### **MINUTES**

For the meetings of the IUPAC Analytical Chemistry Division Committee and Commissions' Chairs and Secretaries at the 40<sup>th</sup> General Assembly, Berlin, 1999

#### **Dates and venues:**

1999-08-07 (Sat) 14:00-17:00 in Room J24-22 1999-08-10 (Tues.) 14:00-17:00 in Room KL 25-121B 1999-08-11 (Wed) 09:00-12:00 in Room JK 24-140

## 1. Welcoming remarks and finalization of the agenda

Folke Ingman welcomed all to the meeting and asked the attendees to introduce themselves. There were 25 in all (see attached list with e-mail addresses). He then overviewed the changes in the Division resulting from the SDIC and Bureau decisions of the past two years. In light of the report from the Idstein meeting of the Executive Committee and Commission Chairs, the Bureau approved our plans to modify the structure of the ACD to include Commission Chairs, with the caveat that no elections for new members would be held to replace those ACD members at the ends of their terms in 1999.

## 2. Matters arising, not otherwise on the agenda

Membership lists from each Commission need to be given to Moore by Tuesday for further transmittal to the IUPAC Secretariat.

## 3. Budgets for the 2000-2001 biennium

The ACD budget was increased by 5% (from 1998-1999 levels) to USD 44,400 for the 2000-2001 biennium (subject to approval by Council).

The issue of administrative costs for Commission Secretaries was raised. Moore will bring up the issue with the Secretariat, but the future project oriented format will alleviate some of this problem because those costs can be written directly into the project budget.

## 4. Reports from Interdivisional Committees

Y. Marcus reported on the activities of the IC on the Teaching of Chemistry (CTC). CTC is not certain of its role in the new IUPAC structure, and discussed the matter extensively. The demonstration of the Soleq tutorial software in the joint CTC/V.6 meeting was received very well. It was suggested that a task group between ACD (V.6) and CTC undertake a project to produce a source book or other listing of software for analytical chemistry, especially for teaching of analytical chemistry. There will be a new joint project proposed between V.7 and CTC for the production of educational materials abuot the real hazards of nuclear materials especially low levels in the environment, in order to counter the vast amounts of misinformation in the media.

President Ingman expressed the gratitude of the ACD to Prof. Marcus' for his efforts during his tenure as representative of the ACD on the CTC.

# 5. Reports from Working Parties and Commissions (membership, status of projects, new projects)

(Reports from Working Parties can be found in the parallel minutes, Section 7.)

- 5.1 Commission on General Aspects of Analytical Chemistry (V.1)
- J.F. van Staden will continue as chair. The Secretary General approved the plan to have a post-doctoral fellow of Van Staden, Dr. Raluca Stefan, continue to function as Secretary, and will support her travel to Brisbane. F. Zagatto has been appointed TM, Vessman was named AM, and Hulanicki (Poland) and Soavedra (USA) were appointed NR. Two projects have been published, one was withdrawn, one is in ACD review, and the remainder is in progress for completion by 2001. One new project will be proposed by Danzer

The responsibility for revisions to the Orange Book continues to reside in V.1 (except for chapter 18, which resides with the IWP on Harmonization of Quality Assurance Schemes). The Commission will request electronic copies of the various chapters from the Secretariat or Blackwell to ease this task.

- 5.2 Commission on Micro-chemical Techniques and Trace Analysis (V.2)
- R. Lobinski was promoted to TM and is the new Chair. Danielsson remains as Secretary. Kim (Korea) was dropped as NR (there were two from Korea).

Four projects have been published or are at the Secretariat awaiting publication. Six projects were cancelled. The remaining projects will be finished by 2001.

New projects will be determined by task groups, who will meet and produce the proposals in the next year.

There continues to be an important link between V.2 and the IWP on Harmonization of Quality Assurance Schemes.

- 5.3 Commission on Separation Methods in Analytical Chemistry (V.3)
- R.M. Smith is the new Chair, and J.A. Jönsson is the new Secretary. Garcia Dominguez was promoted to TM. Jinno was made NR (Japan), and Jandera was made AM. One project will be finished at the end of September, 1999. The remaining present projects will be finished in 6 months.

Three new projects will be proposed: an interdivisional project to expand the Division IV project 422/1/98; a joint project with V.4 on hyphenated techniques (see below); and a project with other ACD Commissions on data handling in analytical measurements.

- 5.4 Commission on Spectrochemical and Other Optical Procedures for Analysis (V.4)
- G. Gauglitz is the new Chair, and K. Volka is the new Secretary. The Commission has requested a special extension for Vo-Dinh to remain as a TM for 2000-2001 to finish several documents by 2001. If this proposal is not accepted, Stykov will be promoted to

TM and Vo-Dinh will remain on the Commission as AM. Niessner is assigned to V.4 as a TM from the Pool. Lukosz and Turk were dropped as AM and Curtius was dropped as NR.

The joint meeting between V.5, I.7, and V.4 achieved agreement on general terms important to biosensors. Each of their projects will now proceed without general term discrepancies. There was one project published, two were cancelled (17/95 and 22/95), and all but two (see below) will be finished by 2001.

There will be a joint working party proposed for a nomenclature document on hyphenated techniques. Included will be V.2, V.3, V.4, V.5, and IV.2. Another interdivisional working party will be proposed for a nomenclature document on high throughput screening and combinatorial technologies with inclusion of V.5, I.7, and division VII.

# 5.5 Commission on Electroanalytical Chemistry (V.5)

S. Rondinini is the new Chair, and W. Kutner will remain as Secretary. R. Buck had submitted his resignation before the Berlin GA. His outstanding work as Chair of the WP on pH was acknowledged. Pratt was promoted to TM. Y. Vlasov will be assigned to V.5 as a TM from the Pool.

Three projects were published. One project is in the Orange Book. Two have been through ACD review and are being prepared for publication. Two projects will be finished by the end of September 1999. Project 49/91 will become a part of a new proposal. Part 1 of project 62/97 will be part of the Hyphenation Project (see V.4 above). Project 63/97 will be combined with 49/91 as part of the larger new proposal. The remainder will be finished by 2001.

V.5 has already submitted two new project proposals. The one on uncertainties in pH measurements they would like suspended until further notice. There will be three further new projects: reassessment of pH data with respect to the Pitzer model; statistical analysis of electrochemical analytical data with V.1; and electrochemistry of liquid liquid interfaces with V.3.

## 5.6 Commission on Equilibrium Data (V.6)

Powell has become ACD Secretary, so R. Byrne is the new Chair and K. Popov was made Secretary. May, Arnaud-Neu, and Tabata were promoted to TM, and Felcman and Wanner were changed from NR to AM. Lajunen was changed from TM to AM. Tabata will provide a strong tie from V.6 to industry.

The equilibrium constant database project is mature and has led to an Academic Software product, in its third release now as fully 32 bit Windows compliant. Project 39/95 was unveiled as the Soleq product from Acad Soft at this meeting. Project 37/95 was published. Project 22/87 was dropped. Three projects will be finished in one year, and the remainder by 2001.

There were two task groups in V.6 formed to formulate new projects: speciation of Cd, Cu, Hg, and Pb with common inorganic ligands (with V.1 and V.8); and evaluation of chemical equilibrium software on the market.

## 5.7 Commission on Radiochemistry and Nuclear Techniques (V.7)

There will be no change in officers. Nakahara completed his term as TM and was dropped. Chai was promoted to TM. Four AM were added (DeCorte, Yates, de Groeij, and Nagame). Kim was dropped as NR (there were two from Korea).

One project was published, one was submitted at this GA for ACD review (12/89), two were withdrawn (the author published them elsewhere without ACD review), and the remainder are making good progress to be finished before 2001.

Several new projects are being proposed, including a half-lives database, speciation of Pu in the environment, and nomenclature in radionuclear chemistry and radiopharmaceutical chemistry.

A suggestion was made that there be a formal liaison between IUPAC and IAEA via V.7. Fajgelj will pursue this with IAEA.

The Commission submitted a formal plan for their future within IUPAC (see attachment).

# 5.8 Commission on Solubility Data (V.8)

There will be no change in officers. Cohen-Adad has completed her term and has been dropped as TM. P. Scharlin will be the new TM. Hala and Mather were dropped as AM. M. Gaune-Escard and C. Balarew were added as AM, and three new NR were added. Five projects were published, via the new agreement with JPCRD. Four projects were dropped. Six projects are planned to be published in 2000. The remaining projects will either be finished or will lapse in 2001.

The Commission has submitted a proposal for continuation as an ongoing Commission for the Dissemination of Solubility Data (see attachment). To be effective, the members are discussing means to assemble more coherent groups of projects with common themes. They also propose to organize thematic symposia, especially with emphasis on the interface between producers and users of solubility data. They will also propose a new project jointly with CTC on the use of solubility in the teaching of chemical concepts.

## 6. Restructuring and plans for the future of the Division

In order to have sufficient and complete representation of the breadth of analytical chemistry on the ACD, each ACD member should be expert in and responsible for a certain aspect of the field. They would then become heads of advisory groups who would assist them in making proposals, seeking proposals, and reviewing proposals.

Examples of bodies that should continue in some form are the Interdivisional Working Party on Harmonization of Quality Assurance Schemes, Commission V.8 (both of which have submitted plans to the Secretariat, and have received approval), and V.1.

The concern was expressed about keeping the balance of subject representation within the ACD. Ingman described the election process for new members in 2001, with formation of a nomination committee according to the changed IUPAC Bylaws. The concern about the need for balance was again reiterated, and it was suggested that ACD formulate a written plan, or a part of the Terms of Reference that includes it.

For future project proposals, several people expressed opinions about how best to identify the best links to persons outside or inside IUPAC with whom to collaborate. There are big changes ahead for the ACD Commissions, and strong links need to be forged in the next two years, especially with the Environment and Human Health Divisions.

The opinion was expressed that IUPAC was like the UN of chemistry, and needs somehow to retain that elite image. A key change is to focus on fewer projects of global interest and impact, and to seek collaborations with other international bodies. Global impacts imply collaborations with global companies and international organizations. One way to proceed is to identify the stakeholders before embarking on a proposal, and obtain their input. An example given was the WTO (hormones in food, antibiotics in food, genetically modified organisms, bioanalytical methods, bioengineering, analysis on a chip, nanomethods). Who, for example, is advising WTO about how good analytical data have to be for certain kinds of decisions? Policy makers should probably also be involved. IUPAC can help lawmakers be scientifically sensible.

Another issue raised is that the work of IUPAC is not visible enough. Whether the new structure will alleviate that problem remains to be seen. But ACD can take advantage of web publishing as well as Chemistry International and other journals to expand their product distribution. Maybe PAC needs to change its format, or add additional formats.

In order to come up with the best proposals, several ideas were voiced. The roles of the ACD could be to stimulate the right people to write good proposals. It can do so efficiently in a large number of cases by electronic forms of communication rather than expending funds for travel. How can the right people for each project be identified and attracted to participate? For the larger projects it is apparently easy. What about nomenclature or smaller projects? Can we use our NAOs more efficiently to identify appropriate people? What about using the past and present IUPAC member database – is there a keyword search possibility for certain expertise and experience? The possibility of using a web billboard or some other form of call for experts (to find experts for a project – not task force members) was raised.

When a project is finished, how do we determine its impact? Are typical methods such as citations or web page hits useful? What else is important for a particular project? The project proposal form asks for this information.

7. **Other business:** There was none.

1999-08-11: Dr. David S. Moore, Secretary, IUPAC Div. V