Report of the IUPAC Analytical Chemistry Division (V)
January 2002 – June 2003
David Moore, President

I. Executive Summary

Division V has completed the transition from a Commission-based to a Task Group-based project system, and has added several new managerial tools to enable efficient project acquisition and management. Projects are still being completed and published at a reasonable rate (14 projects published since January 2002; 17 projects either with the ICTNS or in the queue for publication). The Subcommittee on Solubility and Equilibrium Data published two solubility volumes in the Journal of Physical and Chemical Reference Data. However, new project proposals are not arriving at a high enough rate. At present, all the project proposals come from former Commission or Division members. To improve this situation, projects are being solicited via a four-pronged effort. First, the new Division web pages prominently display a call for proposals, with dates for selection and links to further information on the process. Secondly, each Division Committee TM has established a list of advisors to help them solicit new projects or identify needs for projects (although these have been difficult to establish and few results have been achieved to date). Thirdly, Division Committee members are presenting overviews of IUPAC with details on the project system at several international conferences. Fourthly, we have established plans for focus meetings with targeted industry groups, beginning with a focus meeting on Proteomics at the Ottawa GA.

A new competitive project approval system has been implemented, with ranking of project proposals according to specific guidelines. The approval process is performed semi-annually on proposals that are completed and reviewed by a deadline (April 30 and October 31 each year). This process is envisioned to enable the optimal use of IUPAC project funds to achieve the general goals of the Division. The Division Committee has used this system twice in 2002 and once in 2003. Some projects that need more expedient action are approved outside the cycle via e-mail discussion and voting.

Internal and external communication deficiencies have been addressed via 1) a newsletter, "Teamwork," which has been implemented to keep Committee members and others apprised of their responsibilities, upcoming events, new project proposals, and deadlines, and 2) a new mechanism to oversee projects and their dissemination plans.

The on-line version (http://www.iupac.org/publications/analytical_compendium) of the Compendium of Analytical Nomenclature (Orange Book) has been unveiled on the IUPAC web site. To judge the impact, according to "hits" on the directory, the Orange Book accounts for 1/6 (99432) of the total hits (578399) on the IUPAC publication folder (during the first three months of 2003)! A process to update the Orange Book has been implemented, beginning with the electrochemical analysis and separation methods chapters, to be followed by the other chapters systematically over the next few years. The Division is involved in the IUPAC XML project to decide on a plan for eventual conversion of the Orange Book.

II. Division/Committee Activities Jan 2002 through August 2003, Organized by the Six Goals of the IUPAC Strategic Plan

1. IUPAC will provide leadership as a worldwide scientific organization that objectively addresses global issues involving the chemical sciences.

Division V has implemented well-defined roles of committee members, which include the various fields within analytical chemistry: methods (general aspects, separations, spectrochemical, electrochemical, nuclear chemical) and applications (particularly to environmental and human health problems). To enable analytical chemists to choose the methods best suited for specific applications, the roles of the Division encompass

- the critical and comparative evaluation of established and emerging analytical methods (including the harmonization of associated terminology, proficiency testing, and other inter-laboratory comparisons);
- the recommendations for sample collection, preparation, storage and handling;
- the compilation of data used in analytical chemistry and their critical evaluation;
- the definition of recommended methods and proper application of QC and QA procedures.

To optimally perform its required duties, the Division Committee has established several new managerial and organizational initiatives. Roles and responsibilities were established for each category of Division Committee membership. (These are available on the Division web site and were sent to each member.)

- Each Titular Member (TM) of the Division Committee is encouraged to organize an advisory group in order to help them develop and/or select projects in response to pressing needs in a given area. An advisory group should therefore have a global view and experience in a specific area, in order to aid in identifying and soliciting new projects.
- Associate Members of the committee are to provide focused representation in a particular area of analytical chemistry or to establish a tight link to other IUPAC committees, such as the Committee on Chemistry Education (CCE), the Interdivisional Committee on Terminology, Nomenclature and Symbols (ICTNS), or the Committee on Printed and Electronic Publications (CPEP).
- National Representatives are nominated by IUPAC National Adhering Organizations that are not otherwise represented on the committee (up to 6 are appointed). According to their expertise, each National Representative is linked to a TM, with the goal of ensuring and tutoring their participation in project proposal reviews and Division planning activities.

To date the TM Advisory Groups do not function as intended. See the further discussion of this issue in Section III.

2. IUPAC will facilitate the advancement of research in the chemical sciences through the tools that it provides for international standardization and scientific discussion.

A shortcoming and criticism of the IUPAC has been lack of internal and external communication as well as relevance to the community. We have addressed the internal communication issue by establishing a regular e-mail newsletter ("Teamwork") to keep

members apprised of their responsibilities, upcoming events, new project proposals, and deadlines. As discussed below, initiatives to improve relevance have begun with a fresh review and selection process for new projects, and improved external communication has been addressed by better dissemination of project results. Moreover, we have established a directory of expertise database to allow us to locate experts according to a set of keywords related to their own field of expertise. Each person that has served IUPAC Division V on a commission or project task group in the past decade or more is recorded in the database, and new task group and division committee members, as well as experts involved in project review, will be added.

The revised Division web pages include a large sub-set for project solicitation and explanation of the review and funding process. Included on the New Project Submission page is the next selection date, links to the project submission form, and a link to an example submission, which has annotations giving hints to the level of completeness necessary in critical sections as well as a one-page example (given in an Appendix) of clear evidence of advance planning of the project and of the process that will be used to complete the project.

The Division web site also has clear information on the process used in selection of projects for funding. The information includes links to general guidelines for project priority (appropriateness of funding amount; subject area coverage balance; scientific value to user groups per cost – including guidelines and cost sharing with other funding agencies needed to leverage funds; IUPAC objectives met; and visibility and usability of product), a description of the competitive funding process and the next closing date. This process has been used three times since Jan 2002 to decide which new project proposals make the best use of the funds available to the Division, and the next call closes October 31 with voting in November.

While an individual Task Group Chair (TGC) is responsible for the implementation of the project and the management of the project budget, he/she is expected to prepare a project report twice a year. Practically, a TM of the division committee is to be assigned to track a given project, as soon as funding is approved. (We note that in practice this TM oversight is not yet working as intended.) Each TGC is asked to send a progress report to the Division Vice-President semi-annually (end of June and end of December) stating the completion of milestones, indicating whether any difficulties have been encountered, and stating whether the project is likely still to meet its completion date. All these reports are collated and forwarded to all Division members, so that they can add comments when needed.

The dissemination plan is one of the most important parts of any IUPAC project. How will terminology recommendations, for instance, be made known to practitioners or to the intended audience? Therefore, the implementation of the dissemination plan will be monitored. Again, an assigned TM will liaise with the TGC. As each step in the dissemination plan is executed, the TGC is asked to notify the assigned TM. This tracking system is to supplement the semi-annual progress reports and to help the

Division to improve on external communication. Again we note that the TM liaison assignment is not yet working as intended.

3. IUPAC will assist chemistry-related industry in its contribution to sustainable development, wealth creation, and improvement in the quality of life.

Division V has organized a workshop to be held at Ottawa in conjunction with several Congress invited speakers and organizers, specifically to address new developments in analytical methodology applied to the expanding field of proteomics. The focus of this workshop will be on establishing industrial needs and formulating project proposals within Division V to meet those needs.

A new proposal to "Establish an interdisciplinary (IUPAC consolidated) approach to metrological traceability of measurement results" was prepared and sent to ICSU for consideration in the 2003 funding round. The establishment of such an approach is important not only for international chemical trade, but also for international cooperation in nearly every technical field.

4. IUPAC will foster communication among individual chemists and scientific organizations, with special emphasis on the needs of chemists in developing countries.

The on-line version (http://www.iupac.org/publications/analytical_compendium) of the Compendium of Analytical Nomenclature (Orange Book) has been unveiled on the IUPAC web site. A press release about the availability of analytical chemistry terminology in a cost-free portable document format via the on-line version was sent to several prominent analytical chemistry journals. The impact of having this resource on-line is just being realized, as it presently receives more than 1000 "hits" a day, more than 1/6 of the total "hits" on all web-based IUPAC publications.

5. IUPAC will utilize 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.

Associate Members of the committee were selected to complement the Division expertise by providing representation for specific areas of analytical chemistry. The Division has active involvement in the work of other IUPAC committees though appointment of AMs, to the Committee on Chemistry Education (CCE), the Interdivisional Committee on Terminology, Nomenclature and Symbols (ITCNS), and the Committee on Printed and Electronic Publications (CPEP). We are actively participating in the XML project, which will eventually make IUPAC analytical terminology recommendations more transparently useful to the chemical community.

As a specific initiative in Chemical Education the Division has funded one TM to attend the Inaugural Conference for the Southern and Eastern Africa Network of Analytical Chemists (SEANAC), July 2003. This was seen as a means of IUPAC providing support

and encouragement, and for IUPAC to observe and understand the needs of educators who are teaching analytical chemistry with a minimum of resources.

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.

The smaller size of the division membership has also increased the difficulty in maintaining continuity over many years. We have addressed this problem by establishing a revolving election, whereby half of the committee is elected each biennium to facilitate four-year terms. We have also tasked the Nominating Committee members to be very active to ensure a supply of fresh faces, and to do whatever they can to ensure geographical diversity and complete representation of the different branches of analytical chemistry. It will be recommended to the NC that geographical diversity can be aided by avoiding election of more than two people from the same country. One way we plan to accomplish that is to have the NC seek advice from any over-represented NAO in order to limit the number of nominees from the same country to two.

III. Other Information

We have implemented many new managerial tools to help both with acquisition of new projects and to shepherd them to conclusion, publication, and dissemination. However, we note that all the proposals we have received to date have come from former or present Division, Commission, or Task Group members. Even possibilities that have surfaced at conference presentations have not resulted in a proposal unless the TGC has been involved previously with IUPAC. This is a cause of great concern to us.
Our Division Committee TMs have adapted to their changed roles very slowly. We have only one example to date of any use of their advisory groups to solicit new projects. Also, the majority of the effort of shepherding projects to conclusion continues to be born by the Division officers and the Secretariat. We plan to spend significant time on these issues during our Division Committee meetings at the Ottawa GA.
Finally, we note that we have continued to experience a bottleneck in getting reports from completed projects through the ICTNS review. This process has taken up to one year, and is very frustrating for task groups, especially those which have expeditiously completed their projects according to (or sooner than) the schedule given in their proposal.

IV. Tabular Material

Current Projects

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+

2001-021-1-500 - Analytical electromigration techniques
2001-038-2-500 - Recommendations for NMR measurements of high pK values and equilibrium constants in strongly basic solutions
2001-041-2-500 - Recommendation on the use of countercurrent chromatography in analytical chemistry
2001-055-1-500 - Critical evaluation of stability constants of metal complexes of complexones for biomedical and environmental applications
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
2001-075-1-500 - Compilation of k0 and related data for NAA in the form of electronic database
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

IWPQA

2000-033-1-500 - Assessment of uncertainty associated with soil sampling in agricultural, semi-natural, urban and contaminated environments (SOILSAMP)
2001-009-1-500 - Revision in the international harmonised protocol for the proficiency testing of (chemical) analytical laboratories
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

SSED

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
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 haloganated 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

Projects Completed, in ICTNS review, or In-Press:

501/8/97 - Protocol for In-house Method Validation
510/37/98 - Essential Information for Characterizing a Flow Analyser
510/38/98 - Recommendations for the use of the term 'recovery' in analytical procedures
540/16/95 - Chemical Analysis of Complex Samples using Supersonic Jet Spectroscopy
550/58/95 - Compilation of K(A,B)pot Data
550/63/97 - Lead-Based Second-Kind Electrodes in Aqueous Medium and in Aqueous-Organic Solvent Mixtures
551/1/97 - The Measurement of pH - Definition, Standards and Procedures (revised title)
560/24/87 - Hydroxycarboxylic Acids Part 2: Aliphatic Hydroxycarboxylic Acids
581/26/90 - Ethyne (Acetylene) and Other Gaseous Alkynes
1999-038-1-500 - Solubility phenomena - Applications for environmental improvement
2001-001-2-500 - Dimensionality in analytical chemistry
2001-025-1-500 - Critical evaluation of the state of the art of the analysis of light elements in thin films
2001-037-1-500 - Chemicals in the atmosphere: Solubilities in aqueous media
2001-040-1-500 - Critical evaluation of stability constants and thermodynamic functions of metal complexes of crown ethers
2001-071-1-500 - Critical evaluation of the chemical properties of the transactinide elements
2001-074-1-500 - Critical review of analytical applications of Mössbauer effect
2001-084-1-500 - Experimental determination of solubilities

Publications

Elias A. G. Zagatto, Jacobus F. van Staden, Nelson Maniasso, Raluca I. Stefan, and Graham D. Marshall, Pure Appl. Chem. Vol. 74, No. 4, pp. 585-592 (2002) Information essential for characterizing a flow-based analytical system (IUPAC Technical Report)

Patrizia R. Mussini and Torquato Mussini, Pure Appl. Chem. Vol. 74, No. 4, pp. 593-600 (2002) Sulfate-sensing electrodes. The lead- amalgam/lead-sulfate electrode (IUPAC Technical Report)

Michael Thompson, Stephen L. R. Ellison, and Roger Wood, Pure Appl. Chem. Vol. 74, No. 5, pp. 835-855 (2002) Harmonized guidelines for single-laboratory validation of methods of analysis (IUPAC Technical Report)

Yoshio Umezawa, Kayoko Umezawa, Philippe Buhlmann1, Naoko Hamada, Hiroshi Aoki, Jun Nakanishi, Moritoshi Sato, Kang Ping Xiao, and Yukiko Nishimura, Pure Appl. Chem. Vol. 74, No. 6, pp. 923-994 (2002) Potentiometric selectivity coefficients of ion-selective electrodes. Part II. Inorganic anions (IUPAC Technical Report)

Yoshio Umezawa, Phillipe Buhlmann, Kayoko Umezawa, and Naoko Hamada, Pure Appl. Chem. Vol. 74, No. 6, pp. 995-1099 (2002) Potentiometric coefficients of ion-selective electrodes. Part III. Organic ions (IUPAC Technical Report)

Klaus Danzer, Jacobus F. van Staden, and Duncan Thorburn Burns, Pure Appl. Chem. Vol. 74, No. 8, pp. 1479-1487 (2002) Concepts and applications of the term "dimensionality" in analytical chemistry (IUPAC Technical Report)

K. Popov, H. Rönkkömäki, and L. H. J. Lajunen, Pure Appl. Chem. 74(11) 2227, (2002) Critical evaluation of stability constants of phosphonic acids (IUPAC Technical Report). Errata Pure Appl. Chem. 73, 1641-1677 (2001).

F. Arnaud-Neu, R. Delgado, and S. Chaves, Pure Appl. Chem. 75(1), 71-102, (2003) Critical evaluation of stability constants and thermodynamic functions of metal complexes of crown ethers (IUPAC Technical Report)

J. V. Kratz, Pure Appl. Chem. 75(1), 103-108, (2003) Critical evaluation of the chemical properties of the transactinide elements (IUPAC Technical Report)

R. Portanova1, L. H. J. Lajunen, M. Tolazzi, and J. Piispanen, Pure Appl. Chem. 75(4), 495-540, (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)

E. Kuzmann, S. Nagy, and A. Vertes, Pure App. Chem. 75(6), (2003) Critical review of analytical applications of Mössbauer spectroscopy, illustrated by mineralogical and geological examples.

Compendium of Analytical Nomenclature (Orange Book On-line Version
http://www.iupac.org/publications/analytical_compendium/)

SSED

Volume 77: V.P. Sazonov, et. al. "C2+ Nitroalkanes With Water or Organic Solvents: Binary and Multicomponent Systems," J. Phys. Chem. Ref. Data, 2002, 31, No. 1, 1-121 .

Volume 78: V.P. Sazonov, et. al. "Acetonitrile Binary Systems," J. Phys. Chem. Ref. Data, 2002, 31, No. 4, 989-1133.