

Report of the IUPAC Analytical Chemistry Division (V)

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This report deals with the activities of the Analytical Chemistry Division since the General Assembly in Geneva in 1997. It is comprised of an introductory part on general activity and structure of the Division and then information on subsequent activities of the Division Committee and all Working Parties and Commissions. It closes with the list of projects published during that period. The Division presently consists of 8 permanent Commissions and 2 Working Parties dealing with projects of special importance for the whole of IUPAC.

Working Parties:

Interdivisional Working Party on Harmonization of Quality Assurance Schemes for Analytical laboratories

Working Party on the Definition of pH Scales

Commissions:

V.1 General Aspects of Analytical Chemistry

V.2 Microchemical Techniques and Trace Analysis

V.3 Chromatography and Other Analytical Separations

V.4 Spectrochemical and Other Optical Procedures for Analysis

V.5 Commission on Electroanalytical Chemistry

V.6 Equilibrium Data

V.7 Radiochemistry and Nuclear Techniques

V.8 Solubility Data

The membership of these commissions and working parties is listed in the IUPAC Handbook 1997-1998 as well as the IUPAC web site URL <http://www.iupac.org>.

These commissions and working parties provide a broad representation of Analytical Chemistry. It should be noted that the terms of reference of Commissions V.6, V.7, and V.8 exceed the "core business" of Analytical Chemistry. Projects extend into Physical Chemistry, Inorganic Chemistry, Organic Chemistry, and even Physics.

Commissions V.3, V.4, V.5, and partly V.7 cover the whole field of methods and technologies used in Analytical Chemistry.

Commission V.2 is more problem oriented, although it also deals with methodological questions to a substantial extent. This commission is concerned with some of the most urgent problems of contemporary Analytical Chemistry: trace analysis and speciation of environmental pollutants, quality assurance in trace analysis, and surface analysis.

The existence of the three Commissions V.6, V.7, and V.8, whose terms of reference are much broader than just Analytical Chemistry serves for the whole chemical community, in particular by providing critically evaluated data of general chemical and physical importance.

The Analytical Chemistry Division (ACD) encompasses a broad spectrum of duties that should justify its structure. Here, the Interdivisional WP on Quality Assurance and Commission V.8 may be given as examples of bodies where continuously on-going work is co-ordinated by a few

IUPAC TMs but undertaken by a much larger number of volunteering non-IUPAC members. A similar example is the development of teaching tutorials in Commission V.6, where two TMs serve as co-ordinators for work undertaken by volunteers worldwide - and mainly outside IUPAC.

Activities of the Analytical Chemistry Division Committee

In order to prepare for the reorganization of the IUPAC and evaluate the role the ACD will play in the new structure, a meeting of the officers of the ACD and the Commission Chairs (or their representatives) was held in January 1998. The report from that meeting (submitted with the 1998 Annual Report) outlined a proposed new Division Committee structure, to be composed of a President, Secretary, Past President or President Elect, and the Commission Chairs (or their representatives), leading to more open communication, cross-fertilization of projects, and easier formation of horizontal collaborations. Subsequent events and plans from the SDIC and IUPAC Bureau lead the ACD officers to propose an interim Committee structure of the previous ACD Committee plus the Commission Chairs. This structure was approved by the Bureau in September 1998 and will continue until the IUPAC nomination and election process over the next biennium.

The ACD has strong participation in several Interdivisional Committees and Working Parties. Y. Marcus represents the ACD on the Standing Committee for the Teaching of Chemistry. He represented the Division at the Pittsburgh Conference in New Orleans (March 1998) when the new Eurocurriculum textbook on Analytical Chemistry was presented. The textbook originates from work undertaken by Analytical Division of the Federation of European Chemical Societies and is an important step in harmonising the teaching of chemistry in Europe.

The Interdivisional Working Party on Materials Science is kept abreast of Analytical Chemistry projects and expertise by F. Adams. He is helped in this task by members on several different Commissions.

The importance that the Division attaches to the Interdivisional WP on Quality Assurance Schemes was manifested by adjoining its Chairman, Ales Fajgelj, to the Division Committee and by assigning a Divisional Pool Member to the WP at Geneva.

There are many on-going activities in the ACD that deserve consideration in the new IUPAC structure: 1) Commission V.1 carries the responsibility for keeping the Orange Book up to date; 2) Commission V.6 is involved in keeping the equilibrium database up to date and also does critical evaluations of equilibrium data from an analytical chemistry point of view. The on-going work involves many scientists who are not formally members of IUPAC but is coordinated by a couple of TMs of V.6; 3) Commission V.8 is responsible for the Solubility Data Series. This on-going activity involves well over 100 scientists, just a few of them members of V.8 who assume a coordinating role. Conferences on Solubility Data are also organized by the body; and 4) The Interdivisional Working Party on Harmonisation of Quality Assurance Schemes has been very productive during past years and involves members representing ISO, IRMM, IAEA, EC, FDA, NIST, IUPAC Divisions I, V, VII, etc. The WP arranges symposia on QA with mainly outside funding to discuss issues pertaining to its projects. These on-going activities will require some level of constant IUPAC presence and support, such as advisory groups under a member on the ACD Committee or their Chairs being members of the ACD Committee.

Divisional pool titular members:

Two divisional pool members were continued at the Geneva General Assembly as follows:

Reinhard Niessner (assigned to V.4), coordinator for project 540/20/95, Identification, Coordination and Extension of Bioanalytical Sensors Projects.

Richard Ramette (assigned to V.6), coordinator for project 560/39/95, Development of Materials for teaching of Solution Equilibria (together with H. K. J. Powell). The project received an ICSU grant for 1997 amounting to USD 15 000 and the product will be unveiled at the GA in Berlin.

The third pool Titular Member was assigned to Roger Wood for the Interdivisional WP on Harmonisation of Quality Assurance Schemes

Interdivisional Working Party on Harmonization of Quality Assurance Schemes for Analytical laboratories

The working party collaborates closely with ISO, and all documents published by this party have been agreed between IUPAC and ISO. Other partners with whom there is active cooperation are CITAC, AOAC Int. and Eurachem. There is also a close contact with other divisions of IUPAC, particularly with Divisions I, VI and VII.

The Working Party has new direction, now under the chairmanship of A. Fajgelj. M. Parkany prepared a "History of the IUPAC WP on Harmonisation of Quality Assurance Schemes for Analytical Laboratories".

Two of the new projects undertaken at Geneva: Protocol for in-house method validation and Compilation and clarification of quality assurance related nomenclature will be published soon. A Workshop to complete the third project: Protocol for In-house Method Validation is planned for November 1999. The WP organized a "Workshop on the proper use of reference materials in chemical analytical processes" at the occasion of the BCR 25th anniversary, Brussels, November 9-13, 1998 and held a Workshop on Proper Use of Environmental Matrix Reference Materials in April 1999 in Berlin. The proceedings from the Berlin meeting will be published by the Royal Society of Chemistry.

Working Party on the Definition of pH Scales

The pH Working Party met twice in Durham, England during 1998, and once in Milan, Italy in 1999. Complete reports of the progress at these meetings, and of the WP in general, have been submitted to the Secretary General by the WP Chair. In Spring 1999, after one year of planning and writing, a third meeting was called to read, amend, and combine sections, or to make suggestions on how to make all sections scientifically equivalent in detail. Except for one cell whose error analysis was missing, the WP has compiled some 11 tables of error analyses (all of which may not be shown in the final document). The text was argued over for 10 hours each day, until it was completely revised. The "read-through" of the original was amended and "added-to" in many places. The resulting document will be presented at the GA in Berlin, which can be considered a "best effort" by the WP in the absence of input from the pH World at Large. In the opinion of the members of the WP, this has been a cooperative program and it has produced many points of contention that were resolved in due course.

Commission on General Aspects of Analytical Chemistry (V.1)

The commission held its even year meeting in Basel (Sept. 2-4). The commission assumed responsibility for all projects relating to Quality Control in Analytical Chemistry. They also have

assumed responsibility for keeping the information in the Compendium of Analytical Nomenclature (Orange Book) up to date.

Of the present projects, 510/25/91 was published in PAC. 510/29/95 was withdrawn. Two near-completed projects were split into two parts, with the second parts appearing as new projects (Guidelines for Calibration in Analytical Chemistry, Part 2. Multicomponent Calibration, and Analytical Aspects of Chemical Process Control, Part 2. Evaluation of Methods). Another new project was accepted: Biochemical and Biological Tests (Biotests) for the Determination of Toxicity in Aquatic Systems: Characteristics, Utility and Prospects.

Commission on Microchemical Techniques and Trace Analysis (V.2)

V.2 has had a large turnover in its membership. It has a new secretary, and has just lost its Chairman. The working parties were abandoned since they were found to be too small to be effective. Five projects were cancelled in Geneva. Four more, on quality aspects, were made into chapters in a book. Three projects were published in 1998, two will be published in 1999, and one more has received ACD approval. During the even year meeting in Veszprem August 98 it was decided to merge two projects on selenium into one. One further project was formally cancelled with the intention to revitalise the project within the new IUPAC project framework.

Considerable progress has been made on STE 523/8/93 which is a joint project with several other commissions and which includes nomenclature aspects on speciation. A draft was discussed at the even-year meeting. The 8th draft has been approved by the commissions involved and is presently being reviewed by external experts. Final discussions between the authors are planned for the Berlin meeting.

Commission on Chromatography and Other Analytical Separations (V.3)

The commission held its even year meeting in Madrid, Spain, in August. The work of the Commission focuses on the most modern separation methods including electrochromatography, field flow fractionation and capillary electrophoresis.

One project has been published since Geneva. Three new projects were established in Geneva: Field flow fractionation (530/11/97), Hold-up volume in column chromatography (530/12/97), and Retention parameters in gas chromatography (530/13/97).

Commission on Spectrochemical and Other Optical Procedures for Analysis (V.4)

The even year meeting was held in Münster, Germany, 20 March, 1998.

Project 540/14/93 will be published in 1999. Project 540/5/85 was published in 1998. Work continues on the eleven current projects (Critical Assessments).

Commission on Electroanalytical Chemistry (V.5)

Most of the effort of this Commission has centered on the Working Party on pH (see separate section above). In addition, two projects have been published (550/52/91 and 550/55/93), one will be published in 1999 (550/57/93) and one has received ACD approval (550/61/97). The joint project on Electrochemical Biosensors is being finalized for publication in 1999.

Commission on Equilibrium Data (V.6)

Commission V.6 has been shifting the emphasis of its work from the compilation and critical review of equilibrium data to the application of equilibrium data. The aim of the Commission is to improve the scientific community's understanding of the importance of speciation and the related application of equilibrium data. The outcome will be research scientists better resourced to (i) effect measurements and modelling calculations in labile systems where speciation is important, and (ii) apply the principles of equilibrium speciation in industrial, environmental and bio-inorganic applications. The Commission is also involved in several continuously ongoing projects concerned with the collection of equilibrium data, e.g. the stability constants (SC) database. The work of this Commission is thus of importance for the chemical community in general and not only for Analytical Chemistry.

Project 560/39/95 is finished, and the resulting CD will be unveiled at the GA in Berlin. In addition, three projects have been published since Geneva.

Commission on Radiochemistry and Nuclear Techniques (V.7)

V.7 had its even year meeting during the 13th Radiochemical Conference in Marianske Lazne . The Commission is working out suggestions for the ACD to help identify and select the "hot spots" in the field of radiochemistry and nuclear techniques

One project has been published since Geneva, and another will be published yet in 1999. Two new projects were initiated at the even year meeting.

Commission on Solubility Data (V.8)

A new agreement for publication of the Solubility Data Series was negotiated by V.8 with the Journal of Physical and Chemical Reference Data and approved by the Union. Under this agreement publication resumed in mid 1998 after an 18 month interruption. During the first year of this agreement four volumes (the agreed upon number) have been submitted:

Vol. 66 Ammonium Phosphates, J. Eysseltová and T.P. Dirkse, editors.

Vol. 67 Aliphatic Halogenated Hydrocarbons in Water: Part II: Halogenated Ethanes and Ethenes with Water, A. Horvath and F.W. Getzen, editors.

Vol. 68 Aliphatic Halogenated Hydrocarbons in Water: Part III: Halogenated Aliphatic Compounds C3-C14 with Water, A. Horvath and F.W. Getzen, editors.

Vol. 69 Ternary Systems Containing Alcohols, Hydrocarbons and Water, A. Skrzecz, A. Maczynski and D.G. Shaw, editors.

Volume 66 has already been published and the remaining three volumes are expected to be published before the end of 1999. Four volumes to be submitted between July 1999 and June 2000 will be drawn from projects close to completion.

Negotiations are also underway between V.8 and the US National Institute of Standards and Technology (NIST) concerning electronic dissemination of evaluated solubility data. Although these negotiations are not yet concluded, we are optimistic that the experience of NIST in operating web-based chemical databases can be extremely helpful in making an electronic solubility database a functioning reality.

The International Symposia on Solubility Phenomena (ISSP) were organized with IUPAC sponsorship. These biennial meetings provide opportunities for presentation of original research

and the discussion of topics related to solubility. They also provide venues for participants in the work of V.8 to meet and discuss the progress of Commission projects. The Eighth ISSP was held in Niigata, Japan, 5-8 August 1998. Preparations are well underway for the Ninth ISSP to be held in Hammamet, Tunisia, 25-28 July 2000. The Tenth ISSP is scheduled for Sofia, Bulgaria in August 2002.

Commission V.8 decided that it is in the best interests of the international scientific community and the participants in the solubility data project to continue within IUPAC in a form that is consistent with the new organization of IUPAC. A proposal was recently submitted to the Union for creation of a new Commission on the Dissemination of Solubility Data.

Publications since August 1997

Guidelines for Calibration in Analytical Chemistry Part 1: Fundamentals and Single Component Calibration (V.1) *Pure Appl. Chem.*, 70, pp.993-1014, 1998

Determination of Tin Species in Environmental Samples (V.2) *Pure Appl. Chem.*, 70, pp.2051-2064, 1998

The Determination of Mercury Species in Environmental and Biological Samples (V.2.3) *Pure Appl. Chem.*, 70, pp.1585-1615, 1998

The Determination of Iodine Species in Environmental and Biological Samples (V.2.3) *Pure Appl. Chem.*, 70, pp.1567-1584, 1998

Nomenclature, Symbols, Units and Their Usage in Spectrochemical Analysis - XIV. Laser-based Atomic Spectroscopy: Proposal for a New Notation (V.4) *Pure Appl. Chem.*, 70, pp.517-526, 1998

pH Measurements in Non-Aqueous and Mixed Solvents: Predicting pH(PS) of Potassium Hydrogen Phthalate for Alcohol-Water Mixtures (V.5) *Pure Appl. Chem.*, 70, pp.1419-1422, 1998

Analytical Aspects of Chemically Modified Electrodes: Classification, Critical Evaluation and Recommendations (V.5) *Pure Appl. Chem.*, 70, pp.1301-1318, 1998

Critical Survey of Stability Constants of Metal-Imidazole and Metal-Histamine Systems (V.6) *Pure Appl. Chem.*, 69, pp.1549-1570, 1997

Critical Survey of Stability Constants of Complexes of Thiocyanate Ion (V.6) *Pure Appl. Chem.*, 69, pp.1489-1548, 1997

Critical Evaluation of the Use and Analysis of Stable Isotopes (V.7) *Pure Appl. Chem.*, 69, pp.1753-1828, 1997