



International Union of Pure and Applied Chemistry
Analytical Chemistry Division

Division Committee Meeting
APAT, Via Curtatone 3, Rome, Italy
29 February to 1 March 2008

Minutes

Present

Dr Ales Fajgelj (Division President)
Professor Ryszard Lobinski (Division Past President)
Professor Walter Lund (Division Vice President)
Professor D Brynn Hibbert (Division Secretary)

Prof Maria Belli (APAT)
Prof. Maria F. Camões
Prof. Zhifang Chai
Prof. Paul De Bièvre
Prof Attila Felinger
Dr Heinz Gamsjäger
Prof. Dana Knox
Prof Maciej Jarosz
Prof. Jan Labuda
Prof. Shoji Motomizu
Dr Zoltán Mester
Prof. Pentti Minkinen
Dr Tatania Maryutina
Prof José Pingarron
Monica Potalivo (APAT)
Dr Paolo de Zorzi

1. Welcome and arrangements

AF (President) welcomed the participants and thanked local organizers, Dr Belli and Dr de Zorzi (APAT), for their generous offer to host the meeting. The President noted the exceptional attendance, particularly from Associate Members. He hoped to build on the achievements of previous committees and progress the work of the ACD.

2. Approval of Agenda

Approved.

3. Membership of Division Committee, SSED and WPHQA in 2008-2009

a. Introduction of Members

b. Presentation of ACD past activities and future (Past and Current President)

RL (Past President) gave an overview of the work of IUPAC and ACD, based on his presentation to the IUPAC Council (Annexe I, PowerPoint presentation). He highlighted the IUPAC web site

as a major resource of information. His presentation was followed by a short discussion about projects' funding. It was unanimously agreed that only project proposals of good quality should be funded. The typical recommended individual project funding of maximum \$5,000 from the Divisional funds is kept by the Division also for the future. (Larger scale projects would need to have cross Division support or be funded from the Strategic Opportunities Fund (see item 6). A question about the attendance of a representative of Academic Software at the next ISSP to discuss the future of the stability constants database was referred to the President/Secretary for action.

c. Presentation of SSED past activities and future (Past and Current Chairmen)

HG – the past Chairman of the Subcommittee on Solubility and Equilibrium Data (SSED) gave an overview of the activities of the Subcommittee (Annexe II, PowerPoint presentation). The SSED and its predecessors in IUPAC have taken on the task of making reliable solubility data available as widely as possible to chemists and non-chemists. There are four tools available: the solubility data series, standard reference texts, international symposia on solubility phenomena, and the new glossary of terms related to solubility, recently published in PAC (Vol. 80, No. 2, 2008).

DN – the new Chairman of the SSED then continued the presentation with a report on activity since the GA in Turin, and future directions (Annexe III, PowerPoint presentation). He announced the next International Symposium on Solubility Phenomena and Related Equilibrium Processes (ISSP) meeting in Dublin in July 2008, and invited any members of the ACD who would like to attend.

d. Presentation of WPHQA past activities and future (Past and Current Chairmen)

AF – the past Chairman described a history of the working party, which had initially consisted of members from AOAC, ISO, and IUPAC. (Annexe IV, PowerPoint presentation).

PdZ – the new Chairman continued and indicated that future directions would include his own interests in sampling.

Discussion: AF noted that new priorities in the working party as a result of the change in chairmanship were good and indicated a healthy progression of interests. PDB raised concerns about funding. The working party has no funds of its own, but the Strategic Priorities Fund is to target interdivisional (and other) major initiatives, and could be a source of project funding. Concerns were raised about proliferation of documents that attempt to define the same terms, often for different concepts. Concern was expressed that ICTNS might not be in a position to control the situation, as it hardly recall earlier work when reviewing newly submitted recommendations. In general, IUPAC is doing a good job in this area, but more should be done.

To sum up, the President is assured that SSED and WPHQA will continue their successful work. Both groups were encouraged to try to raise funds also external to the Division and IUPAC.

4. Reports from workshops (DK and MB)

DK – Report on *Metrological traceability in solubility measurement results*. (Annexe V, PowerPoint presentation, and agenda)

Outcome – There was an agreement to develop metrological traceability chains for some simple solubility measurements. Contacts, one from SSED (to be announced) and BH. The exercise will be initiated within next few months and with a draft to be available for ISSP in Ireland in July 2008.

MB – Report on talks given earlier in the day at the IUPAC-WPHQA Workshop “Trace elements analysis: role of grain size distribution in solid reference materials”. (Annexe VI, agenda).

Outcome – Continuation of the project has been proposed.

5. Review of Project Progress Reports

The full list of projects, including SSED, WPHQA and interdivisional ones is attached as Annexe VII.

WL – the Vice-President introduced the state of the Division's projects by noting that majority of projects were progressing well with current reports. Out of 56 projects 30 project reports this reporting period had been received. However many of the projects that had not reported were either ones with zero funding, or new projects that had not been in existence long enough to generate sufficient outcomes for reporting yet. The standardized reporting form is still appropriate. WL noted that his reminder doubled the reply rate. For projects with no reports the Division will request prolongation to September 30th 2008 and give 3 month deadline to the task group chair to provide details of progress or intended actions.

Individual projects of concern were dealt with under item 6. The general discussion considered the circumstances under which projects should be terminated. The present rule is if three project reports are missed, a request for information is sent out and the project terminated if a good reason (or proper report) is forthcoming. This was endorsed, noting that each case must be considered individually and in special cases exceptions could be made.

ZC asked why are projects so slow? He believed there should be a limit of 5 years. The committee noted the lack of the clear IUPAC policy. It was noted that the year starting the project code was the first year that the proposal appeared in the system and not the actual commencement of the work.

6. Projects under completion (projects for which there are concerns about progress)

WL – 2006-022-1-500 project of Moore to convert the Orange Book into glossary format. For different reasons, the majority of the task group members is no longer available.. Action: BH to contact David Moore as part of new interest group on electronic tools.

AF – 2003-015-2-500 project of Bonardi has a budget of \$21,000 with no money spent at all. These funds cannot be recovered. The President will consider approaches to help the task progress and consume at least part of the funding.

Other projects that had not offered progress reports will be contacted by the Vice President and given 3 months to provide information.

7. New project proposals

a. ACD strategy and policy related to projects

B.H. the Secretary, noted the increased cost of projects for task group members travelling from Asia and USA, and the weakening American dollar. It was agreed that there is a need to efficiently use funds. It was also noted that there has been only one submission from ACD this round. Every member of the ACD should be involved in at least one project.

WL – The Past President (RL) had workshops to help generate new projects. Were these successful? The Vice-President also considered that the system is rather bureaucratic and there should be more discrimination to allow greater funds to be directed towards better projects.

RL – The rules were because in former times there were more proposals than funds.

Concerning the earlier discussion on quality and funding, the President, supported by the Past President, urged the committee to consider how to make a project that would be successful in gaining funds from the Strategic Opportunity Fund.

The President concluded that there should be no set limit for project funds, but we must be conservative to keep some reserve. If there are not enough projects then we should promote new proposals.

8. Review of actions arising from the ACD meeting in Turin 2007

This had been covered elsewhere in the agenda.

9. Review of Division structure, operations, work plan 2008-2009

The President gave an overview of the Division, its processes and future plans (Annexe VIII, PowerPoint presentation). He started by paying tribute to the excellent work done by the Past President.

a. Division funds

The Division had been given a small increase in funding this biennium. However it appeared that increasingly IUPAC was choosing to augment the Strategic Opportunities Fund. The President will talk to Kip Powell (Chair of the projects committee) about how to put up competitive projects.

After discussion that noted some disparity among allocations to Divisions, both for operating budgets and project funds, AF will review projects for each Division and funds and investigate the criteria used to allocate funds to Divisions.

b. Division priorities and core business

The discussion started with a question from ZM – what is the contribution of ACD to “Advancing Worldwide Chemistry”? There are many branches of analytical chemistry. Should we identify any areas? Categories in the present terms of reference (<http://old.iupac.org/divisions/V/membership/ToR.html>) read like a textbook. He proposed we should have selected priorities that change every biennium to take account of emerging issues. How do we manage the two views of analytical chemistry – the techniques and the applications? We tend to be strong on the former (most areas in terms of reference are technique oriented), while the world’s interest is on the latter. IUPAC should lead in a scientific advisory role in establishing regulations in the world (PDB). The dot points in the terms of reference should be revised.

The terms of reference are updated every two years. Last time was in Rome in 2006.

c. Task Groups

The Past President gave a short history of the “Task Groups” that appear on the front page of the Division web site (<http://old.iupac.org/divisions/V/index.html>). They were set up to encourage new projects in targeted areas, and cover the interests of the current committee. Unfortunately the term ‘Task Group’ was coined by the secretariat and some confusion has occurred with the project system. It was always intended that the groups reflected current core interests of the Division; they are not funded and serve only to channel ideas and efforts to create suitable projects.

The President introduced his proposal for new groups:

- **Communication?**
- **Critical evaluations of data**
 - Knox (leader)
- **Electronic Resources for IUPAC terminology work**
 - Hibbert (leader), Smith, Moore, Shaw
- **Emerging analytical issues**
 - Lobinski (leader), Chai, Karst, Labuda, Mester
- **Metrology**
 - De Bievre (leader), Fajgelj, Hibbert
- **Standardization in nuclear and related techniques**

- Chai (leader), Bode, Fajgelj

After debate, the following structure was agreed

- **Communication**
 - Lund (Teamwork)
- **Critical evaluations of data**
 - Knox (leader), discuss with SSED
- **Electronic Resources for IUPAC terminology work**
 - Hibbert (leader), Smith, Moore, Shaw
- **Emerging analytical issues**
 - Lobinski (leader), Chai, Karst, Labuda, Mester
- **Metrology**
 - De Bievre (leader), Fajgelj, Hibbert
- **The analytical potential of nuclear techniques**
 - Chai (leader), Bode, Fajgelj

Notes:

1. *General.* The interest groups serve for the biennium when they will be reviewed. On the web page, the titles will be displayed with a link to more information on another page. Interest group leaders should write regular reports for Teamwork.
2. *Communication.* This has been a way of creating visibility for the Division. Teamwork will continue, so this interest group can remain under WL to maintain this presence_[DBH1].
3. *Critical evaluation of data.* James Sangster has a critically -evaluated database on $\log(K_{O/W})$ values (more than 20,000), which he maintains and updates. This could be considered by the group for taking over by IUPAC (unless this conflicts with NIST). Dana Knox can lead the group to keep an overview of all kinds of data that can be critically evaluated.
4. *Electronic resources.* With concerns about the Orange Book and developments in presenting terminology in the Gold Book, it is important that the Division maintains an interest in the area. BH is keen to lead the group and will be the point of contact for such matters.
5. *Emerging analytical issues.* The emerging issues group had provided new members to the ACD (e.g. ZM) and had generated projects from within its members. The committee agreed that it should continue in its role to seek new areas of analytical chemistry, and encourage their development through organising workshops, and proposing new projects. It was suggested that a nano-analytical interest group (Mester, Felinger, Maryutina, Pingarron) could come under 'emerging issues'_[DBH2]. Other new areas, such as bio-analytical or process analytical chemistry could also appear here.
6. *Metrology.*
7. *The analytical potential of nuclear techniques.* The specific aim of the President in proposing this Interest Group was to provide a channel to create Standards for the sector (in a similar way to Division VII). However it can also function more widely and should encompass nuclear related phenomena such as synchrotron radiation.

d. Role and responsibilities of Division Members

There is a responsibility of each member to be involved in projects, and to contribute to the work of the Division. See <http://old.iupac.org/divisions/V/membership/info.html> for responsibilities of

officers and members. The presence of a large number of members at the meeting was applauded by the President. Specific duties and tasks of members is detailed throughout these minutes.

10. Division key products

a. Stability constants database

This was largely discussed in the SSED report above (item 3c). The database is now under an interest group. The past chair of SSED reported that they were rather skeptical about taking responsibility. However they will consider this at the SSEP meeting in Dublin in July. Kip Powell had informed HG that people from Phys. Chemie (Berlin) will attend the ISSP meeting in Ireland in July. (AF to confirm).

b. Orange Book

The Secretary introduced the concerns about the Orange Book and opened the debate about whether the Division should attempt to update it. The main argument for continuing the Orange Book was because it provided terminology in an hierarchical way that was useful for analytical chemistry. Therefore although the Orange Book needs converting to glossary format in order to provide terms that can be abstracted into the Gold Book, it could have a life in addition to that. A print copy also gives the Division status and visibility. A project to update the Orange Book would be a major undertaking of the Division. In addition to updating the structure and some old chapters, all chapters would need to be consistent with new VIM terminology.

It was agreed that the Division would investigate the required effort and desirability of updating the Orange Book. The Secretary will coordinate the process.

The following members agreed to read a chapter and give an assessment of the worth of the material and what updating would be necessary. All members were urged to read the text as a whole and offer general comments. Replies to BH by 1st July.

PDB – All terms related to metrology

HG/DK – Ch 3 Solution Thermodynamics

SM – Ch 7 Automatic Analysis

JP/JL – Ch 8 Electrochemical Analysis

AF – Ch 9 Analytical Separation Methods

WL – Ch 10/11 Spectrochemical Analysis, Other Optical Methods

ZM – Ch 12 Mass Spectroscopy

ZC – Ch 16 Radioanalytical Methods

PdZ – Ch 18, Quality Assurance of Analytical Processes

Other useful information will be sought: when was each chapter last revised? how many hits has the web version had?

c. Division brochure

The Division brochure is available in the form of a PowerPoint presentation, which is maintained by RL. There might be need for a paper version, like David Moore's poster from some years ago. The Past President will take responsibility for disseminating the electronic brochure and will advise on the need for hard copies of something.

d. CI articles

Project announcements automatically appear. We can contribute editorials, but at present there is nothing specific. The ACD has a good record of CI articles and all members were encouraged to contribute.

e. Web page

The site is maintained by the Secretariat, but it is our responsibility to provide content. Project progress reports should be sent to Fabienne Meyers (by WL) for incorporation in the web site. It was hoped that the present membership of the Division would be soon added to the site.

f. Teamwork

The problem is sourcing regular input. Each copy of Teamwork is mailed out to a list of IUPAC and external recipients, and is also put on the web. The files are large and there has been some problems of multiple posting and dead e-mail addresses. It was suggested that with improved technology a version with colour pictures could be created on the web and the URL e-mailed out to interested people. WL agreed to edit at least two issues during his time as Vice-President. The editor requires material from all, especially when solicited (for example for short profiles of new members).

g. Conferences and workshops

ACD was allocated a symposium in the scientific meeting in Turin 2007. Workshops in Rome (2006) and now in 2008 have been very successful. We should continue this practice. The SSED meeting in Dublin July 2008 (ISSP) has been noted and all members are invited to attend. There will be an International workshop with IAEA in 2009 on proficiency testing schemes for small numbers of laboratories.

h. Any other initiative

PDB raised the issue of whether ACD should lead IUPAC in the adoption of VIM terminology. The President advised this is a matter for higher levels within IUPAC.

11. ACD links with other IUPAC Divisions and external to IUPAC

The President presented a list of our links with other organizations, and particularly welcomed our new member to ICTNS, Maciej Jarosz. It is hoped he can help Division members avoid problems with ICTNS by giving an early opinion on proposed recommendations.

- Interdivisional Committee on Terminology, Nomenclature and Symbols (ICTNS) Prof Maciej Jarosz
- Committee on Chemical Education (CCE) – Prof Roger M Smith
- Committee on Chemical Industry (COCI) – Dr Zoltán Mester
- *Pure and Applied Chemistry* Editorial Advisory Board – Dr. Ales Fajgelj
- International Committee on Weights and Measures/Consultative committee on the Amount of Substance (BIMP/CCQM) – Dr Ales Fajgelj
- ISO-Committee on Reference Materials (ISO/REMCO) – Dr Ales Fajgelj
- International Committee on Weights and Measures/Joint Committee for Guides in Metrology (BIPM/JCGM)
 - Working Group 1 – Prof Brynn Hibbert
 - Working Group 2 – Prof Paul de Bièvre
- Inter-Agency Meeting (IAM) – Prof Ryszard Lobinski
- Joint Committee on Traceability in Laboratory Medicine (JCTLM) – Prof Paul de Bièvre

The strong links with regional European organisations (FECS and EURACHEM) were noted. It was hoped more links to America and Asia could be made. There was some discussion about involvement in meetings, education and training in developing countries. PDB and AF will have discussions with the Secretariat.

12. ACD at the IUPAC GA 2009 in Glasgow

The Past President reported that it was still not clear if there will be a session on analytical chemistry. IUPAC has asked for a parallel session for IUPAC sponsored activities, but there is likely to be competition for this session. The ACD needs to make sure we retain our slot.

An invitation to participate in a session on pharmaceutical chemistry to Roger Smith was noted and RM appointed as Divisional representative

HG – The meeting of SSED overlapped with the Congress in Turin, so members missed the analytical section. It is important to have a schedule in advance to avoid overlap.

It was agreed that the President will invite one member, in addition to the Chair, from SSED and one from WPHQA to the Glasgow ACD meeting.

13. ACD Membership 2010-2011

Nomination committee set up with RL chair and WL member from IUPAC. Three other external members will be appointed by the President after consultation. Names to be reported to Secretariat by 31 May 2008.

14. Next ACD Committee meeting

Next Division Committee meeting will take place at the time of the IUPAC GA in Glasgow in 2009. ACD Officers' Meeting will take place between on 22 and 23 November 2008 in Beijing, China. Kind offer made by Professor Chai to host the meeting was gratefully accepted.

15. AOB

Concluding remarks – AF will take forward the work of previous ACD presidents, but with some adjustments. He was very pleased at the attendance and hoped all had a stimulating and worthwhile meeting. The workshops were scientifically important and at the same time provided a good social function. . He gave thanks to our hosts at APAT (de Zorzi and Belli). In wishing the members well, he reminded all to think about proposing new projects.

List of Annexes to these minutes

Annexe I – RL Introduction to the ACD (based on Report to Council)

Annexe II – HG Overview of the SSED

Annexe III – DK Future directions of ACD

Annexe IV – AF, PdZ – Overview of the WPHQA

Annexe V – DK Agenda and Report from SSED workshop

Annexe VI – MB Agenda of WPHQA workshop

Annexe VII – WL Current projects of the ACD

Annexe VIII – AF Introduction to the main agenda items of the ACD