



# International Union of Pure and Applied Chemistry

## Analytical Chemistry Division (V)

### Report to IUPAC Bureau March 2008

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*Note: The last full report from the Analytical Chemistry Division (ACD) was provided to the Council at the IUPAC General Assembly in Turin in August 2007. In present report only issues arising from the ACD Committee meeting, held in Rome, Italy, between 28 February and 1 March 2008 are covered, with emphasis on issues where some changes might have been introduced.*

#### **1. Membership of Division and Committees (SSED and WPHQA) in 2008-2009:**

In biennium 2008-2009 the ACD is facing the change of ACD officers as well as the change in chairmanship of both associated groups, namely the Subcommittee on Solubility and Solution Equilibrium Data (SSED) and Interdivisional Working Party on Harmonization of Quality Assurance (WPHQA). Therefore at the ACD Committee meeting in February 2008 a review of past and future activities has been organized:

##### ***Presentation of ACD past activities and future***

Ryszard Lobinski (Past President) gave an overview of the work of IUPAC and ACD, based on his presentation to the IUPAC Council 2006-2007.

##### ***Presentation of SSED past activities and future***

Heinz Gamsjaeger, the past chairman of SSED gave an overview of the activities of the subcommittee. As products of SSED activities there are now four important tools available: the solubility data series, standard reference texts, international symposia on solubility phenomena, and the new glossary of terms related to solubility. Dana Knox, the new president of SSED presented future directions. He also announced the next International Symposium on Solubility Phenomena and Related Equilibrium Processes (ISSP) meeting in Dublin in July 2008.

##### ***Presentation of WPHQA past activities and future***

Ales Fajgelj, the past chairman presented a history of the working party which originated from trilateral membership of the AOAC Int., ISO and IUPAC. Paolo de Zorzi, the incoming president indicated some future directions, which include also new areas of interest, e.g., sampling.

#### **2. Division priorities and core business 2008-2009**

Division members have reviewed its activities and discussed the possible orientation for the new biennium. It was agreed to change the name Task Groups to Interest Groups to avoid misunderstanding with the Project Task Groups. Interest Groups should be operative and dedicated to specific issues not covered by projects. For the biennium 2008-2009 the following interest groups and activities were identified:

- Communication (W. Lund (Teamwork))
- Critical evaluations of data (D. Knox (leader), discuss with SSED)
- Electronic Resources for IUPAC terminology work (B. Hibbert (leader), R. Smith, D. Moore, D. Shaw)
- Emerging analytical issues (R. Lobinski (leader), Z. Chai, J. Labuda, Z. Mester)
- Metrology (P. De Bievre (leader), A. Fajgelj, B. Hibbert)
- The analytical potential of nuclear techniques (Z. Chai (leader), P. Bode, A. Fajgelj)

Notes to the establishment of Interest Groups:

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, and W. Lund will lead the group.
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. B. Hibbert will 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 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'. Other new areas, such as bio-analytical or process analytical chemistry could also appear here.
6. *Metrology.* To allow for and assure proper dissemination of IUPAC work in metrological traceability area when the related project is accomplished (mid 2008)
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.

### 3. Core activities of SSED and WPHQA in 2008-2009

To address the activities of SSED and WPHQA two workshops were organized in conjunction with (before) the ACD meeting. These two workshops were attended by all ACD Officers, TMs and some AMs, and provided an excellent opportunity for the ACD members to receive the information on these two important integral parts of the Division.

**Workshops on Metrological traceability in solubility measurement results** was organized by the SSED. As an outcome there was an agreement to develop metrological traceability chains for some simple solubility measurements. Cooperation with the IUPAC project task group working on metrological traceability is foreseen.

**Workshop on Trace elements analysis: role of grain size distribution in solid reference materials** was organized by the WPHQA. As one of the outcomes, activities in new areas of interest, e.g. sampling have been strengthened.

### 4. Projects

Divisional project status reporting system works well. Walter Lund, the Vice-President noted that out of 56 current ACD projects 30 project reports for the past reporting period had been received. However many of the projects that had not reported were either ones under the SSED with zero funding, or new projects that had not been in existence long enough to generate outcomes worth reporting. The new standard form is working well. For projects with no reports the division will request prolongation to September 30<sup>th</sup> 2008 and give 3 month deadline to the task group chair to provide details of progress or intended actions.

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.

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

2006-022-1-500 project of Moore to convert the Orange Book into glossary format. The majority of the task group were no longer available for different reasons.

2003-015-2-500 project of M. 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 the funding.

Project team leaders of projects with no progress report submitted will be contacted by the Vice President and given 3 months to provide information.

**5. 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 investigate with the Bureau members how to put up competitive projects.

**6. Role and responsibilities of Division Members**

ACD has a well established structure of responsibilities, which can be found at the link <http://old.iupac.org/divisions/V/membership/info.html> Members have agreed that there is no need in changing this description at the moment.

**7. Division key products**

***Stability constants database***

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.

***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.

***Division brochure***

The Division brochure is available in the form of a PowerPoint presentation, which is maintained by R. Lobinski.

***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 further contribute.

***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 for incorporation in the web site. It was hoped that the present membership of the Division would be soon added to the site.

***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. W.

Lund agreed to edit at least three editions during his time as Vice-President. The editor requires material from all, especially when solicited (for example for short profiles of new members).

**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.

**8. 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) M. Jarosz
- Committee on Chemical Education (CCE) – R. M. Smith
- Committee on Chemical Industry (COCI) – Z. Mester
- *Pure and Applied Chemistry* Editorial Advisory Board – A. Fajgelj
- International Committee on Weights and Measures/Consultative committee on the Amount of Substance (BIMP/CCQM) – A. Fajgelj
- ISO-Committee on Reference Materials (ISO/REMCO) – A. Fajgelj
- International Committee on Weights and Measures/Joint Committee for Guides in Metrology (BIPM/JCGM)  
Working Group 1 – B. Hibbert  
Working Group 2 – P. De Bièvre
- Inter-Agency Meeting (IAM) – R. Lobinski
- Joint Committee on Traceability in Laboratory Medicine (JCTLM) – P. 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.

**10. 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.

**11. 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.

**12. Next ACD Committee meeting**

The next ACD Committee meeting will take place at the occasion of the IUPAC General Assembly in Glasgow 2009. ACD Officers' Meeting is planned in November 2008 in Beijing, China.