

International Union of Pure and Applied Chemistry
41st General Assembly, Brisbane 2001
Physical and Biophysical Chemistry Division Committee, PBCDC.
Minutes of Meetings 29 June and 3 July

Present: Peter Atkins, Georg Atkinson (elected member DC), John Bertie, Christopher Brett, David Buckingham, Tomislav Cvitas (past president), R. Fernández-Prini (elected member DC), Jeremy Frey, Steven Girshick, Robert Goldberg (I.7), Luuk Koopal, Gerd Olofsson (secretary), John Ralston (vice president), Michel Rossi, Gus Somsen, Herbert Strauss, Ron Weir, George Wilson (president). Observers: Brian Grady, Luke Hanley, Timothy Wallington, Tamae Wong.

AGENDA (Provisional)

Friday, June 29

- 9:00 – Introductions/Announcements (Wilson)
- a. Administrative developments (DC Electorate, etc.)
 - b. Division financial situation
 - c. Appointment of AMs and NRs
- 9:30 – Approval of Agenda
- Approval of Minutes of Wageningen Meeting April 1-2, 2000
(www.iupac.org/divisions/I/I_00min.pdf)
- 9:40 - Biennium Division Report/Review of Progress on On-going Projects (Appendix I)
(www.iupac.org/news/archives/2001/41st_council/Item_10_Div_I.pdf)
(www.iupac.org/news/archives/2001/41st_council/Item_10_Div_I_Append.pdf)
- Review of Projects Submitted through the Review System (Wilson) (Appendix II)
- 10:00 – How well did the project initiation and review system work? (Wilson)
- a. Steps in project initiation and review (Appendix III)
 - b. Review of proposed criteria for project review (Appendix IV)
- 11:00 – The Project System from the View of the Secretariat (Meyers)
- 11:30 - Progress Reports (15 min. ea)
- a. Free Radicals (Bérczes)
 - b. Plasma Chemistry (Girshick)
 - c. Data Evaluation for Atmospheric Chemistry (Rossi)
 - d. AFM for Measurement of Colloidal Forces (Ralston/Koopal)
 - e. Other projects?
- 13:00 – LUNCH
- 14:00– Proposal for International Committee on Thermodynamics (DPC-11)
(Weir)(Appendix V)
- 14:30 – Other Proposals
- a. Reduction potentials of radicals (Brett, Goldberg) (DPC-14)(2001-015-1-)
 - b. Traceability of pH measurement(Brett)(DPC-13)(2001-012-1-)
- 15:00– Special Topics Issues of PAC (Bull)

15:15 – What should the Physical and Biophysical Chemistry Division be doing in the future? (Wilson/Ralston)

18:00 – Adjourn

Tuesday, July 3

14:00 – Appointment of Associate Members/National Representatives (Wilson)

14:15 – Date/Place of Division Committee Off-Year Meeting (Ralston)

14:30 - Division Rules (Ralston)

15:30 – Responsibilities of Division Committee (Ralston)

16:00 – Interdivisional Activities

a. Interdivisional Committee on Coordination of Environmental Projects (Brett)

b. Ad-hoc Committee on Materials (Koopal)

c. Interdivisional Committee on Coordination of Environmental Projects on Biomolecular Chemistry (Goldberg)

d. IDCNS (Cvitas)

e. Committee on Teaching of Chemistry (Atkins)

17:00 – Action on Projects

18:00 - Adjourn

Friday, 29 June

Wilson opened the meeting and welcomed those present. He started by presenting the results of the election of titular members of the Division Committee that had been carried out by email earlier in the spring. The following were re-elected for a two-year term: Christopher Brett, Luuk Koopal and Ron Weir. The following were elected for a four-year term: George Atkinson, Ruth Lynden-Bell, Roberto Fernández-Prini and Joachim Maier. The newly elected members were invited to participate in the General Assembly in Brisbane and Atkinson and Fernández -Prini were present. Wilson reviewed the Interdivisional Meetings that were going to take place during the G. A. It was agreed that Atkinson and Goldberg would attend the meeting on Biomolecular Chemistry, Brett and Rossi the meeting on Coordination of Environmental Projects and Buckingham the meeting of the Ad hoc Committee on Materials.

Wilson reviewed the various actions to be taken by the Council. There will be a new Division on Systematic Nomenclature and Structure Representation. The Commission on Physicochemical Symbols, Terminology and Units will be recreated in the PBCD but should in the future cover the whole IUPAC. The present IDCNS will be renamed to Interdivisional Committee on Terminology, Nomenclature and Symbols, ICTNS.

The procedure for election of Division Committee members will be decided. {*Comment by secretary*: from IUPAC web site: “The council approved the following change in Bylaw 4.103: The Titular Members of each Division Committee shall be chosen by an electorate comprising the Titular Members, Associate Members and National Representatives on the Division Committee, together with the members or officers of such bodies within the Division that the Bureau may specify. The number of Titular Members shall not exceed ten unless otherwise determined by the Bureau. (Continue unchanged to end of current text.) New paragraph following current text: Additionally, a Division Committee may elect no more than six National Representatives on the nomination of Adhering Organizations, with no more than one representative from a given

Adhering Organization. The term of a National Representative shall be two years, with the possibility of renomination and reelection consecutively for only two more years. Exceptional circumstances must be established and special permission obtained from the Bureau for the election of a National Representative from a country already represented on the Committee by a Titular or Associate Member.” }

The next General Assembly will take place in Ottawa, Canada, 8 - 17 August 2003.

1. The provisional agenda was approved.
2. Minutes of Wageningen meeting. Change of item 6, end of first section: Wühtrich found it appropriate *and consensus was reached to accept the addition*. With this addition the Minutes were approved.
3. Wilson asked the Commission Chairmen to go through Appendix I listing publications and meetings organized by the PBCD during 2000-2001 and give corrections to him on Tuesday. Comment to Appendix II containing summary of projects reviewed or under review: project DPC-7 will be funded (\$ 5000) by the Project Committee as an interdivisional project. A discussion followed of how to disseminate results of work that has been carried out. Publication in Pure and Applied Chemistry does not give wide enough distribution. Bertie was congratulated for the good job he had done in spreading the documents resulting from work in his Commission. *Fabienne Meyers, IUPAC Secretariat*, joined the meeting for a discussion about the support that can be expected from the Secretariat in, for instance, maintaining the web site and the project review process. Meyers commented that a lot of work is needed to keep the web site updated. The Secretariat cannot operate a database but can offer a server and can help to set up a database but doesn't have any scientific expertise. Strauss asked if the Green Book could be put on the website. Meyers thought it would not be feasible straight away as it was doubtful how useful it would be. A discussion followed about how interactive a web version should be made etc. Koopal considered that the Green Book in the form of a pdf file would be useful to students, as many of them will not have the printed version. Meyers wondered what would remain on the web site after the New Year. Ralston asked about how to create a database of possible reviewers. The general opinion was that an attempt should be made to create a list of persons that could be asked to review project proposals. Atkins suggested that Chemical Societies in various countries could be approached. Buckingham commented that good people usually are becoming less willing to review.

Progress Reports

- a. Free radicals (Selected Free Radicals and Critical Intermediates: Thermodynamic Properties from Theory and Experiment). The chairman, Tibor Berczes, presented the project that will be a joint effort by six experimentalists and seven theoreticians. The project progresses well. Four papers have been published in leading journals and four more are in preparation. The first joint meeting will be held in September 2001 with discussion of data sheets of 12 free radicals. A second meeting will take place in May 2002 when data sheets for the remaining 20 radicals will be discussed. Preparation of the final version of the data sheets will be made at a third meeting to be held in November 2002. The selected values will be used when modelling atmospheric chemistry and combustion. It is the largest project currently carried out within the Division
- b. Plasma Chemistry. Girshick, chairman of the Subcommittee on Plasma Chemistry, considered the Subcommittee to have had an oversight role for the plasma science community. Now it will be abolished and will be replaced by the “International Plasma Chemistry Society” to be constituted at the ISPC-15 conference in Orleans, France, 9 - 13 July 2001. These biennial international symposia

on plasma chemistry have been organized for 30 years under the auspices of IUPAC. This year's symposium will be preceded by a three day Summer School. There will also be a workshop on Industrial Applications. About 650 participants are expected to attend the symposium. Girshick mentioned a number of topics that could be suitable IUPAC projects and should be considered. However, the question of funding is not so easy to solve.

c. Data Evaluation for Atmospheric Chemistry. Rossi described the project. The main purpose is to make the large amount of data evaluated and selected by the Subcommittee on Gas Kinetic Data Evaluation for Atmospheric Chemistry easily available to the scientific community in the form of an interactive database on the www. Data have been published in monographs and a series of papers in J. Phys. Chem. Ref. Data. These data are of direct interest, for instance, when modelling the climatic change from air pollution. Issues of maintenance and copyright are not yet fully resolved.

d. AFM for measurement of colloidal forces. (Recommendations for the use of AFM in the Direct Measurement of Colloidal Forces). Koopal commented on the excessively long time the reviewing process had taken. Such delays must be prevented. Work on the project will start 1 July 2001 and a first draft is expected to be ready at the end of the year. A revised draft will then be prepared and sent out for review. After two years a document should be ready.

How well did the project initiation and review system work?

Wilson described the various steps in the project review and publication processes presented in Appendix III to the agenda. He stressed the importance of having a speedy and efficient way of handling project proposals.

Somsen suggested that incomplete proposals should be returned directly by the Secretariat. Koopal commented that the Secretariat must fulfill the needs of the Divisions, otherwise secretarial help should be given to the Division Presidents.

It was generally agreed that the initial review by two DC members was not always necessary.

Those present suggested leaving it to the discretion of the President to decide if it should be sent out to two DC members or not. If sent out, it is essential that the members respond quickly.

The present recommended length of about 250 words for the project description was considered too short and should be increased to 500 words.

In order to achieve a speedy handling of the review process the Secretariat should be briefed by experienced persons. In order to get response from reviewers the Secretariat should follow the procedure of journals by, for instance, sending out reminders by email. It is essential that things are kept going.

Bertie suggested that reviewers should only be asked the question "what is the scientific impact of the project?"

Ralston proposed that three reviewers should be approached with one of them maybe from industry.

Wallington raised the question about deadlines for submission of proposals. Those present agreed that it would be of advantage to have a deadline but this cannot be decided by the PBCD alone. The question of deadlines is to be discussed by the Division Presidents or by the Bureau.

The meaning of the word "endorse" was unclear to many but Somsen confirmed that it meant "support by money".

Concerning rules for publication: it can be noted that the Division President is responsible for the technical content of a Technical Report.

Wilson promised to raise the question at higher levels in IUPAC of the long procedure for publication of Recommendations.

James Bull, editor of the Special Issues of Pure & Appl. Chem., visited the PBCDC meeting and described the work with the Special Issues. So far two issues containing refereed articles have been published. Not so easy to find willing authors.

Proposal for International Committee on Chemical Thermodynamics (PDC-11, Appendix V to the Agenda)

The PBCDC approved the allocation of \$ 5000 to the newly established International Committee on Chemical Thermodynamics, ICCT, to support the infrastructure during the coming two years until industrial funding is secured. These funds will be taken from the Division 2002-3 Biennium Budget. It should be understood that no further financial support will be given. The ICCT will apply to become an Associated Organization of IUPAC. The main purpose of ICCT will be to initiate projects in the area of chemical thermodynamics and to function as advisory board for the biennial IUPAC Conference on Thermodynamics. (Comment: The expenditure has not been approved by the Secretary General).

Other proposals.

a. *Reduction potentials of radicals (DPC-14)* Brett and Goldberg had looked at the proposal. They considered it a good project as did other DC members. It is a big project which maybe is not so well focused. Wilson promised to forward the proposal to the Project Committee if Division II is willing to support it as seems likely.

The PBCDC approved support for two years with \$ 8 300 per year. Progress report will be evaluated before funding for the third year will be decided.

b. *Traceability of pH measurement (DPC-13)* The proposal was considered not to be well written and needs to be better focused. The recommendation was to send it back to the proposers.

What should the Physical and Biophysical Chemistry Division be doing in the future?

The remaining part of the afternoon was used to discuss this topic. Wilson introduced the discussion by showing the IUPAC Statement and Long-range Goals. Buckingham noted that nothing was said about what to do to increase the interest of young people in chemistry and in our case physical chemistry. Various suggestions were made but Atkins strongly urged that the Division should stay in the area of its competence, that is science. However, IUPAC can encourage publishers, TV, radio etc and PBCDC should in that case work via mass media.

Rossi commented that by tradition IUPAC has kept a low profile in "hot topics". Should IUPAC change its behaviour? It should be borne in mind that people are not going to seek out IUPAC expertise but we need to make ourselves better known.

Tuesday, 3 July

Wilson thanked the following members who are leaving the DC at the end of the year for their service to the Division and IUPAC and for the work they have carried out: Peter Atkins (hoping for

continued interaction), John Bertie (Commission I.5), Tomislav Cvitas (Green Book), Gerd Olofsson (secretary), Gus Somsen (latest contribution being the Nominating Committee) and Herbert Strauss (Green Book). Wilson thanked Steven Girshick for taking time to attend the PBCDC meeting.

The "Green Book"

It is the formal responsibility of the PBCDC to approve the Green Book.

Any comments to the present version of the book should be given as soon as possible and at the latest by 15 August. Frey responsible for collecting comments from the Commission Chairmen.

Project funding.

There are possibilities to receive further funding this year for projects. Project proposals must be submitted before 15 September. Absolutely necessary to fill out the forms completely and correctly. The proposals should be sent to Wilson who will forward them to the Secretariat. Koopal was of the opinion that ongoing projects should have priority so that they could continue to work.

Associate members. (Comment: according to bylaw 4.103: A Division committee may elect Associate members, who shall have full voting rights. The number of Associate Members should not exceed six. The term of service shall be two years, with the possibility of reelection consecutively for two more years only.)

The PBCDC is of the opinion that if the Secretariat wishes to categorize the members they can do so, but the PBCDC will treat all members in the same way. The Associate Members are expected to participate in the work of the Division in the same way as the Titular Members. It was generally agreed that it was important when electing the Associate Members to consider both their scientific expertise as well as geographic distribution and gender. Names of possible candidates were mentioned. Wilson undertook to handle the election. Wilson also agreed to handle the matter of National Representatives.

Next PBCDC meeting. The next meeting of the Division Committee will take place 19 - 21 April 2002 in Lausanne, Switzerland. Rossi will make arrangements for the meeting.

Reports from Interdivisional Meetings.

Brett from the meeting on *Coordination of Environmental Projects*.

Topics discussed: a) green and sustainable chemistry, b) environmental implications of endocrine active substances, and c) solubility of gases in water.

Brett commented that the project on Environmental implications of endocrine active substances is very big and can have economical and political consequences. The political fallout may be important. Somsen said that the Bureau was unaware of this.

Fernández-Prini and Rossi will receive a copy of the report on gas solubilities in water.

The Divisions I (physical chemistry), III (organic and biomolecular chemistry) and VI (chemistry and the environment) will form an Interdivisional Subcommittee with P. Tundo (Div. III, chairman) and J. Miyamoto (Div. VI, vice-chairman).

Interdivisional Committees do not operate under a Division but outside and are responsible directly to the Secretariat. They deal with specific topics initiated by a group of interested persons. So far such Committees have not been particularly successful.

Buckingham from the meeting of the *Ad hoc Committee on Materials*, John Corish (Div.II, chairman). Report indicated low activity. New materials is a strong area and IUPAC could be expected to be active in the field. The activities would be interdivisional and 19 possible areas were suggested.

Koopal mentioned that a whole new area opens up with nano materials. Frey commented that material scientists do not consider themselves chemists and they have their own societies and journals. This should be of concern for IUPAC.

Goldberg from the *Interdivisional Meeting on Biomolecular Chemistry* (U. Pandit, Div III chairman). Status of interdivisional projects: a) Organization of a one-day symposium during the 37Th IUPAC Congress in Berlin, 1999. b) An interdivisional project (Div III, VII and COCI) on the Molecular Basis of Biodiversity, Conservation and Sustained Innovative Utilization” is almost completed, the final text will be discussed during the G.A. in Brisbane. The Committee invites proposals for new projects. As a summary it can be said that the idea behind this interdivisional committee appears not to have taken hold.

Operation of PBCDC in the future.

The last part of the PBCDC meeting was spent discussing how to find ways for an efficient operation in the future. Its new role is to cover the work of the seven Commissions that are abolished. What is the responsibility of the individual members of PBCDC?

Ralston suggested the following distribution of areas of responsibility among members of the PBCDC during 2002–2003:

John Ralston	Surface and colloid chemistry
David Buckingham	Theory
Michel Rossi	Environmental chemistry/Kinetics
George Wilson	Electrochemistry/Biophysical chemistry
Jeremy Frey	Spectroscopy
George Atkinson	Laser spectroscopy/Photochemistry
Ruth Linden-Bell	Theory&Experiment (Condensed Phase Matter)
Chris Brett	Electrochemistry /Environmental chemistry/ chemistry
Analytical	
Luuk Koopal	Colloid and surface chemistry and (aqueous) Environmental chemistry
Joachim Maier	Solid state chemistry
Roberto Fernández- Prini	Solution chemistry
Ron Weir	Materials

Each person needs to establish networks surrounding themselves with an advisory group of between 3 to 12 members of varying background (industry - academia). It will be the responsibility of the Committee members to establish these groups till the meeting in Lausanne and further to Ottawa. This new function of the DC means a lot of responsibility for the members. It is essential for each member to create a personal network that can act as informal or formal advisory groups including persons with competence outside that of the DC member. This work must start without delay. By the end of October the networking activities should have been considered and the creation of constructive groups planned. By the time for the meeting in Lausanne (April 2002)

communication should have been established so results can be reported at the meeting. Project ideas resulting from network interaction are anticipated.

Atkinson suggested that information about the various reference groups could be collected and put up in a Division News Letter. "Compilation of knowledge" could be made once or twice a year. Koopal commented that we will need to reach out to enlist people, as they will not seek us. Rossi suggested that National Chemical Societies could be approached. Atkins said that the Royal Society of Chemistry has an IUPAC liaison committee that meets twice a year. There are at the present 93 persons in the Division. By keeping them informed about what is happening in the Division they may be stimulated to become involved. A Division News Letter could fill this purpose. It was generally felt that such a News Letter would be useful and be of help in the future operation of the PBCDC.

It was decided to make an attempt to create at the Secretariat a database of physical chemists and their expertise that could be used when there is need to involve persons from the outside to review proposals, participate in Task Groups etc. The advisory groups of the DC members should be included. For this a list a Key Words is needed. A first rough draft had been prepared based on the list of key word used by the Journal of Physical Chemistry kindly provided by Mostafa El-Sayed. The original list is much too detailed and a simpler list must be prepared. Wilson asked the DC members to go through the draft list and provide additions and comments.

Brett asked what is the message to be if we make presentations at conferences and symposia? Ralston promised to see to it that a few transparencies about the Division were prepared.

RE Project proposals: there will be no deadline for submission. Submitted projects proposals will be considered February 1 and September 1 by the PBCDC. It should then be possible to reach decisions in April and October, respectively.

20 Nov 2001 G. O.