

Minutes of the

## Physical Chemistry Division Committee Meeting

Wageningen, April 1 - 2, 2000

Present: David Buckingham, Christopher Brett, John Dymond (secretary I.2), Jeremy Frey, Peter Klæboe (secretary I.5), Luuk Koopal, Gerd Olofsson (secretary), John Ralston (vice president), Michel Rossi, Gus Somsen, Herbert Strauss, George Wilson (president), Kurt Wüthrich

### Agenda

1. Review of Progress on On-going Projects (Commission Chairmen)
2. Procedure and Criteria for Project Review (Somsen/Wilson)
3. The Secretariat/General Secretary View of IUPAC Operations (Wilson)
4. Status of Commission I.1 (Green Book) (Strauss/Frey)
5. Future Management of Data Bases (Dymond/Rossi)
6. New Projects/Initiatives (Buckingham–theoretical chemistry/Wüthrich–biophysical chemistry)
7. The Structure of the PCDC after 2001 (Wilson/Ralston)
8. Year 2001 PCDC Elections (Ralston)
9. Interdivisional Activities (Brett–Environment/Koopal–Materials)
10. Young Observers (Wilson)
11. GA Brisbane: Regular meeting format?

Wilson opened the meeting and welcomed Buckingham as member of the Division Committee. The Agenda was approved with the change of item 2 to include “Review of projects submitted under the new system”.

*1. Review of Progress on On-going Projects.* The “Current Project Summary” listing the projects that are presently worked on or undergoing the review process was distributed. It contains the 40 projects of the Physical Chemistry Division listed in the IUPAC Handbook 2000–2001 plus 6 new projects that are under review. Wilson asked the Chairmen or Secretaries of the Commissions to check that correct names were given for the coordinator and to complete the questionnaire to describe the status and funding for each project and hand in the material before the end of the meeting. Projects extending beyond the year 2001 should be resubmitted and will be handled in the same way as new projects. The discussion of projects was postponed till Sunday morning, April 2.

*2. Procedure and Criteria for Project Review.* The Physical Chemistry Division Committee, PCDC, will be responsible for projects in the future. Projects are listed on the IUPAC web site. Information about project proposal and evaluation can be found on the IUPAC web site.

The discussion of procedure and criteria for project review dealt with the following items:

- 2.1 Submission of proposal to the Secretariat
- 2.2 PCDC Internal Evaluation (re-review if necessary)
- 2.3 External Review of Proposal  
(2.1 - 2.3, *cf.* Project Review Procedure pp. 203 - 205 in Handbook):
- 2.4 Approval of Proposal by PCDC/Funding
  - a. Division funding – less than \$ 5-6K
  - b. Funding from Secretary General
  - c. Funding from Project Committee
- 2.5 Project Committee – Interdivisional
- 2.6 Funding Level Established – Possibilities of external funding?

- 2.7 Review by other Commissions/Divisions
- 2.8 External Review of Manuscript – 15 reviewers including journal editors
- 2.9 ICDNS – if recommendations on nomenclature/symbols/terms are involved
- 2.10 Provisional recommendations – put on web site and publish synopsis in CI – (recommendations only)
- 2.11 Revision and publication of manuscript

Items 2.1 to 2.7 dealing with project proposals were discussed in detail. For items 2.8 to 2.11 dealing with reports and manuscript reference is made to the IUPAC Handbook.

#### 2.1 Proposals should be submitted to the IUPAC Secretariat.

The proposer should be aware that other Divisions may be interested in the project.

2.2 Two members of the PCDC will be asked to review an incoming proposal. Based on the review the Division President will either forward the proposal with the reviewer's report to the Secretariat for further action or send it back to the proposer. Wilson proposed that the PCDC should decide how we want to administer projects and then try to harmonize our approach with the Secretariat and the other divisions. Projects of interest to two Divisions (or more) will be handled by the Project Committee. The role of the President is critical for the successful work of the Division.

PCDC needs to formulate a set of criteria for the review of project proposals. A draft (prepared by Wilson) containing the following items was distributed to the participants and will be used on a provisional basis until adopted in some form in Brisbane:

1. Goals and Objectives –
  - a. Are the goals and objectives consistent with those detailed in the IUPAC Strategic Plan?
  - b. Are the goals and objectives consistent with the priorities of the PCD?
  - c. Why IUPAC?
2. Implementation Plan –
  - a. Administration
  - b. Communication
  - c. Dissemination
3. Personnel –
  - a. Is the expertise of the Chairman and Task Group members well suited to carry out this project? Should additional members or consultants be recruited?
  - b. How will this project be integrated into PCD activities, i. e., is there sufficient expertise concerning IUPAC activities?
4. Impact –
  - a. What impact will this project have on the scientific community? How might impact be assessed a posteriori?
5. Budget –
  - a. Administration
  - b. Travel
  - c. Other Expenses
  - d. Alternative/additional sources of funding?

Item 1.b needs to be worked out as PCD defines its interest areas. 1.c is an important item but not so easy to answer. "Why IUPAC support" should be included in the proposal. The international consensus is important in the evaluation and judgement by an international panel. Dymond commented that a feasibility study should be carried out before a project is approved. Wilson agreed that feasibility studies should be carried out at least for substantial projects, and in the future the PCDC can make such grants from internal resources.

Rossi commented that those judging IUPAC projects should be aware that all work carried out is unpaid work by volunteers and, therefore, it is difficult to state in advance a realistic estimate of the time required.

Task Groups should have at least three named, committed members. The PCDC will come back to the question of the size of Task Group.

2.3 PCDC identifies external reviewers and the Secretariat sends out the proposal (together with a copy of Advice for Project Reviewers). Koopal suggested that the letter to the external reviewers is very important and should be signed by the Division President. Such a procedure would have to be worked out with the Secretariat, since they are responsible for soliciting the external reviews. Further, things should be made as easy as possible for the reviewers, considering that one is asking for a favour. It is important that the proposal reaches the reviewer in a convenient way, regular mail may be preferable to electronic mail. Rossi stressed the importance of external reviewers. Wilson mentioned the problem that many external scientists are ignorant about IUPAC and therefore every effort must be made to clearly explain the review criteria to them.

2.4 The three degrees of funding are listed under 2.4 a-c.

- a. The PCDC can allocate up to maximum \$ 5 000 to 6 000 to projects from the Division money.
  - b. The extra funding to the Benzene project (International Thermodynamics Tables of the Fluid State, Vol. 14) (DPC-3) is an example of funding from the Secretary General.
  - c. The Project Committee deals with large projects and interdivisional projects.
- Decision must be taken about source of funding for each project.

2.5 For Terms of Reference for the Project Committee, and procedures for project submission, see page 276 in Handbook.

2.6 Basic funding from IUPAC should and could be used in applications for external funding.

3. *The Secretariat/General Secretary View of IUPAC Operations.* The suggestion to the Secretary General of October 12, 1999, that a half-time *Scientific Liaison Officer* should be assigned to the Physical Chemistry Division had not met with any enthusiasm. The Secretariat is not yet persuaded that such administrative help is needed. However, the President and Vice President will continue their efforts to acquire administrative support for the PCDC from 2001 when the project-oriented organization will take full effect.

*Budget allocations 2000–01.* The allocation to the Physical Chemistry Division is USD 52 700. The allocation to the Inorganic Division is \$ 39 200, Organic 40 900, Macromolecular 35 700, Analytical 44 400, Chemistry and the Environment 55 200, Chemistry and Human Health 49 599 and Biotechnology 7 500.

The operating reserve for 2001 - 01 is USD 275 000 for the Secretary General and the same amount for the Project Committee. This money will be made available on a competitive basis for additional project funding.

4. *Status of Commission I.1 (Green Book).* PCDC decided to start the procedure to create a new Commission to fill the function of Commission I.1 on Physicochemical Symbols, Terminology, and Units in the new system. Its name should be “Commission on Quantities, Units, and Symbols in Physical Chemistry”. The tentative number of members is three. In addition there can be National Representatives. The procedure to be followed can be found in the IUPAC Handbook (By-Laws Section B4.301 and B4.302) and requires eventual approval by the Bureau and the Council.

The Commission Chairman should probably be a member of PCDC. Frey will prepare a draft of the new Terms of Reference and suggest duties the Commission should fulfill and new projects for a two-year period.

Strauss reported that the typing of the manuscript for the new edition of the Green Book is close to completion. The reviewing procedure should be the same as for the earlier version, that is the manuscript will be read by one or two persons within IUPAC. The manuscript will also be sent to all members of Commission I.1.

Negotiations are underway with University of Oxford Press (New York) and Wiley (New York) about publication. The situation about contract is uncertain. It is also uncertain when and how the Green Book can be made electronically available. The question of getting the material on the web site and who should be responsible for the upkeep, taking care of comments and making corrections need to be decided.

#### *Review of proposed projects.*

DPC-1. Electrochemistry and interfacial chemistry in environmental clean-up and green chemical processes (I.3; Brett, Rusling, Ardizzone).

The Project has received ICSU funding of \$ 4 000 but the remaining request of \$ 17 000 is too large for the Division budget. PCDC advised a rewriting of the proposal to cover 1 workshop and thereby reduce the remaining request to \$ 8 000, or a total of \$ 12 000 for the project. (*Update note:* This project has now been funded at the level of \$ 12 000 as of May 2000.)

DPC-2. Recommendation for the use of AFM in the direct measurements of colloidal forces (I.6; Ralston).

The proposal was approved and will be sent to the Secretariat for external review.

DPC-3. (already funded)

DPC-4. Size effects on electrochemical reactivity. (I.3; Ahlberg, Feliu)

PCDC found the proposal not properly focused, it aims at too much. It needs to be rewritten, and the budget reduced.

DPC-5. Kinetic models/data for chemical processes under extreme conditions. (I.4; Breet).

PCDC recommends rewriting to make the proposal more focused. The budget needs to be substantially cut.

DPC-6. Evaluated kinetic data for atmospheric chemistry. (I.4; Cox).

The project is actually the transfer of the printed tables in J. Phys. Chem. Ref. Data to the web site. This transfer needs hired help. After correction of the budget the proposal should be sent for review and then further to the Project Committee.

DPC-7. Standardization of methods for the characterization of inorganic membranes. (I.6; Ma).

PCDC recommends it for external reviewing. The budget should be rewritten mentioning that the first workshop to be held in summer 2000 is supported from the budget of Commission I.6.

Corish, President of Inorganic Division, should be approached.

Deadline for rewritten proposals was set to May 1.

The comments of the external reviewers will be sent to the appropriate Commission Chairmen before further action is taken.

The participants in the meeting stressed that projects in the area of physical chemistry should be dealt with by PCDC and not by other Divisions without involving PCDC. This raises the question how to ensure exchange of information between the various Divisions in the future.

*5. Future Management of Data Bases.* IUPAC and data bases. There are big unresolved questions about ownership, maintenance, cost etc. concerning IUPAC and data bases. PCDC is

of the opinion that ownership should mean the obligation to maintain the database. Dymond mentioned the Cp data base in Prague as an example of a large data base that IUPAC cannot take over. The opinion was that IUPAC needs to be more active in the field of data bases and should put together a group of people to look after the matter. Dymond was asked to prepare a proposal about the Transport Property Data Base to test IUPAC in this matter.

*6. New Projects/Initiatives in theoretical chemistry and biophysical chemistry.* Buckingham commented on the difference between theoretical chemistry and computational chemistry and indicated that when PCD says theoretical chemistry as in Subcommittee on Theoretical Chemistry it usually means computational chemistry. There is the danger that computational chemists talk only to themselves and, likewise, theoretical chemists should not be isolated. IUPAC could play a role in the education of chemists about the various computational models, their strengths and limitations. Computational chemistry also includes molecular mechanics. Evaluation of commercial programmes will face problems with finding people not tied to any special programme. Computational chemistry is of definite interest for the Division in the future. Wüthrich pointed out that biophysical chemistry covers the whole field of physical chemistry and merits its own Division. Ralston asked about the reaction to the change of name of the Division to “*Division of Physical and Biophysical Chemistry*”. Wüthrich found it appropriate. Such a request will be made to the Secretary General. The Protein Data Base is a possible project for IUPAC to get involved in, either alone or in collaboration with IUPAB.

*7 and 8. The Structure of the PCDC after 2001 and Year 2001 PCDC Elections.* After 2001 the PCDC should consist of up to 16 members, of which IUPAC will pay for 10 to attend General Assemblies, and, probably, up to 6 National representatives. 16 plus 4 to 6 is a large group for effective meetings but has the advantage that it can give breadth of expertise. Ralston is in favour of 12 to 14 members but says he can cope with 16. A Nominating Committee consisting of Gus Somsen (chairman), David Buckingham, Mostafa El Sayed, Toyoki Kunitake and David Eisenberg was selected with Winfried van Gunsteren and Makoto Misono as reserves. Wilson will ask the suggested members of the Committee if they are willing to serve. (The Committee needs the approval of the Bureau). The Nominating Committee will present to the PCDC for approval in advance of the nominations and elections a plan indicating the number of positions to be filled and the suggested number of candidates.

The way of operation of the new PCDC was discussed. Wüthrich commented that it is desirable in the future to have few but well funded projects and Ralston envisaged a PCDC with 10 members dealing with 6 to 10 high-visibility projects.

The creation of an Advisory Committee with say four members was discussed.

The desirability of having new members of the PCDC attending the General Assembly in Brisbane was pointed out. It should be possible to get some funding for this from the Secretary General under the heading “Restructuring cost”.

*9. Interdivisional Activities.* Neither Koopal nor Brett had any progress to report from the interdivisional activities in materials and environment.

*10. Young Observers.* The comments from the Young Observers that had attended the General Assembly in Berlin were positive. Rossi had found it a positive experience to have a Young Observer attend the Commission meetings.

*11. GA Brisbane: Regular meeting format?* The meeting schedule during the General Assembly in Brisbane was discussed. The general (or Open) meeting of the Division will be more extended and more important than earlier. The following tentative schedule was decided: day 1: 16. 00 to

about 18: meeting of the whole Division in lecture hall (or equiv.) for election of the new PCDC followed by buffet and drinks; day 2, 9.00 to 11.00: results of election, future work, discussion. (Comment July 2000: For various reasons we will follow the scheme of earlier GA:s so there will be only one meeting in the evening of Day 2)

Koopal commented that the IUPAC fellows constitute an important reservoir of experienced people who will be needed in the future. Wilson promised to locate a list of fellows.

The President thanked Koopal on behalf of all the participants for the excellent arrangements for the meeting and closed the meeting.