

**Minutes of the IUPAC Analytical Chemistry Division Committee at the 42nd General Assembly, Ottawa, 9-10 August 2003**

**Present:**

*Titular members:* D. Moore, K. Powell, R. Lobinski, F. Ingman, R. Smith, Y. Umezawa, K. Matsumoto, Y. Vlasov, V. Kolotov,

*Associate members:* A. Fajgelj, H. Gamsjager, B. Hibbert, W. Kutner,

*Observers:* M. Bushey, K. Murray, D. Shaw

*Saturday, August 9<sup>th</sup> 2003*

**1. Welcome and agenda approval**

David Moore welcomed the ACD Committee members and the IUPAC observers (M. Bushey and K. Murray). He made sure that everybody received the agenda of the meeting, his presentation to the Council and the report on project proposals prepared by K. Powell. D. Moore suggested a number of additions to the agenda which included:

- approval of the minutes of the ACD Committee meeting in Tübingen,
- matters arising from the ACD officers meeting on the previous day concerning: new projects in the pipeline and budget implications,
- matters arising from the morning briefing of the Presidents and Secretaries: project sending for review by the Secretariat and sponsorship of conferences.

The above items were added to the agenda.

**2. Approval of the minutes of the previous meetings: Tübingen, Brisbane and Research Triangle Park**

D. Moore apologized for not having sent the minutes of the Brisbane and Tübingen ACD committee meetings to the observers (M. Bushey and K. Murray). W. Kutner noticed that he had not received the minutes of the ACD officers meeting in RTP Raleigh-Durham. D. Moore promised to send the documents. The minutes of the ACD Committee meetings in Tübingen and Brisbane and of the ACD Officers meeting in RTP Raleigh-Durham were approved unanimously by vote.

**3. President=s remarks**

D. Moore presented a number of problem areas on which a discussion has focused afterwards. They included:

- a) matters raised during the Division Presidents and Secretaries morning meeting with J. Jost and E. Becker.
  - streamlining the project review process
  - a new process for IUPAC sponsored conferences
  - 2002-2003 project funds still available. A small strategic meeting can be readily funded out of this money. Good project should be quickly approved and funded.
  - DC can be proactive in seeking nominations from NAOs. However, only NAOs can nominate a national representative.
  - the Secretary will provide a list of the new Division members to the Secretariat by August 12th (NB the list was provided by R. Lobinski on August 11th).
  
- b) project tracking. The idea to assign a TM member to a project to track it as approved in Brisbane seems not to have worked properly. Further, the tracking of a project is completely lost when a report approved by the Division is submitted to the Secretariat to be reviewed by ICTNS prior to its approval for publication in PAC. Apparently the track of 6 projects was lost in the ICTNS. W. Kutner suggested an internet tracking system be introduced like in most of the journals. D. Moore assured to have raised this issue during the Presidents and Secretaries morning briefing with J. Jost and E. Becker. It was decided to rediscuss this matter profiting from the visit of E. Becker later in the afternoon (see item 8.4)

- c) proposal solicitation and development. Historically, proposals came from the commissions, now it is imperative that ideas come from outside. D. Moore pointed to difficulties with obtaining ideas from outside. All the proposals to date came from the IUPAC structure. D. Moore prepared an information brochure on what the ACD does and how projects can be submitted. The brochure appeared not to be widely known even among the DC members (W. Kutner asked for a copy). A. Fajgelj noticed that outside people are not aware about the possibility to make project proposals which he finds quite understandable since time has been short. He found it important to spread the news to external people so that they can submit projects. W. Kutner suggested an approach in which a speaker is contacted after his/her lecture by a Division officer, should the latter see a potential for an IUPAC project. It was stated that the ACD should look for ideas not projects.
- d) TM election process. D. Moore summarized problems with the e-mail ballot. 9 persons had not received the ballot during the initial mailing. The ballot had been resent to them so that they had the opportunity to vote.
- e) ACD delegates were appointed for the interdivisional meetings on Tuesday: Human health and biomolecular chemistry (R. Lobinski), Environment (D. Shaw, K. Powell)
- f) D. Moore worried about the Division capacity of spending money on new projects. 19 k\$ is left to be allocated for the present biennium. A possibility to inject some money into the already running projects was indicated. The need to be proactive in generating and managing projects was emphasized.

#### **4. Review of the ACD structure, operations and responsibilities**

The points raised by the President triggered off a discussion animated by K. Powell.

##### **4.1. Advisory groups**

First, the role of advisory group was examined. Currently 3 advisory groups organized around V. Kolotov, Y. Vlasov and Y. Umezawa are active. Y. Kolotov found his advisory group very useful to set up the project on radiopharmaceuticals (M. Bonardi). He emphasized that his AG was consulted actively and regularly but admitted that the original idea was born in the Commission some time ago. Y. Vlasov also established an AG (20 people) that was occasionally contacted but has not go successful in promoting a project. H. Gamsjager shared his good experience with discussions on the project related to the octanol-water partition coefficients in the environment in the frame of Y. Vlasov advisory group. R. Smith suggested the issue of octanol-water partition coefficients should also be consulted with the Human Health Division. D. Moore volunteered to serve as a contact person.

A. Fajgelj asked for the difference between advisory groups and the directory of expertise assembled by K. Powell. D. Moore explained that the original idea was to assure continuity when TMs change. The Directory of Expertise should be considered as an aid but not necessarily be bound to advisory groups. The proper size of an advisory group should be kept small (5-7 persons). The need for stimulating contacts with advisory group members and two-way communication between AGs and TMs arose. R. Smith suggested that a questionnaire containing clear and precise questions might be a correct way to improve the communication. It was agreed that TMs should look for ideas whereas the role of advisory group should be to help a task force to setup a project.

##### **4.2. Project solicitation and initiation**

Possible ways for project solicitation and initiation were outlined by K. Powell. They include:

- organising a forum of discussion with invited speakers from outside. K. Powell indicated his willingness to associate such a forum (workshop) with the ACD meeting in February 2004 in order to find ideas around which projects could be developed.

- using the ACD web page to solicit ideas. The possibility to create a link (a pop up window) from the on-line Orange Book, in addition to the one already serving to alert to inconsistencies (100 000 hits)
- using chapters in the Orange Book itself is a source of projects, e.g. in the separation methods and electrochemistry areas. R. Smith listed: peak symmetry, electroanalytical techniques, countercurrent chromatography as examples.
- being proactive in adding to task groups the names of people who can inject projects into the system. The Division can pay for that.
- consulting journals editors on emerging problems concerning terminology. K. Powell expressed his willingness to contact A. Manz, the Editor of the Lab-on-a-chip journal.
- using press releases (consulted with L. Abernathy) sent to the key analytical chemistry journals as for example ANews from the Analytical Chemistry Division@. K. Powell indicated that it would be good to have a database containing the name of the journal, contact person and a few keywords. Each ACD member was encouraged to send this information concerning 5 the most representative journals from his field.

A Fajgelj inquired how the ACD compares with other divisions in terms of projects, what is our capacity? The ACD always ran more projects than other Divisions. Now we have 16 projects running whereas other Divisions have 7 to 15. To that a number of 25 fast-pipeline (older projects beeding to continue to completion without funding) projects needs to be added. A big problem is the very small number of new starting projects. Only 6 projects have been approved in the biennium. A sum of \$17 000 is still available. K. Powell indicated that the Secretariat monitors attentively the budget for projects allocated to Divisions. If divisions have good projects they can create pressure for more money. It was estimated that the current Division budget would allow for 5-6 new projects to be funded before the end of 2003.

#### **4.3. Task group membership**

The Division could be proactive in terms of expanding the composition of task groups so that they become more representative. It was suggested to examine the approved projects and to propose additional funding to allow the participation of young members. One or two TMs should be involved in each task group, especially in the case of big projects. This might bring a tangible interaction between the task groups and the ACD Committee. K. Powell defined two levels of involvement: 1) working member of task group with financial implications; 2) a corresponding member of a task group (no financial implications). The role of a corresponding member would be to assure that the project is running on schedule. The involvement of TMs in the running projects was reviewed and only 1 out of 6 projects approved in the biennium (Duncan Burns= project on robustness) did not involve a TM. It was decided to add to the project form another line with a request to nominate a corresponding IUPAC member.

D. Moore emphasized the necessity of engaging stakeholders and endusers in the projects, i.e. people who would be affected by, and use the project=s results, respectively.

#### **4.4. What is our core business?**

A discussion was initiated by D. Moore on the core business of the ACD in the following key areas: nomenclature and terminology issues, validated data and standard procedures, and education and public appreciation of chemistry. A. Fajgelj described how he saw the role of his Working Party. D. Shaw noticed confusion between the role of the DC and the role of task groups. The mission of the DC was to manage the best possible portfolio of projects. As an example the Ain-house method validation protocol@ was cited. The role of IUPAC is not to validate methods but to give tools to endusers to do it. R. Smith gave the example of the proliferation of acronyms in electroanalytical techniques. The inventor has the right to name one, but IUPAC needs to generate a name with the consensus. A. Fajgelj suggested a closer look at the Terms of Reference in the near future.

D. Moore passed a request from the IUPAC executive and, especially, from G. Wilson that ACD promotes the publication on pH. A. Fajgelj inquired about mechanisms that can be developed to approach the legislative bodies with the results of our projects. One working example goes via Codex Alimentarius. He will submit his inquiry to E. Becker.

#### **4.5. Streamlining project review process**

In order to accelerate the project reviewing process, a project received by the Secretariat is immediately sent out for review by F. Meyers. A problem may be that she sends the project to the reviewers whose names were given by the proposer. Such a review cannot thus be considered as independent. This issue was further discussed with E. Becker and F. Meyers (*cf.* item 8.4).

#### **5. A visit of Peter Atkins (CCE)**

Peter Atkins, the chairman of the Committee on Chemistry Education (CCE), paid a 15-min visit to the ACD meeting. He expressed his will to establish joint projects on the public understanding of chemistry. K. Powell assured that as the ACD representative to CCE he has watched all the projects of the Division from the angle of their interest for the CCE. K. Powell also emphasized that the ACD took an initiative and sponsored a titular member to visit Botswana to share experience or resources in analytical chemistry. P. Atkins suggested that the IUPAC report on Weapons of Mass Destruction should contain an educational component but did not make any precise suggestion how.

#### **6. Visit of E. Becker, F. Meyers, L. Abernathy, and J. Bull (PAC Editor)**

The ACD hosted a delegation of the IUPAC Bureau. E. Becker presented three current areas of concern of the Bureau: i) money available left, (ii) new system for sponsoring conferences and symposia, and (iii) Pure and Applied Chemistry editorial matters. After the presentation by E. Becker a discussion on other matters of interest for ACD started.

##### **6.1. Funds still available**

E. Becker indicated that there is still money available left for projects. It would be preferable to use it this year, since cuts are likely in the next biennium. He agreed that money can additionally be injected into a running project if necessary. However, money left on a project nominally completed will not be returned to the Division.

##### **6.2. IUPAC sponsorship for conferences**

In general, IUPAC sponsorship of conferences in developing countries attests to its quality but does not carry financial support. However, Divisions and Standing Committees of IUPAC may apply for financial support via two programs: New Directions in Chemistry (NDC) and Conferences in Developing and Economically Disadvantaged Countries (CDEDC). The NDC program is to provide funds on a competitive basis to support conferences in innovative fields or cutting-edge research topics. Such conferences may be held in any country that is a Member (NAO) or Associate Member (ANAO) of the Union. Application shall only be submitted with the recommendation of an IUPAC Division or Standing Committee. The CDEDC program is to provide funds to support conferences in developing and economically disadvantaged countries that are either NAOs or ANAOs. Alternatively, this program can also be used to support an "IUPAC Lecturer" to give talks at conferences otherwise not supported by IUPAC in developing and economically disadvantaged countries. Divisions and Standing Committees will identify eminent scientists who are willing to participate in conferences and perhaps also present talks at universities in the host country. An application for support must be initiated by an IUPAC Division or Standing Committee. A question about a need for a centralized register of IUPAC speakers was raised. K. Powell obtained clarification whether the Division should take the initiative in seeking funding for a conference.

##### **6.3. Supply of information for chemistry via PAC**

J. Bull is now the editor of PAC where part of his function is to deal with the proceedings of conferences. He indicated that the paper should be properly reviewed. H. Gamsjager evoked the symposium his working party is organizing in Portugal and asked whether he could count on some help from PAC with reviewing the material. J. Bull said that communication is greatly facilitated if as soon as the conference is approved, a proceedings Editor is appointed.

#### **6.4 Questions from the ACD**

A discussion was raised by the fact of projects being sent for review by F. Meyers immediately upon reception. D. Moore emphasized that it is the function of the ACD to know what proposals come in and how to prioritize. If we need to be pertinent we need to be present in the beginning. It was agreed that F. Meyers sends the projects for reviews at the same time as she sends them to the ACD Committee. The system seems to work.

Regarding the tracking of complete projects within the Secretariat, F. Meyers is going to search for an appropriate tool and an improvement can be expected in the near future.

#### **7. Reports from conferences**

ACD TMs gave their accounts on different conferences during which they promoted the ACD. D. Moore presented a poster during the FACCS meeting, Providence, Rhode Island, R. Lobinski gave a talk on the role of IUPAC during the EUROANALYSIS meeting, Dortmund, Germany. K. Powell offered a workshop on IUPAC project preparation during the Flow Analysis Conference in Melbourne, Australia, but the offer was not taken in by the organizers. His impression was that although there was an interest in the work of the ACD, there was none in project submission. Y. Umezawa published a paper in *Bunseki Kagaku* on what ACD does. R. Smith was satisfied with his participation in the session on analytical chemistry in the developing world. He pointed to the need for more assistance to the scientists and technicians who operate equipment on site. A question was raised on obligations of conference organizers using the IUPAC logo. The registration fee of an IUPAC representative should be waived and a lower registration fee be available for participants from the developing countries made available. Also, an IUPAC representative should get a 5-min slot during the opening ceremony to present the mission of IUPAC.

#### **8. Report on the progress of current projects**

K. Powell gave an account of the progress of current projects. The account is attached as an Annex to the minutes. The progress report raised no comments with the marked exception of the project on analytical electromigration techniques by J.A. Jonsson. The origin of this discussion was a recommendation of the ICTNS to reject the project unless it is extensively reviewed. K. Powell raised a question about interactions with ICTNS and D. Moore considered the ICTNS decision as difficult to understand. He said that the authors were demoralized and thinking whether they should revise the report and bring the project to completion.

W. Kutner said he had not seen the project on the Division and the first time he got it was accompanied by voluminous review material. According to him the guidelines to how the project should be revised were very precise and a revision feasible.

D. Moore suggested a help from Division might be useful to finalize the project. R. Smith accepted to get involved as an additional person sponsored with ca. 750 \$. The Division gave a green light to additional funding (1000 \$) for the SIT project (Pettit)

The canvas of this particular project raised a number of questions on the relations of the Division with ICTNS. The delays were judged too long. This point was to be raised again by D. Moore in the Division Presidents meeting and the Bureau meeting.

Another project discussed in more detail was that run by S. Sjöberg on Chemical Speciation of Environmentally Significant Heavy Metals and Inorganic Ligands. The project has expanded, it is going to produce not one as initially expected but possibly 6 publications.

### **9. Report on the Orange book**

The revision of the orange book is a determined process that should go via determined roads. An ideal situation in future would be one database of terms.

*Sunday August 10<sup>th</sup> 2003*

### **10. Workshop on challenges to analytical chemistry**

R. Lobinski summarized the idea of having external speakers during an ACD Committee meeting in order to introduce to the hot topics in analytical chemistry that could give ideas to new task groups. The persons who graciously accepted the invitations were Aled Edwards, Director of the Genomic Consortium, University of Toronto, Jim McLaren, Director of the Chemical and Mechanical Standards, National Research Council, Ottawa, and Heinz Schimmel, IRMM, Geel, Belgium. The topics retained were analytical chemistry in proteomics and genetically modified organisms. R. Lobinski brought the topic of the needs of analytical chemistry for biotechnology to the Subcommittee meeting on biomolecular chemistry on the following day.

A. Edwards presented the increasing role of mass spectrometry in a multibillion industry of identification and prediction of disease states. He evoked the need for standardization of analytical mass spectrometric methods, qualitative fingerprinting and quantitative determination. J. McLaren and H. Schimmel talked about the needs for accurate measurements of DNA in view of the increasing role of genetically modified organisms and regulatory trends.

Summarizing the workshop D. Moore stimulated the identification of areas to which ACD may contribute. A. Fajgelj said that the ICSU proposal could be expanded to include the traceability aspects in GMO measurements. Other topics included:

- evaluation of analytical method performance in biotechnology
- compare the use of terms: preconcentration/sample preparation in GMO analysis to that in classical analysis (K. Matsumoto)
- an insight into techniques for metabolomics with the objective to bridge the gap and regaining ground from biologists
- mass spectrometry terminology (K. Murray)
- terminology related to analytical chemistry of metal forms in biological systems, metallomics (R. Lobinski)

### **11. Report from Working Party on Quality Assurance**

A. Fajgelj presented briefly the activities of the WPQA. The latter currently includes 7 members and is involved in 6 projects. The project on Harmonized guidelines has been published in PAC. A. Fajgelj suggested a stronger link between the Working Party and the ACD. He will prepare a detailed report of the WPQA activities.

### **12. Report from the Subcommittee on Solubility and Equilibrium Data**

H. Gamsjager presented a report of the activities of the SSED chaired by him. The report is enclosed as an annex to the minutes. The contribution of H. Gamsjager to this area was recently reflected by a special issue (2003, 134, Vol.5) of Monatshefte für Chemie dedicated to him on the occasion of his 70<sup>th</sup> birthday. H. Gamsjager presented the silhouette of W. Hummel, Paul Scherrer Institute, eager to join HG group as an editorial consultant for the carbonate

project. D. Moore noticed that W. Hummel is an ideal example of enduser. The question of the visibility of SSED within IUPAC was discussed.

### **13. Report from Interdivisional Committee on Terminology, Nomenclature and Symbols**

W. Kutner presented the activity of the ICTNS which is a link between the Secretariat and Pure Appl. Chem. He presented the recent changes in the composition of the ICTNS (J.W. Lorrimer replaced T. Cvitas as President, whereas V. Metanomski was replaced by B.J. Herold as Secretary. The change in chairmanship may overcome the factors responsible for the increased delay in handling the projects by ICTNS. W. Kutner noticed that in addition to the passive activities (tackling the projects coming in) the ICTNS has also its own projects, citing the example of a recent project on the correct use of symbols and fonts.

D. Moore will supply W. Kutner with the list of 5 projects of which track was lost apparently in ICTNS. They include: Nomenclature in XRS (Y. Goshi), Guidelines in calibration Part 2 (Danzer), speciation in soils (Hlavay), Piezoelectrical sensors (Lindner), Critical Evaluation of the State of the Art of the Analysis of Light Elements in Thin Films (Friedbacher).

### **14. Report from the Committee on the Chemistry Education**

K. Powell could not go to Beijing. The interface between the CCE and ACD was already discussed on the occasion of the P. Atkins visit (see item 5)

### **15. Division membership**

The ACD committee noted the retirements of G. Gauglitz, V. Kolotov and F. Ingman. R. Smith agreed to be appointed as the Secretary under the condition that he will stay as the Secretary for two terms and then quit. According to the election results (unanimous) from February 2003 the Division officers for the term 2004-2005 are K. Powell (President), R. Lobinski (vice-president), R. Smith (Secretary) and D. Moore (past president). F. Ingman (Chairman of the Nominating Committee) resumed the work of the nomination committee composed of F. Adames, B. Byrne, B. Cattrill and A. Hulanicki producing a ballot reflecting discipline and geographical discipline consideration. Problem with some people who have not received the ballots was discovered and saw to. The election (18 ballots received) brought the following composition of the ACD committee: MauroBonardi (nuclear methods, 18 votes), Ales Fajgelj (general aspects, 10 votes), Maria-Lisa Riekkola (separation techniques, 11 votes), Elias Zagatto (environmental chemistry, 11 votes), Brynn Hibbert (electroanalytical chemistry, 11 votes), Kazuko Matsumoto (human health, 18 votes).

The appointment of associate members (a total of 6 is possible) was then discussed. The ACD nominated H. Gamsjager, W. Kutner, Z.F. Chai, Y. Umezawa, V. Vlasov and K. Murray as associate members.

The following representatives of the Division were nominated: CCE (R. Smith), Subcommittee on Materials Chemistry (B. Hibbert), Joint Committee on Traceability in Laboratory Medicine, JCTLM (P. DeBièvre). D. Moore stays an ACD representative on the Evaluation Committee that evaluates the impact of projects.

The nominations were voted unanimously.

Nominations for NRs could not be decided at the meeting. F. Ingman was tasked with the preparation of a summary list with nominations from the NAOs. On the basis of this list the ACD selects the NRs.

### **16. Other business**

V. Kolotov announced that the 2006 ICAS conference will be held in Moscow, and its chairman, B. Spivakov wish is to organize it in close collaboration with the ACD.

**17. Next meeting**

The even-year meeting of the ACD committee is going to be held in the second week of February, the meeting place was traditionally left at the discretion of officers.