

Report of the IUPAC Analytical Chemistry Division Officers and Commission Chairs

From their meeting in Idstein, Germany, 17-18 January, 1998

Executive Summary

This first ever meeting between the officers of the ACD and the Chairs (or Secretaries) of the various Commissions was held to discuss and plan for the future role of the ACD in a reorganized IUPAC. To this end, several background documents including a draft strategic plan from the SDIC were used. The ensuing very open and thoughtful discussions were extremely fruitful, resulting in development of a diagram that designates the role IUPAC and particularly the ACD plays in international chemistry, as well as proposed new structures for both the ACD Division Committee and the Division itself. The proposed new Division Committee structure, which would be only composed of a President, Secretary, Past President or President Elect, and the Commission Chairs (or their representatives), will result in more open communication, cross-fertilization of projects, and easier formation of horizontal collaborations. The new Division structure more clearly lays out which parts of the division perform what roles, as defined here.

1. Description of the present status of the Analytical Chemistry Division

The present Division consists of a President, a Secretary, and a Division Committee, composed of six TMs and nine AMs. The primary jobs of the Division Committee are to provide strategic direction and advice, review documents produced by the Commissions, and to assess the activities of the Commissions. There are then eight Commissions: V.1 General Aspects, V.2 Microchemical Techniques and Trace Analysis, V.3 Separation methods, V.4 Spectrochemical and Other Optical Methods, V.5 Electroanalytical Chemistry, V.6 Equilibrium Data, V.7 Radiochemistry and Nuclear Techniques, and V.8 Solubility Data. At the present time there are 46 TMs and 63 AMs, as well as 74 NRs and 64 co-opted members on subcommittees, involved in the work of the Commissions. These volunteers work at present on just over 100 different projects and have a range of collaborations and networks with the other Commissions in the ACD, as well as in the Physical, Organic, Macromolecular, Chemistry and the Environment, and Chemistry in Human Health Divisions. The projects are developed and completed through contacts and cooperation with the scientific community (academia, industry, other research institutes) and are aimed at a diverse set of users (educators, instrument developers and users, national and international standardization organizations, political bodies, popular media, and society in general). The recommendations are generally accepted to be the ultimate global authority on analytical chemical issues, produced free from political influences.

2. Discussion

With the foreseen reorganization of the IUPAC, however, it was thought prudent to examine exactly what we think the ACD ought to be doing and why, and for whom the results of ACD projects are meant and whether they are reaching them.

The discussion began by attempting to define for ourselves just what distinguishes analytical chemistry from the other branches of chemistry. One attendee offered that analytical chemistry is an assisting science for many different fields and that the word science should be emphasized. It has been said that "Lots of physical chemists today are doing high quality analytical works", a comment that received much rebuttal, including the fact that the purposes are different: many scientists apply chemical and physical measurements to chemical problems, but Analytical Chemistry is a scientific discipline of its own, which involves the science of measurements, including solving the problems of applying measurements to real world problems and the verification and validation of the results.

The definition of Analytical Chemistry developed by the Federation of European Chemical Societies, Division of Analytical Chemistry is: "Analytical Chemistry is a scientific discipline that develops and applies methods, instruments and strategies to obtain information on the composition and nature of matter in space and time". There was a consensus in these discussions that an additional phrase is needed about the "value" of the measurements, i.e., uncertainty, validation, and/or traceability. The role analytical chemists play in science was seen by the group to be as information broker to end users, clients, or interested parties, for example through technology transfer, education, critical reviews of technologies to provide guidance, and the international implications and underpinnings of all of the above.

A list of such clients or stake holders was developed, and includes important international organizations (IAEA, OECD, WHO, EURACHEM, etc.), educators (education), accreditation bodies, standardization bodies, chemical societies, and society / broader community. These can be broken down into two general groups: users and beneficiaries. The idea of education includes QA education in industry, for example. Also of particular concern are the unique requirements of countries in development.

At present, the ACD has a portfolio of projects that demonstrably reach out to this client community. Each of these projects has a specific aim and a defined deliverable. However, some projects need a client partner to achieve a usable end product, and most often this should be established in the initiation stage.

Finally, the question of "what should the IUPAC ACD be doing?" was debated. The results of this discussion are best represented as in Fig. 1:

In words, a multiplicity of information sources, vast amounts of data, inconsistent nomenclature, newly developed and changed methods and techniques exist in analytical chemistry. The role of the IUPAC ACD is to sort through, analyze, codify, review, and harmonize this input into consistent and useful recommendations or reports for and through interactions with the scientific community, end users, and other stake holders. It also promotes interactions between the scientific community, users, and other stake holders.

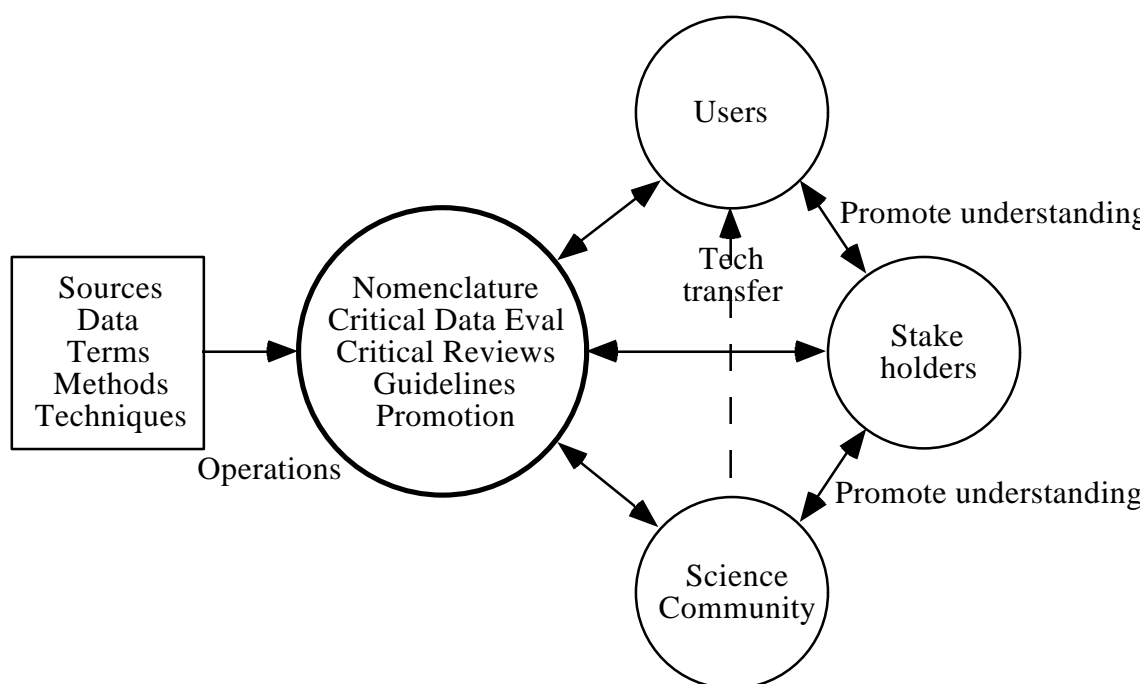


Fig. 1: A representation of the role and position of the IUPAC ACD. The center circle shows the product of actions by the ACD members. The square represents the input. The arrows in the diagram are the interactions catalyzed by the IUPAC and the ACD.

In order to perform these tasks effectively and efficiently, a strong engagement of scientists with specific knowledge and reputation is mandatory. In addition, as all work is performed on a voluntary basis there must be a strong motivation for these scientific colleagues to contribute to IUPAC work. Apart from scientific determination and curiosity, it is certainly the experience to belong to a select international group of top class scientists and a prevailing spirit of congeniality, even camaraderie, which act as such driving forces for taking part in IUPAC work. So IUPAC and its Commissions have a strong corporate identity, which must be fostered and continuously maintained. It is difficult or even impossible to achieve such a productive corporate feeling with a short term and totally fluctuating membership structure. This difficulty has been experienced by nearly all ACD Commissions in the problems of incorporating new members into Commission work. This integration process was, however, much easier for TMs and sometimes AMs, who had the perspective of serving for a reasonable time on the Commissions and, thus, the ability to provide a substantial input, than for co-opted members or NRs. The need for a mechanism to provide special motivation for scientists, particularly non-IUPAC members, to work on projects is a major concern that should be taken into account in any reorganization. A majority of ACD Commissions expressed this concern. Therefore, the group concluded that a basic structure for the ACD with a certain number of standing Commissions and members (TMs) serving up to 8 years is need to provide continuity of operation and stability.

3. Proposed structure of the ACD Division Committee

The attendees at this meeting observed and experienced very much improved communication between the Division Officers and the Commissions, as well as among the

Commissions. The idea was expressed that the work of the Division could be made much more efficient and streamlined by making a significant structural change. It was therefore unanimously recommended to propose that the future AC Division Committee be only composed of a President, Secretary, Past President or President Elect, and the Commission Chairs (or their representatives).

The principal function of the Division Committee members is to develop strategy and coordinate the functions of the Commission. This function can be performed more effectively in the new structure. Further important tasks are to review documents and to assess the activities of the Commissions. The review of documents would be done by a number experts in the field. The ACD will assume full responsibility for the final content of the publications. Documents that need to be reviewed by IDCNS would, as at present, be dealt with according to IDCNS rules. An advantage of the new structure will be the closer coordination of projects. The presence of the Commission Chairs on the ACD Committee will provide a more direct link to the stakeholders via the members on the Commissions and their scientific colleagues, etc.

4. Proposed ACD structure

Analytical Chemistry at present is involved in a large number of interdisciplinary projects, including understanding speciation from a variety of points of view, measurements, and implications. Speciation is presently under examination by V.1, V.2, V.6, V.7, C&HH, C&Env, and elsewhere. There are a number of other examples of such horizontal projects, such as Sensors (V.2, V.4, V.5, I.3, I.7, C&HH, C&Env), Chemometrics (V.1, V.4), Electrochemical FIA (V.1, V.5), Electrophoresis of metal complexes (V.1, V.2), Orange Book (V.1-8), Tutorial program (V.6, V.5, V.8), QA (V.1-8), and Trace analysis (V.2, V.3, V.4, V.5, V.7, C&HH, C&Env.). To enhance cross fertilization and coordination of these and other similar projects, there needs to be a mechanism to coordinate all joint commission meetings, based on their mutual overlaps in current projects.

The group feels strongly that some basic pillars or core functions need to be present in the division. The first pillar involves the role of the IUPAC as official international advisor to regulatory bodies such as ISO and BIPM (State treaties with 70 nations) as well as strong interactions with regional harmonization groups such as EURACHEM. The ACD offers globally agreed upon recommendations regarding the value or quality of analytical measurements, standard analytical practices, and reference materials. This function can be referred to as fundamental, and also includes other general aspects of analytical chemistry.

The second pillar is termed methodological. A set of standing commissions are necessary to provide an infrastructure to recognize, assess, and rapidly respond to stakeholder needs. The rapid development of instrumental methods creates a need for harmonization, classification, critical evaluation, and recommendation of nomenclature, terminology, units, and symbols and their proper use. Such a methodological pillar also would allow efficient dealing with new and future methodological developments in analytical chemistry such as sensors, laser-based spectroscopic methods, screening tests, and complex analytical procedures involving, for example, combinations of separation and spectroscopic methods for speciation, etc. By such a structure the ACD can provide the best possible input to problem oriented projects carried out within the IUPAC particularly for programs in the environmental, life science, and material science arenas, as well as

other future areas. Methodological core groups will also be very beneficial for development of tutorials program and educational tools, especially for developing countries.

The third pillar is fundamental data for analytical chemistry. Core groups to coordinate the work of co-opted members and other volunteers to assemble, assess, and evaluate such data already are in place and perform this function efficiently and effectively. The leverage provided by the present structure is enormous.

The fourth pillar is a small core group that provides broad coverage of the fields of analytical chemistry particularly with respect to diverse applications to recognize problems and needs and coordinate working parties to respond. The function can be described as science observation in chemistry to identify and react to the big issues.

The consensus was that all the principal pieces to accomplish the above objectives were already within the ACD as it is presently structured, but that it needed to be redistributed and refocused. The structure given in Fig. 2 evolved, and encompasses the discussed elements or pillars and the desired product given in Fig. 1:

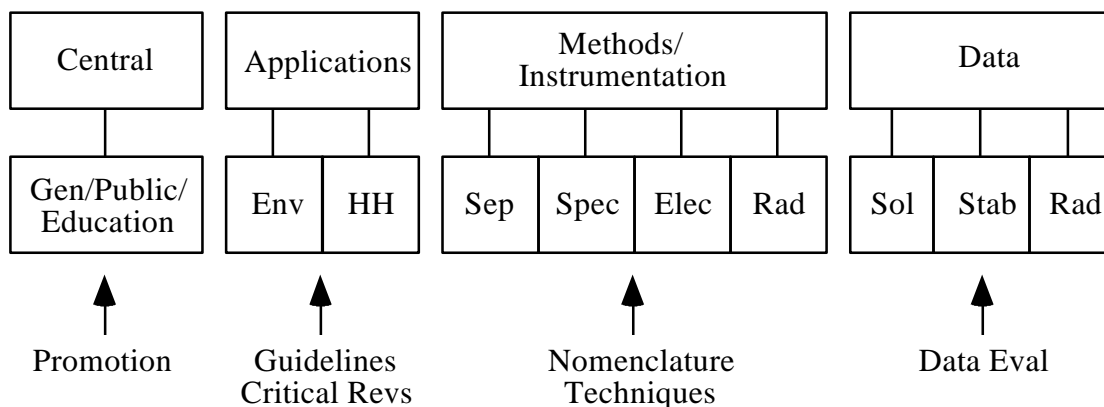


Fig. 2: Suggested ACD structure. Gen - General, Env. - Environment (connection to C&Env Division), HH - Human Health (connection to C&HH Division, and including Pharma), Sep - separations, Spec - spectrochemistry, Elec - electrochemistry, Rad - radiochemistry, Sol - solubility data, Stab - stability constants. The upper layer represents the core functions or pillars of the work of the ACD. The duties of standing commissions are depicted in the middle layer and the terms at the bottom correlate this structure to the parts of the product of the ACD defined in Fig. 1.

The group deemed it very necessary to have a core of standing commissions or committees. These are necessary to provide the means to identify projects and identify people to do the work, as well as perform a coordination role. An sufficient number of TMs in standing commissions are needed to provide a core of expertise and a continuity that can respond to tasks by selecting and coordinating specialists to carry out a project. They should also be seeking areas where it would be appropriate for IUPAC to respond and act. As now, they would rotate out of the Commissions on a reasonable time scale.

However, the Chairs and ACD Leadership realize that there will probably need to be reshuffling or redistribution of personnel between the various bodies to optimize their function.

5. Support for Division Presidents suggestion of a three part Bureau structure.

The suggestion of the Division Presidents (given in their report from the Brighton Meeting) for a three part structure of the Bureau with responsibilities as depicted in Fig. 3 was met with great approval.

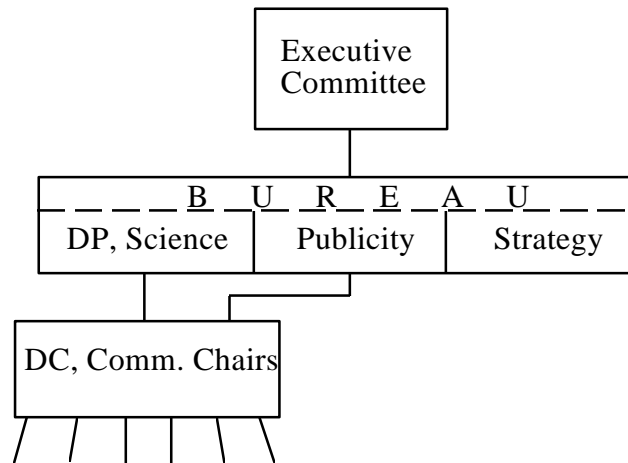


Fig. 3

Two important issues improved by this structure were noted: communication with clients and education. The structure flattens the levels, catalyzes interactions, and reduces overhead expenses. The foreseen necessity of good direct communication between the Divisions (Committee Chairs) and the Publicity Bureau Sub Committee resulted in the additional recommendation of a direct link between the two groups (rather than through the Science Sub Committee).

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