.*

The Division's commitment to education is expressed through its representation on the Committee for Teaching of Chemistry and on the Education Strategy Development Committee. It has taken a leading role in tertiary education (an area not previously covered by the CTC) through the production of the SolEq (Solution Equilibrium) tutorials on CD.

5. *Make special efforts to assist the career development of young chemists.*

The Division included a 'young scientist' (Prof. Linda McGown) on its 2001 Nominations Committee. It has appointed a 'young scientist' (Prof. Michelle Bushey) to attend its meetings at

the 2001 General Assembly. The Division's current Vice-President established his links with the Analytical Division through a similar appointment in 199*. In creating a Directory of Expertise in Analytical Chemistry, it has specifically instructed Commissions to provide names of 'emerging' active analytical chemists.

6. *Encourage world-wide dissemination of information.*

The Division is actively engaged in preparing the highly successful 'Orange Book' (Compendium of Analytical Chemistry) for public access on the web. It is also developing protocols for the timely updating of its content.

Several of the Division V Commissions, and its Working Party on Quality Assurance, produce documents on Nomenclature and Terminology. As part of the standard review process these documents appear on the web for comment from the wider scientific community.

The Commission on Solubility Data has negotiated with the National Institute of Standards (NIST) for electronic dissemination of its evaluated solubility data (the IUPAC-NIST Solubility Data Project), utilising the experience of NIST in operating web-based chemical databases.

7. *Assure sound management of IUPAC's resources to provide maximum value for the funds invested.*

The Division has gained much experience through 2000-1 in assessing new Project Submissions, in providing applicants with advice regarding definition of goals and milestones, and in formulating meaningful outputs. Commencing in 2002 the Division will assess and fund new Project Submissions in three categories and on a contestable basis to ensure that both funds and Division support are channelled into the most meaningful projects.

III. Division Strategy and Direction

Structure:

The Division has given much thought to its evolving structure and to the fulfilment of its responsibilities. It sees as its core business: Nomenclature and Techniques, Quality Assurance, Data Evaluation and Critical Reviews. To achieve its objectives, seven Titular members will be elected, each with expertise and responsibilities in one of the following areas. In addition, each TM will have responsibility for links with other Divisions and interest groups (shown in italics):

- Electrochemical analysis: *links with Division I, Physical chemistry.*
- Environmental analytical chemistry (speciation; trace analysis): *links with Division VI, Environmental chemistry.*
- General aspects of Analytical chemistry (nomenclature; chemometrics; quality assurance; equilibrium and solubility data): *responsibility for the Orange Book and links with sub-committees on QA and solubility data.*
- Human health (analytical methods for assessing human health): *links with Division VII, Human Health.*
- Nuclear chemistry: *links with Division VII, Human Health.*
- Separation methods: *links with the Pharmaceutical industry (from which 1 or 2 of the Advisory Committee members should be appointed).*
- Spectrochemical analysis: *links with Division I, Physical chemistry.*

Together with the Executive (President, Past-President, Vice President and Secretary), appointed AMs and invited Advisory Groups the TM will maintain a portfolio of good projects that cover the core areas.

They will identify emerging topics, promotional opportunities, nomenclature issues and needs for databases and their evaluation.

The Terms of Reference for the Division have been updated to accommodate the revised Division structure (8 Commissions replaced by 7 designated TMs and associated Advisory Committees, and 4 broad areas of responsibility). To ensure transfer of knowledge and experience from the wide membership base of 8 Commissions through to the much smaller membership base of the Division Committee, each Commission is preparing a contribution to an Analytical Division Database of Expertise.

Stakeholders and visibility:

The Division is aware that it must be more pro-active in identifying and working with stakeholders. In the past it has tended to 'follow' rather than 'lead' and has therefore lost leverage with stakeholders. It is committed to working with stakeholders to find consensus on contentious issues and to encouraging them to comment on IUPAC recommendations before they are published. The activities of the WP on Quality Assurance (working closely with ISO, IRMM, IAEA, EC, FDA, AOAC International, CITAC, EURACHEM, CCQM/BIPM and IUPAC Divisions I, V, and VII), the WP on pH, and Commission V.8. (working closely with NIST) provide examples of successful linkages. They are also examples of bodies in which work is coordinated by a few IUPAC TMs but undertaken by many more volunteer non-IUPAC members.

The Division Executive has given some thought to project development in partnership with stakeholders and to mechanisms for ascertaining the needs of the analytical chemistry community. Preliminary discussions have centred on sponsorship of a Round Table meeting between representatives of one industrial sector pertinent to the Division's portfolio and an appropriate group of Division members. It is appreciated that such meetings must have a clearly defined focus to be successful. Over a period of time these meetings could draw on a range of industries and canvas several geographic areas.

The Division actively encourages the use of workshops and conferences as one means of dissemination of project outcomes.

The Division has made recommendations to the Secretary General regarding the need for improved visibility of IUPAC at major national and international conventions at which stakeholders will be represented, e.g. Pittcon, Achema and Analytica. Such venues are a forum for IUPAC to listen to stakeholders and to promote its products.

New Projects:

Projects approved since August 1999 under the new Project Submission system are:

- Solubility phenomena – applications for environmental improvement.
- Revision of the Compendium of Analytical Chemistry (Orange Book).
- Terminology for the description of peak asymmetry in chromatography.
- Chemical speciation of environmentally significant heavy metals and inorganic ligands.
- Ionic strength corrections for stability constants.
- IUPAC Stability Constants database – completion to 2000+.
- Dimensionality in analytical chemistry.

IV. Publications since August 1999:

Books:

Principles and Practice of Method Validation. Eds. A Fajgelj and A. Ambrus. The Royal Society of Chemistry. 2000. [ISBN 0 85404 783 2]

Pure and Applied Chemistry:

Classification and Use of Terms for Amplification and Related Reactions, *Pure Appl. Chem.*, 71 (1999) 1331.

Electroanalytical data on U, Np, Pu ions in acidic aqueous solution. S. Kihara, *Pure Appl. Chem.*, 71 (1999) 1771-1807.

Phosphorus speciation in water and sediments. H. Muntau, B. Spivakov. *Pure Appl. Chem.*, 71 (1999) 2161.

Nomenclature, symbols, units and their usage in spectrochemical analysis. Part XVII. Laser-based molecular spectrometry for chemical analysis. *Pure Appl. Chem.*, 71 (1999) 2189.

Analytical Aspects of Chemical Process Control. Part 1. Fundamentals and Terminology. *Pure Appl. Chem.*, 71 (1999) 2303.

Electrochemical biosensors: recommended definitions and classification. D.R. Thevenot, K. Toth, R.A. Durst, G.S. Wilson. *Pure Appl. Chem.*, 71 (1999) 2333-48.

Temperature dependence of the Westcott g-factor for neutron reactions in activation analysis. N. Holden. *Pure Appl. Chem.*, 71 (1999) 2309-2315

Species-selective determination of selenium compounds in biological materials. R. Lobinski, J.S. Edmonds, K.T. Suzuki, and P.C. Uden. *Pure Appl. Chem.*, 72 (2000) 447-461.

Guidelines for terms related to chemical speciation and fractionation of elements. Definitions, structural aspects, and methodological approaches. D.M. Templeton, F. Ariese, R. Cornelis, L-G. Danielsson, H. Muntau, H.P. van Leeuwen, and R. Lobinski. *Pure Appl. Chem.*, 72 (2000) 1453-1470.

Micro-electrodes: definitions, characterisation and hints for their use. K. Stulik and V. Maracek, *Pure Appl. Chem.*, 72 (2000) 1483-92.

Spontaneous fission half-lives for ground state nuclides. N.E. Holden. *Pure Appl. Chem.*, 72 (2000) 1525-62.

Potentiometric selectivity coefficients of ion-selective electrodes. Part I. Inorganic cations. Y. Umezawa, P. Bühlmann, K. Umezawa, K. Tohda, and S. Amemiya. *Pure Applied Chem.*, 72 (2000) 1851.

Chemistry International:

Report on the IUPAC/ISO REMCO/BAM/EUROLAB-D Workshop on Proper Use of Environmental Matrix Reference Materials, Berlin, Germany 22-23 April 1999, *Chem. International*, 21 (1999) 142-143.

Report on the EURACHEM 10th Anniversary Meeting and the EURACHEM Full Committee Meeting, Helsinki, Finland, 16-19 June 1999, *Chem. International*, 22 (2000) 35-36.

Report on FAO/IAEA/AOAC Int./ IUPAC International Workshop on Principles and Practices of Method Validation, 4-6 November 1999, Budapest, Hungary, *Chem. International*, 22 (2000) 71-73 and *CITAC News*, February 2000, pp. 6.

Report on International Bureau of Weights and Measures (BIPM) – Consultative Committee of Amount of Substance (CCQM) Meeting and Workshop on Measurement Uncertainty, 29 November to 3 December 1999, Paris, France, *Chem. International*, 22 (2000) 76-78.

SolEq: Solution Equilibria, Principles and Applications. 1999. New Products from IUPAC and Academic Software. *Chem. International*, 22 (2000) 24.

Solubility Data Series:

Volume 68: Halogenated Aliphatic Compounds C3 - C14 with Water. A.L. Horvath and F.W. Getzen. *J. Phys. Chem. Ref. Data*, 28 (1999) 649-777.

Volume 69: Ternary Alcohol-Hydrocarbon-Water Systems. A. Skrzecz, A. Maczynski and D.G. Shaw. *J. Phys. Chem. Ref. Data*, 28 (1999) 983-1236.

Volume 70: The Solubility of Gases in Glassy Polymers. R. Paterson, Y. Yampol'skii, and P.G.T. Fogg. *J. Phys. Chem. Ref. Data*, 28 (1999) 1255-1451.

Volume 71: Binary Nitromethane Systems. V. Sazonov, G.T. Hefter and K.N. Marsh. *J. Phys. Chem. Ref. Data*, in press.

Other refereed journals:

Harmonized Guidelines for the Use of Recovery Information in Analytical Measurement. *Eurachem Newsletter* No. 15, pp. 2, and *Accred. Qual. Assur.*, 4 (1999) 512.

Information on the activity of the IUPAC Interdivisional Working Party on Harmonisations of Quality Assurance Schemes for Analytical Laboratories 1997-1999, *Accred. Qual. Assur.*, 4 (1999) 520-521.

Terminology and definitions: Alphabetical index of defined terms and where they can be found Part I, *Accred. Qual. Assur.*, 4 (1999) 525-530; Part II, *Accred. Qual. Assur.*, 5 (2000) 77-82; Part III, *Accred. Qual. Assur.*, 5 (2000) 159-164.

Other:

SolEq: Tutorials on Solution Equilibria. Published as a CD by Academic Software/IUPAC, 1999.

'In Press' (Submitted to PAC):

Critical Evaluation of Stability Constants of Phosphonic Acids. L.H.J. Lajunen and K. Popov.

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. R. Portanova, L.H.J. Lajunen, M. Tolazzi and J Piispanen.

Molality-based primary standards of electrolytic conductivity. K.W. Pratt, W. F. Koch, Y. C. Wu, and P. A. Berezansky.

On the web for public review:

Selectivity and specificity in analytical chemistry. J. Vessman, et al.

Commission representation at Conferences:

5-th International Conference on Nuclear and Radiochemistry (NRC5), September, 3-8, 2000, Pontresina, Switzerland.

RADSITE-SCOPE meeting, December, 4-7, 2000, Brussels, Belgium.

8th International Conference on Flow Analysis, 25-29 June, 2000. Warsaw, Poland.