

**Minutes of the meetings of the Analytical Chemistry Division Committee, Brisbane,
June 29 - July 2, 2001**

Present:

F. Ingman (President), D. Moore (Vice-President), L. Currie, A. Fajgelj, J. van Staden, R. Byrne, V. Kolotov, R. Smith, B. Spivakov, D. Shaw, S. Rondinini, R. Lobinski, R. Durst, K. Powell (Secretary). In attendance: M. Bushey and R. Stefan.

[For minuted items 8-16 the Division Committee was joined by Commission and WP Secretaries (W. Kutner, K. Volka, Å. Johanssen, P. Benes, K. Popov, H. Gamsjäger and P. de Bièvre) and for some items by Y. Vlasov, Y. Umezawa and G. Friedbacher.]

1. Welcome.

F. Ingman welcomed members to the last meeting of the Division to be held under the 'old system'. He extended a special welcome to Prof. Michelle Bushey (Trinity University, San Antonio) who was attending as a Young Observer.

2. Agenda.

The Agenda as circulated was approved.

3. Minutes of Berlin Meeting.

The minutes were accepted as a correct record of the proceedings in Berlin (Durst/Byrne). There were no 'matters arising'.

4. President's remarks.

F. Ingman reported on the productive meeting of Commission Chairs and the Division Executive in Manchester, May 2000, and on the meeting of the Division Executive in Raleigh in December 2000. Minutes of both meetings had been circulated.

He reported on the General Assembly briefing meeting for Division Presidents and Secretaries. John Jost (Executive Director) spoke about the objectives of the three inter-Divisional meetings on the new system for project proposals: the first outlining the application process, the second to explore ways of establishing wider involvement in new projects and the third on management of projects by Divisions.

Ted Becker (Secretary General) indicated that all sub-committees and working parties would be terminated at the end of this year and that a new case must be made by the Division for the re-establishment of these groups. He indicated that the period until the end of this biennium would be an opportune time to initiate proposals for new projects, as funding would be available from sources other than the Division budgets. This would also ensure that existing interests of Commissions could be carried forward. He indicated that existing projects that would not be completed by the end of the year would have to be re-initiated using a simplified (fast-track) Project Submission. If such projects require additional funding then a full Project Submission will be required.

5. Future structure and function of the Division Committee.

The Division will have 10 TM. It can add 6 AM and up to 6 NR. Only the TM will be funded from the Operational Grant. The Division must be structured and function in such a way that it can effectively promote and nurture new projects.

5.1 Division Rules and Terms of Reference

The Terms of Reference drafted in December 2000 were discussed. There was a general concern that the draft listed Methods and Applications under a single heading. It was agreed that the draft should be modified on the basis of changes notified in writing at the meeting. It would then be distributed to the Division for further comment.

5.2 Mechanisms for soliciting and initiating new projects.

The task of the TM and AM will be to identify important areas for new work, to identify qualified people to form Project teams and to encourage the submission of Project Proposals. It will be necessary for each TM to maintain an informal network of Advisors to broaden the competence and resources of the Division.

Commissions were asked to comment on the composition and function of an Advisory Group (or Groups) and to present recommendations for membership of this Group. The ensuing discussion considered several possible models. It was resolved that the Advisory Group(s) should consist of the retiring DC members and Chairs and Secretaries of Commissions. Such a group would assist in the transfer of knowledge and experience from the 'old system', and could be of particular benefit to the new Division Committee members.

It was suggested that the information flow within the Division could be improved. For example, by use of a non-public URL on the IUPAC web site, all TM could have access to all referee comments on each Project Proposal and information about approved funding.

Concern was expressed about the need for early 'initiation' of new TM to their responsibilities as members, and to the general functioning of the Division Committee.

6. Commission reports on the status of "old" (Commission-sourced) projects.

These reports are summarised in appendix A.

7. Commission reports on progress of projects approved under the new Project Submission scheme.

These reports are summarised in appendix B.

8. Status and membership of Sub-committees and Inter-Divisional working parties.

8.1 The Solubility Data sub-committee

Draft Terms of Reference, prepared by Commission V.8. were tabled (see Appendix C). It was agreed that this new sub-committee should also serve the interests of the previous Equilibrium Data Commission, with its new name reflecting this partnership. Following informal discussion by the Commission chairs the name "Solubility and Equilibrium Data sub-committee" was proposed. The sub-committee membership will be: H. Gamsjäger (chair), M. Salomon, P Scharlin, D. Shaw, W. Voigt, S Sjöberg, P. May.

8.2 Inter-Divisional working party on Harmonisation of Quality Assurance

The Working Party will retain its name (abbreviated to WPHQA). The ACD will take responsibility for moderation of WPHQA activities. Ales Fajgelj will continue as the Chair. The WP will shortly submit revised terms of reference to the Division.

A. Fajgeli presented a report on the activities of the WP. He outlined the three projects that have been active in this biennium. It is clear that the WP is highly visible in that their workshop, proceedings and other publications have led to invitations to conferences and for further articles. The WP has strong and active links with official Analytical Chemistry bodies and has had success in obtaining external funds. The inter-Divisional nature of its work also gives it access to Project Committee funds.

A. Fajgeli expressed concern about the selection of external reviewers. What is IUPAC policy? The network linking Commissions to leaders in their fields is no longer available. For review of its work IUPAC needs access to an independent, fiercely critical scientific community. He also questioned the criteria against which IUPAC projects are evaluated. What are the IUPAC-specific criteria? Will these be met when a document is published in a journal other than PAC?

8.3. Inter-Divisional working party on redefinition of pH scales

A 'final' version was completed in May 2000 and submitted for public review and for approval by the Division I and V Presidents. The document is a fundamental article on methodology, with due emphasis on traceability. It provides a foundation for future work. The contentious issue of authorship had now been resolved with the addition of C. Brett's name. The work of this WP is now complete and the group has been disbanded.

S. Rondinini noted that pH is a very important topic. She suggested that it may not be adequately served by the new project proposal system as it is unlikely to bring together the necessary comprehensive input from a large group of experts. She requested that the Executive consider the possibility of a more permanent place or group within the Division for oversight of this topic.

9. Submission of new projects

How many projects can be approved/funded in a biennium? The major constraint will be limitation of funds – approximately \$40,000 for the biennium. There will be strong encouragement for Task Groups to source funds additional to those sought from IUPAC.

The policy on submission, review and funding of projects needs to be transparent and therefore clearly specified on the web site.

S. Rondinini questioned why the new Project Proposals submitted by W. Kutner had not been funded in the present biennium. It was noted that they had been deferred (not rejected) because of the large number of V.5 projects that were unfinished at the time of application. It was agreed that these projects could now be reconsidered.

In future, all persons involved in project Task Groups will be recorded in the Blue Book. On completion of their project they will become Fellows of IUPAC.

9.1 Division policy for Project Submission and Review.

Although project proposals may be submitted at any time, it was agreed that the funding decisions for Project Submissions should, in general, occur twice each year. Exceptions would be for projects that requested zero or minimal funding, those projects requiring collaboration with other Divisions and those of very high priority. It was agreed that for all other cases the project funding should be contestable in each funding period. This will require prioritisation of projects, which in turn will require concurrent access to all referee reports. Prioritisation will include the value of the project in terms of scientific impact. The Division Committee should draft guidelines for establishing priority.

R. Smith proposed that submission of an outline of the project proposal to the Executive should be encouraged in advance of a formal submission. Following assessment by the relevant ACD members, comments and suggestions could be made to the Task Group leader in advance of a formal Project Submission. This is not too different from the current review process which involves (a) review by the Division, (b) return of the document to the Task Group chair for refinement (if necessary), (c) review by external referees. The same objective will be met by retaining step (b).

Clear reasons should be given when a project is rejected or deferred.

The review process at both the Project submission stage and completion stage will be facilitated by access to the **Directory of Expertise**. Commissions V.6. and V.7 submitted contributions for this Directory at the meeting. Other Commissions were working on their contributions and agreed to forward them to the Secretary.

9.2 Division policy on specification of Task Groups and presentation of project outlines and budgets.

It was noted that project proposals often lack details regarding the steps and amount of work involved and the assigned responsibilities of each Task Group member. In some cases the membership of the Task Group has not been finalised (e.g. 'additional Task Group members will be added as required'). In future these matters must be explicit. The proposal by S. Sjöberg was cited as an example of a project that, on an additional 1 page submission, had given adequate specific details of the tasks and (pre-agreed) responsibilities for each Task Group member.

Funds assigned to a project remain available for the full life of the project. At the time of project approval they are deducted in full from the Division Budget and entered into a specific ledger for the project. For

each project the Task Group leader will be responsible for approval of expenditure. If a project is terminated, or if there are unspent funds, the outstanding balance will not be returned to the Division budget. However, if there are justifiable cost over-runs on a successful project the Division may present a case for additional funding.

9.3 Division policy for management of new projects.

It was agreed that Task Groups should provide the Division with a brief report in June each year.

10. Proposals for a Solubility Data Program.

A meeting between F. Ingman, D. Moore, D. Shaw and T. Becker had produced an agreed mechanism for new project proposals that could preserve elements of the solubility data program's *modus operandi*. Separate proposals will be required for approval of a Series and for approval of individual projects (volumes) of a series.

For a Series: A "phantom" Project Submission will be completed, seeking approval for the Series. It will establish the area to be covered and its significance, indicate the user group(s) and suggest appropriate external referees. The Project Submission will undergo the normal review by the Division and by external referees.

For individual projects (volumes) in a series: a fast-track proposal will be made, which need not restate the case for the series.

For current projects (volumes) that are near completion, or require no funding, a simplified (fast-track) Project Submission will be made and the Division will determine if external review is necessary.

11. Proposals for an Inter-Divisional Commission on Biotechnology

F. Ingman reported that he had received favourable comments from Division members. The possible outcome will be formation of a sub-committee within the Organic Chemistry Division.

It was resolved that the Division should be pro-active in seeking representation on this sub-committee because of the relevance of quality assurance and the importance of analytical techniques such as electrospray mass spectrometry.

The Division makes a strong recommendation that the name for the sub-committee should include the identifier 'chemistry'. An appropriate name may be the Sub-committee on Biochemical Technology.

12. Orange Book

The unedited electronic version of the Orange Book is now ready for placement on the web. At this time the Index is in a separate PDF file which can be searched by key word to locate the relevant section of the Orange Book. Interfacing of the Index with the main text may be achieved through a summer student project.

A non-public URL will be provided to allow Division members to identify items that require revision in the light of more recent terminology recommendations. Where need for substantial change is identified the Division may need to initiate new projects via the Project Submission process.

In future, where approved IUPAC projects recommend a new or changed Terminology, the Task Group will be responsible for checking the Orange Book and then for advising the President of required changes when the final project documents are submitted. This process will become a standard part of the project implementation plan. The IDCNS process will ensure that there is adequate editorial oversight.

13. The Special Topic Project.

James Bull made a presentation on the status of the Special Topic Project. He indicated that a ST issue may be based on the proceedings of an IUPAC sponsored conference but with additional IUPAC-invited

or contributed papers. The latter are subject to the usual IUPAC review process. There were two ST issues of PAC in 2000, each based on conference proceedings.

The Division indicated that it would be helpful if TM who review AIQ's were fully aware of the need for suitable material for Special Topic publications.

Another possibility is that authors may be invited to write authoritative special feature articles. To date this has not been successful. The Division enquired whether an honorarium would be available for an invited author, or whether funding through the Project Submission procedure (e.g. for a meeting of review writers) may be possible (and if so, from what budget would the allocation be made?)

14. Division membership

14.1. Retirements

The following Division members will retire at the end of 2001: F. Adams, R. Byrne, R. Durst, S. Rondinini, B. Spivakov, J. van Staden, L. Currie, R. Niessner, B Schrader.

14.2. Titular members

For 2002-3 the elected TM are R. Lobinski, R. Smith, G. Gauglitz, V. Kolotov, Y. Vlasov, K. Matsumoto, Y. Umezawa. In addition, F. Ingman (past President), D. Moore (President) and K. Powell continue as elected officers. K. Powell was nominated and elected as vice-President and R. Lobinski was appointed as Secretary for 2002-3.

14.3 Associate members

The chair of the WPHQA (A. Fajgeli) and the chair of the Sub-committee on Solubility and Equilibrium Data (H. Gamsjäger) were appointed as AM. The remaining three AM positions will be filled after consideration of 'gaps in expertise' and by consultation with the current TM.

14.4 Division representatives

Division members were appointed as follows:

IDCNS: W. Kutner (AM); CTC (CCE): K. Powell; Committee on Chemistry and Materials: F. Ingman; Committee on Chemistry and the Environment: R. Lobinski; representative on BIPM/CCQM, ISO/REMCO: A. Fajgelj.

15. Date and venue of the next meeting

Ottawa, 8-17 August, 2003.

16. Other business.

F. Ingman reported that the vice-President, President, Past President and Secretary General had all praised the work of the Division through the restructuring process. He thanked the retiring Division Committee Members for their work during the past biennium.

Appendix A

Commission reports on the status of "old" (Commission-sourced) projects.

This summary is restricted to projects that are 'in progress' or to be terminated.

Commission V.1.

510/31/95: Nomenclature for X-ray Emission Spectroscopy. (Y. Gohshi)

External review comments will be discussed in Brisbane.

510/39/98: Selectivity and Specificity in Analytical Chemistry. (J. Vessman)

Approved by Division President. Open for public comments until 30 September 2001.

510/38/98: Recommendation for the use of the term recovery in Analytical Procedures. (D. T Burns).

With external reviewers. Only two replies to date.

510/37/98: Essential Information for Characterizing a Flow Analyser. (E. Zagatto)

External reviewer comments discussed at the GA.

2001-001-2-500: Dimensionality in analytical chemistry. (K. Danzer). Commission review of the document is complete.

510/36/97: Terms and Definitions Used in Connection with Ecotoxicological Investigations of Aquatic Systems. (H. Muller). Finalised by the Commission. Ready for Division review.

510/33/95: Downsizing in Chemistry and Chemical Research with Special Reference to Analytical Chemistry (Y. Gohshi). To be terminated.

510/34/97: Analytical Aspects of Chemical Process Control. Part 2: Evaluation methods. (J. van Staden). To be terminated.

510/35/97: Guidelines for Calibration in Analytical Chemistry. Part 2: Multicomponent Calibration. (K. Danzer). The Commission expects to complete first draft at the GA.

510/40/98: Uncertainty in Analytical Chemistry. (W. Horwitz). To be terminated.

Commission V.2

523/2/89: Determination of trace elements bound to soil and sediment fractions. (J. Hlavay). Approved by the Commission and sent to three external reviewers. The manuscript and reviewer reports will be sent to the Division.

Commission V.3

530/10/95: Analytical Electromigration Techniques. Near completion at Commission level. A fast-track project proposal will be submitted to ensure its continuation.

530/12/97: Hold-up volume in column chromatography. Public review complete. Should be finished at the GA.

530/13/97: Retention parameters in gas chromatography. Public review complete. Should be finished at the GA.

Commission V.4

540/17/95 (Moore), 540/20/95 (Niessner), 540/21/98 (Laserna), 540/23/97 (Velhorst) and 540/24/98 (Imasaka) have been terminated. D. Durst commented on the importance of 540/20/95 and 540/23/97 and asked if new Project Submissions would be made. The meeting was advised that it had been impossible to assemble a satisfactory task group.

540/15/95: Waveguides/Optical fibres (G. Gauglitz). Under review at Commission level. A fast-track Project Submission be lodged.

540/18/95: Hyphenated techniques (Velhorst). A new Project Submission will be prepared.

540/19/95: Optical sensors/bioprobes. (Vo-Dinh). Has been reviewed by Commission but revised document not received. A fast-track Project Submission will be prepared.

540/25/98: High throughput screening/ combinatorial techniques (G. Gauglitz). A new Project Submission will be made.

540/26/98: Liquid organised media (Shtykov). Under review by Commission. A fast-track Project Submission will be prepared.

540/27/98: Surface analysis (K. Volka). Under review by Commission. A fast-track Project Submission will be prepared.

Commission V.5

550/49/91: Critical assessment of the contribution of liquid junction potentials to analytical potentiometric measurements (A. Covington). The future of this project will be considered in the light of the work by the WPPH.

550/58/95: Potentiometric selectivity coefficients for ion-selective electrodes, Parts II and III. (Y Umezawa). At external review stage.

550/62/97: Electroanalysis with piezo-electric devices. (E Lindner). Under external review. A fast-track Project Submission will be required.

550/63/97: Lead-based second kind electrodes in aqueous medium and in non-aqueous solvent mixtures. (T. Mussini). Responding to external review comments.

550/64/97: Non-selective sensor arrays. (Y Vlasov). Under external review. A fast-track Project submission will be required.

550/65/97: Electrochemistry since Volta. (S. Rondinini). Terminated.

Commission V.6.

560/40/97: Critical evaluation of stability constants and thermodynamic functions of metal complexes of crown ethers. (Arnaud-Neu). The project is under review by Commission and should be completed early in 2002. A fast-track Project Submission will be made.

560/41/97: Critical evaluation and prediction of stability constants of metal complexes of complexones for biomedical and environmental applications. (K. Popov). Parts of this document have been reviewed by the Commission but others are still in preparation. A new Project Submission will be made to ensure continuation and completion of this work.

560/36/93 (S. Ishiguro) and 560/38/95 (M. Tabata) have been terminated.

Commission V.7

570/18/93: Critical Evaluation of the Chemical Properties of the Transactinide Elements. (J.V.Kratz). External review complete but conflicting reports difficult for author. Has been sent to two independent reviewers who have suggested a compromise. A new Project Submission will be made.

570/19/93: Critical Evaluation of Resonance Integral for Activation Analysis (N.Holden). Terminated

570/21/93: Low Activation Materials for Fusion Technology: State and Prospects (V.P.Kolotov). Under Commission review. A new Project Submission will be made.

570/22/95: Determination of Alpha-emitting Radionuclides in Diet. (H. Nakahara). Responding to external review comments.

570/24/95: Critical Review of Analytical Applications of Mossbauer Effect. (A. Vertes). Responding to external review comments.

570/26/98: Compilation of K_0 and related data for NAA in the form of electronic data base. (F. De Corte). Under Commission review. This project will lead to a CD and a short article in PAC. A new Project Submission will be made.

570/27/98: Effect of humic substances on the environmental migration of radionuclides. (P.Benes). Terminated.

Commission V.8

580/43/92: Experimental determination of solubilities. (G. Hefter). Near completion. To be published by Wiley as part of a series on Solution Chemistry. A fast-track Project submission will be required.

581/26/90: Ethyne and other gaseous alkynes. (P. Fogg). Journal (JPCD) review process complete.

582/43/97: Nitromethane with water or organic solvents. (V. Sazanov). Submitted to JPCD.

583/34/92: IA and IIA azoles, cyanates, cyanides and thiocyanates. (J. Hal). Submitted to JPCD.

All other V.8 projects will either be terminated or the basis of a fast-track or new Project Submission.

WPQA

501/8/97: Protocol for in-house method validation. Second draft in circulation. [Chair: will a fast-track Project submission be used?]

501/10/97: Description of chemical test methods. To be terminated.

Appendix B

Commission reports on progress of projects approved under the new Project Submission scheme.

DCA-4: Solubility phenomena – applications for environmental improvement. Work is progressing. A workshop is planned at the International Symposium on Solubility Phenomena.

DCA-5: Orange Book. See Minute item 12.

DCA-6: Terminology for the description of peak asymmetry. A draft document to be discussed at the GA.

DCA-7: Chemical speciation of environmentally significant heavy metals. Some of the Task Group met in August 2000. Contributions from two group members have been circulated. Other contributions are at an early stage. Work is progressing well but the completion date may not be realistic.

DCA-8: Ionic strength corrections for stability constants. Programming is complete. A trial version has been evaluated by experts and may be down-loaded from www.acadsoft.co.uk

DCA-9: IUPAC Stability Constants database. Structures for all ligands are now included. Searching routines based on ligand structure or structure fragments are now complete and tested. Data collection is up to schedule.

Appendix C

Terms of Reference: Solubility and Equilibrium Data Subcommittee

The Solubility and Equilibrium Data Subcommittee (SEDS) coordinates projects in the area of compilation and critical evaluation of published experimental data on the chemical solubility of well defined substances and other equilibrium systems. The SEDS also coordinates the dissemination of evaluated solubility data through traditional (journal) and electronic (internet-accessible database) means. The SEDS works with the Analytical Chemistry Division and the US National Institute of Standards and Technology (NIST, the Solubility Data Series publisher) in the selection of chemical systems for treatment. It encourages the formation of Task Groups to perform compilation and evaluation, and it assists Task Groups in carrying out their projects.