

**Meeting of the IUPAC Analytical Chemistry Division Committee  
Rome, March 4-5, 2006**

**Venue:** APAT (Agency for Environmental Protection and Technical Service)  
EUR - Via Vitaliano Brancati, 48

**Time:** Saturday, March 4<sup>th</sup>, 9.00 – 17.00 and Sunday, March 5<sup>th</sup>, 10.00 - 14.00

**Present**

Prof. R. Lobinski (Division President), Dr A. Fajgelj (Vice President ), Prof. K. Powell (Past President), Prof. R. M. Smith (Division Secretary), Prof. P. De Bièvre, Prof. H Gamsjäger, Prof. D. B. Hibbert, Prof. J. A. Jönsson, Dr. S. Kocaoba, Prof. J. Labuda, Dr Z. Mester, Prof P. Minkkinen.

**Apologies**

Profs M. Bonardi, ZF. Chai, U. Karst, W. Kutner, B. Spivakov, E. Zagatto

In attendance. P. DeZorzi

**1. Welcome and arrangements**

The Division President welcomed Analytical Chemistry Division (ACD) committee members and especially thanked those who came on their own funding. He thanked Maria Belli and Paulo De Zorzi for their help in organising the venue and transport and APAT for the use of the room.

**2. Matters arising, not otherwise on the agenda:**

A technical presentation made by APAT staff describing the work of the organisation was included. The agenda was approved.

**3. President's remarks**

a) Review of the ACD Committee and Operation

ACD Committee Composition;

Currently 10 TM (including 4 officers), 6 AM and up to 10 NR are permitted (currently 8)  
Two Working Parties/subcommittees are represented on ACD Committee

Subcommittee on Solubility and Equilibrium Data (SSED) (Heinz Gamsjäger  
Chair)

Working Party on Harmonisation and Quality Assurance (WPHQA) (Chair is  
currently Ales Fajgelj (TM) changing to Paulo De Zorzi)

b) Budget: project and operational funding

The ACD operational funding of 56400 USD is used for meetings etc and organisation (< 30% of total) and the rest supports projects (70% of total). Once a project is approved, the project's budget is allocated centrally from the Division to the Project as a block and is lost to ACD. Any unspent funds on a project returns to the central reserve. This reserve is used by the Project Committee and the ACD can apply for extra funding. ACD has used some money to facilitate workshops and funding for speakers.

The IUPAC funding can be used for travel, meetings and expenses, but not for chemicals or practical experiments etc. In applying for funds the project should consider contributions from alternative sources. To receive funding, expenses have to be submitted but the accounting needs are minimal.

- c) The status of WPHQA and SSED was discussed. The ACD is home to Interdivisional WP for Harmonization of Quality Assurance - its remit is wider than that of a subcommittee and the naming is historical (Chair is usually a TM or AM of the ACD). SSED is a subcommittee of ACD and encompasses a number of projects (Chair is usually an AM)
- d) The Division President reported that a former ACD TM Professor Matsumoto had been elected to VP (and will become the President of IUPAC) which is an honour to the Division.

#### **4. Division Objectives and Organisation for 2006-7**

- a) Review of the current objectives: division priorities and core business

The Division President reminded the meeting that in 2004 (at Vienna meeting), the ACD had decided to concentrate on four core activities: communications, critical evaluation of data, quality assurance, terminology, and on four emerging areas: process analysis, nanotechnology, bioanalysis, developing countries.

The ACD had allocated Teams to each of these areas to be proactive and devise new projects. It was felt that this approach had been partially successful. The generation of projects externally to IUPAC has not been successful. The ideas continued to develop and expand but it was felt that a further biennium was needed to evaluate correctly the success of this approach. Discussion followed on the need for a slight re-definition of the objectives and the best ways to achieve them.

It was agreed that each activity should be supported by a team whose overall role is to develop and initiate projects, take part in forward planning, coordinate activities, and seek new participants for projects and task groups. The modifications included:

- to expand the work of the Terminology team to include electronic resources so it would cover the Orange/Gold book (electronic resources) including stability databases and NIST databases (Sol EQ) (related to critical evaluation) (and possibly educational resources).

- following a discussion pointing to the fact that bioanalytical and nano/process were really not emerging issues but were now reasonably well established fields, the current description of these teams was found inappropriate. What was required was a new Team, specifically looking not at core topics but concentrating on where to go next and to have a role of development. Consequently a new core activity: emerging analytical issues was defined. It will be lead by the Division President and would select membership from among the ACD. Its main task will be finding new areas where work is needed. Its mission would be to find new ideas for the future, maintain and develop areas and be outward looking.
- to create a core activity: emerging analytical communities based on the former team dealing with activities related to the developing countries. There was a desire to involve more developing countries. A number of names were suggested by Paul DeBièvre as possible contacts.

In summary the focus of the Division in the 2006-2007 biennium will be six core activities, each dealt with by a specific team. The composition of the teams was decided to be:

**Communication**

Powell (leader), Murray, Chai, Kocaoba, Torto, De Bièvre, Dominquez

**Critical evaluations of data**

Gamsjaeger (leader) Bonardi, Balarew, Hibbert, Mikkinen, Watarai

**Quality assurance**

Fajgelj (leader) Hibbert, Mester, Labuda, Mikkinen, Spivakov

**Electronic Resources/ Terminology**

Smith (leader), Kutner, Jönsson, Powell, Gamsjäger, Murray

**Emerging analytical communities**

Jönsson (leader), Lund, Torto, Smith, Zagatto, De Bièvre

**Emerging analytical issues**

Lobinski (leader), Chai, Karst, Labuda, Mester,

The Team leaders will send a letter to its Team's members explaining the objectives of the team to be reached by the end of the biennium and encouraging their involvement.

The Division President will make the core activities, and team composition and related information available on the website as soon as the Minutes are approved.

- b) Review of the current strategies to achieve the Division objectives: efficiency of the Division attempts to generate new projects (teams, workshops, other)

Attempts had been made to generate external interest through articles in Trends in Analytical chemistry and in an electroanalytical journal but with little response. There is a need to engage wider systems (other organisations) and to be aware of work elsewhere.

Teams need to work harder on development areas. One mechanism was to use the TM election to generate new activities and introduce new blood into the system but because the members were elected, the process was not found to be completely managed by the Division. One question was the extent to which the ACD should concentrate on Division goals or whether it should rather focus on interests of individuals.

Of the current work traceability has progressed well but although there had been an aim of increasing work in the bioanalytical area this had not been as successful as expected. An interest in genetically modified analysis had not developed because of limited interest from the wider community. On the other hand, a new project (Mester) was generated in this area as an indirect consequence of the Ottawa (2003) workshop.

It was felt that ACD needs to be a steering committee - to increase its visibility in the outside world. A question was raised of the external view of IUPAC - how much use is made of evaluated data. It was felt that ACD had a role in distinguishing junk from valid science, particularly in areas, such as data validity and critical evaluation.

Some areas had a significant external impact such as the work of the WPHQA because its direct applicability in real life and links to the EU legislation. One misconception of the WPHQA has been that the definition of "quality" assurance does not mean assured quality.

A factor that helped spread the work of ACD was collaboration with other organisations. This helped in achieving a majority consensus on topics and terminology. There have been occasions where there has been a client-customer relationship making use of IUPAC results and policies in which IUPAC brings an international perspective.

In the projects themselves, is there need for practical experience external to IUPAC, so that outputs are more relevant to external users? Should the composition of task groups be modified by adding members to reflect community/stakeholders? For many projects do the aims need to be more focussed to increase the relevance of work to external users? Applications for funding are often very general rather than specifying recipients. Should we be looking for funding support from stakeholders? There is a need for more industrial involvement. The drafting of proposals needs to reflect industrial input to change aspect. The task group may need to ensure representation from industry. Support should not come from a single company in order to maintain independence and unbiased character of evaluation.

#### c) Review of Member Responsibilities

The Terms of reference and duties of the ACD members are listed on the IUPAC website. The Division President would propose revisions to duties to reflect the involvement of all ACD members in Teams; these will be circulated to Officers and then to the Division. In general it was proposed to adjust the description to the current organization of the Division

Titular Members: currently the selection of TMs was defined by their subject expertise to ensure the coverage of all the areas of analytical chemistry. The next Nominating Committee would be asked to review the areas and decide if they were still appropriate or

whether they should be changed. In particular if the areas of general aspects of analytical chemistry should be worded differently.

Associate Members: they would have very similar responsibilities to TMs and would be expected to be involved “as appropriate” in specific interest groups

National representatives: Part of their duties would include the need to seek support from their NAOs to attend meetings. They would also be asked to communicate and interact with their NAOs (this was also seen as a desirable activity of all members).

The duties of the Officers would also change to reflect the earlier changes in the Team structure and the automation of the project tracking process, largely assured by the Secretariat.

## **5. Review of Project progress reports**

### **a) Division projects**

The project reports from Task group Chairs had been circulated in advance and will be posted on the IUPAC website. Most were accepted without comment. It was recommended that Projects involving terminology should be forwarded to Włodzimierz Kutner for comment before sending to ICTNS. The discussion and particular decisions concerned the following projects:

2002-009-2-500 - Optical spectrochemical analysis using waveguides and optical fibres;  
2003-037-1-500 - Optical biosensors and bioprobes  
The revision of the VIM was also reported on.

The above projects were inherited from the old Commission system and no progress reports have ever been received. The Division President will write a letter to the Task Group Chairmen with an intention to finish each project unless a motivated answer for the maintenance of the project in the system is received within one month.

2002-058-1-500 Definitions and fields of application of the terms robust and rugged and the characteristics or qualities of robustness and ruggedness in analytical chemistry

The project had been returned to the authors for revision but no more had been heard. The Division President asked Kip Powell to contact the Task Group Chairman (TGC). The project will be terminated unless a revision (or confirmation of the will to revise the project reports) is received.

2001-072-1-500 - Low activation materials for fusion technology: State and prospects

The project final report apparently exists in Russian. The Division had offered financial assistance for translation but no feedback from the TGC. The Division President will contact the TGC.

2004-016-2-500 - Guidelines for potentiometric measurements in suspensions

Kip Powell needs to contact Professor Rajagopalan to clarify his role in the project. The final report to be submitted as soon as the position is clear.

2005-014-1-500 - IUPAC stability constants database - completion of data collection up to 2006 - project is on-going and may need to be extended into a further project in 2006. Additional members may be needed for task group

b) Report from SSED (Heinz Gamsjäger)

2002-033-1-500 and 2002-034-1-500 to be reorganised

2002-043-1-500 Mather project to continue

Developments and Applications of Solubility. T. Letcher (ed.), The Royal Society of Chemistry, accepted, 2006. (Many contributors from IUPAC Solubility Data Group)

Biom mineralization – Medical Aspects of Solubility. Wiley, in press 2006, edited by E. Königsberger and L.C. Königsberger (IUPAC Solubility Data Group)

2002-036-1-500 Goto and Miyamoto

Requested funding for future work - but an extension of the project needs a new project submission.

Generally task groups need to consider need for funding for travel at start of submission of proposal - details may also result in a more appropriate vector for publication

Cezary Guminski seeks help from Chinese members for envisaged project, DP to facilitate contact.

There was concern at the number of projects which appear to only involve one person. A group may be better at completing a task. A number of task groups were being restructured

The group is involved in the organisation of the 12th ISSP International Symposium on Solubility Phenomena and Related Equilibrium Processes to be held at the Institute of Inorganic Chemistry of the TU Bergakademie Freiberg from July 23-28, 2006.

Three projects had been completed:

2001-052-1-500 H. L. Clever, SDS volume 80

2003-018-1-500 Andrzej Maczynski, SDS volume 81

2002-025-1-500 Jiri Hala, submitted.

A new project was started: 2005-017-1-500 Glossary of terms related to solubility - updates and revisions to the Orange Book, DG Shaw.

Three new projects were planned.

d) Report from WPHQA

2005-019-2-500 Maria Belli to join Task Group

2001-010-3-500 could lead to a UNIDO project on Traceability. Paul De Bièvre will contact UNIDO to formalise links.

Also: with one meeting later in Paris, the revision of the VIM should be finished by the end of the year.

Work of WPHQA needs to be presented in Turin at GA in 2007. One proposal was a workshop in cooperation with the Human Health Division.

## **6. Proposed Projects under review:**

The next funding round will be in April 2006 - projects currently under consideration

2005-035-1 Trace element analysis - role of grain size (Belli)

2005-041-2 Critical evaluation and recommendations regarding the determination of selenomethionine in selenized yeast supplements (Mester) may need to widen task group

2005-048-2 Solubility and thermodynamic properties related to environmental issues (Letcher) lead group not clear - unclear on publication position and royalties. Division President to contact JJ. Principle is contact with editor / IUPAC. Also uncertain of connection with earlier book project - danger of over-commitment

2006-010-1 The adjustment estimation and uses of equilibrium reaction constant in aqueous solution (Sukhno)

The Division President will have assured the completion of the reviews by 30 April for the above projects so that they could be considered during the April funding round.

## **7. Proposals in the pipeline and ideas for new projects**

- a) “metallomics” glossary of terms (Ryszard Lobinski) draft project will be completed in June 2006
- b) Direct methods for metal speciation in solid samples - still unclear on proposed coverage and TGC - no progress since Beijing
- c) ICPMS - Walter Lund to contact J M Marchante Gayon at Oviedo to generate a proposal
- d) Isotope geochronology no progress / contact needed with IUGS. A project proposal to be submitted soon by Division II, with participation of Ales Fajgeli, Mauro Bonardi and Paul De Bièvre.
- e) MIPS - no development and a concern was expressed that this was a field that was not progressing - decided to drop as idea

- f) Process analytical technology - suggested by Caroline Ribes and Mark Schoenfisch - awaiting draft proposal.
- g) Chemometric soft modelling - Brynn Hibbert - possible project with Pentti Minnkinnen
- h) Sample preparation terminology. A proposal will be prepared by Jan Ake Jönsson for the December funding round
- i) Heat capacity factor project was suggested by Heinz Gamsjäger in Beijing but no development since

Other new areas floated as possible projects

Jan Labuda - chemically modified electrodes / biosensors - recommendations on DNA biosensors, related to bioanalysis, chiral interactions, drug evaluations and a number of related areas.

Walter Lund - update of chapter on spectrochemical analysis in Orange book - with David Moore

Pentti Minnkinnen - Process analytical interests / sampling educational aspects/ weak electrolytes constants

Ales Fajgelj – EUROCHEM: interaction sampling uncertainty projects

- j) A project focussing on a “layman’s guide to traceability” was evoked by WPHQA (PDB)

The Division President will write to the potential TGCs and encourage the submission of a project

## 8. Maintenance of the Division key products

- a) Orange Book: report on status and future developments (Roger Smith)

Currently being updated; Chs. 8 (Electrochemical), 10 (Spectrochemical) (but needs new Task group Chairman), 16 (Radioanalytical) already in hand

Roger Smith has been interacting with Aubrey Jenkins who is entering terms into the Gold Book based on the Division terminology papers published since last Orange book.

One problem is that in some chapters, such as spectrochemical analysis, the terms are descriptive rather than definitions. A project on “Conversion of Orange book Chapter 10 to Glossary format” is expected from David Moore.

The Division through the Electronic Resources Team will need to look closely at the format and style of the Orange book and whether it is appropriate for the future in which will largely be electronically based.

- b) *SC-Database* (Kip Powell)



Discussions have been held with Academic Software, regarding the transfer of the management of the project to IUPAC.

The IUPAC Bureau has agreed in principle that the Solubility Data base should become an IUPAC based project. It was agreed that Division V would be in overall charge and control the quality of the data. The IUPAC Secretariat would be responsible for data management, publicity and marketing. This would require a database management expertise to be available, but this could also be required for other database projects. A Business plan had been submitted to the Executive of the Bureau and will be discussed in April. The plan provided for a project income that will cover costs.

## **9. Visibility and image of the Division: public relations**

### a) *CI* articles – present and future.

Jan Ake Jönsson reported on the progress of the series of articles on Emerging Issues in Developing Economies. The list of articles is sufficient until end of year - then plan to end if no particular new areas.

Kip Powell - New series of articles on Tools of the Trade - aim is to highlight tools that IUPAC provides - such as colour books, databases etc, WPQA papers recommendations - All Division presidents contacted asked for interest - only response from Division V so far.

Possible articles on SSED Heinz Gamsjäger - describing output - develop to solubility aspects

Need to ensure Division outputs have high publicity by generating links to PAC from other websites, such as trade journals, analytical journal websites, NAO members journals, including translations -

Brynn Hibbert to approach journals - and pass contacts to Fabienne Meyers

### b) Division web page: scope of enhancement and management;

It was felt that the web site of the Division needs redesign - Division President to revise (interests) (query is there a content management system in place).

### c) Teamwork

The edition of Teamwork (newsletter of the ACD) is going to be taken over by the Vice-President, Ales Fajgelj. The next issue is expected by the end of April.

### d) Conference and workshops

The need for more publicity for the ACD at IUPAC sponsored conferences was emphasised. The Division President is going to represent IUPAC at the ICAS in Moscow and HG at the ISSP. Both are expected to present the Division during the opening session.

e) Other

Article in the TRAC presenting the ACD: BH reported to have received no feed back.

Ales Fajgeli reported that pdf files from PAC had been used in soil sample project and circulated widely. Ryszard Lobinski confirmed that this method worked very well to spread the news about the speciation terminology IUPAC project.

### **10. Initiatives with journal editors: follow-up**

After Beijing - Brynn Hibbert had been in contact with journal editors to try and encourage them to adopt IUPAC terminology in house style. Efforts continuing

### **11. Role and involvement of NAOs and NRs in the ACD work**

As noted above it is felt that NRs need to be more actively involved in projects and to promote IUPAC to their NAOs. It should not be just an inactive role.

### **12. Preparation for GA in Turin 2007**

A proposal had been made for a Metrology symposium - a response from the organisers (Della Gatta) is awaited. A Speciation analysis symposium was also suggested. There seemed to be some communication problems. Ales Fajgeli will approach informally and determine current situation and see if symposia can be included

### **13. Closing remarks:**

The Division President recapped the objectives, including the revised structures, individual and group responsibilities

### **14. Other business**

It was noted that two WPHQA members (Michael Thomson and Roger Wood) were retiring after many years service and there was interest in making a presentation in recognition of their work at an appropriate occasion. Division President will contact the Secretariat to explore the possibilities.