

International Union of Pure and Applied Chemistry
40th General Assembly, Berlin, 1999
Physical Chemistry Division Committee

Minutes of Meetings 7 to 11 August

Present: Peter Atkins (member DC), John Bertie (I.5), Christopher Brett (chairman elect I.3), Tomislav Cvitas (president), Helmut Hauser (I.7), Kozo Kuchitsu (member DC), Luuk Koopal (I.6), Ian Mills (member DC), Gerd Olofsson (secretary), Waldfried Plieth (I.3), Michel Rossi (I.4), Gus Somsen (past president), Herbert Strauss (I.1), Ron Weir (I.2), George Wilson (vice-president)

Apologies for absence received from John Ralston

Draft Agenda

1. Introduction and finalization of the agenda
2. Confirmation of Minutes from Frankfurt
3. Nominations and preparation for elections
4. Vice president's assessment of PCD activities (George Wilson)
5. Status of projects (Commission Chairs)
 - a) what is completed
 - b) what has died
 - c) what needs continuation until 2001
 - d) what needs continuation beyond 2001
 - e) what new projects should be initiated
6. Role and tasks for the future PCDC
 - a) project proposal evaluation
 - b) retro evaluation of projects (?)
 - c) initiation of projects
 - d) allocation of National Representatives
7. Finances
8. IUPAC-PCD web site
9. Education (Peter Atkins)
10. Election results
11. Next meeting
12. Any other business

President Cvitas opened the meeting. The draft agenda was approved.

The minutes of the Frankfurt meeting were approved.

Cvitas told about his trial retro-evaluation of the work of the Physical Chemistry Division which is described in his Report to the Council (August 1999).

Then followed a discussion about the future structure of the Division and the election and recruitment of Division Committee members. The question what should be the duties of the

Division Committee in the future was raised. To invite, review and handle proposals and recruit members? The dissemination of IUPAC material was also discussed.

Nominations and elections.

The Physical Chemistry Division Nominating Committee (Wilson, chair, Atkins, Strauss and M. A. El-Sayed) proposed the election of the following persons as titular members for the period 1999 - 2001:

George Wilson	reelection
Tomislav Cvitas	reelection
Gerd Olofsson	reelection
John Ralston	reelection
Herbert Strauss	reelection

New titular members (= Commission Chairmen)

John Bertie
Christopher Brett
Jeremy Frey
Luuk Koopal
Michael Rossi
Ron Weir
Kurt Wüthrich

No additional nominations had been received.

On Tuesday, 10 August, the Commission Chairmen reported that the members of the Physical Chemistry Division unanimously had accepted the proposal of the nominating committee.

Vice president's assessment of PCD activities (George Wilson).

Instead of reviewing the activities of the PCD, Wilson preferred to comment upon the Long-Range Goals of IUPAC as they have been formulated by the SDIC and how the work of PCD in the future can be related to these goals. Wilson asked the Committee members to discuss focusing areas such as materials and biophysical chemistry. Koopal wondered how to develop a reporting strategy that will include a description how the strategic goals have been fulfilled.

Wilson reported that the *Working party on pH* would complete its work within one month. The project has been successful and shows that IUPAC can react fast when needed.

The question was asked what is the attitude of IUPAC towards translations. IUPAC's policy concerning Reports is expressed in the following way in Pure and Applied Chemistry: "Publication of a translation into another language is subject to the additional condition of prior approval from the relevant IUPAC National Adhering Organization. (The basic condition is that an acknowledgement with full reference to the source along with the use of the copyright symbol, the name of IUPAC and the year of publication are prominently visible.)"

James R. Bull, editor of the Special Topics Issues of Pure and Applied Chemistry visited the PCDC meeting after lunch on August 7. He told about the aim of the Special Topic Issues which is to increase the readability of and interest in Pure and Applied Chemistry, PAC. The issues, up

to 200 pages, can be written by invited authors or can be Workshop publications. The publication time is 9 months and the issues are incorporated into the general publication schedule.

John Ward, treasurer of IUPAC visited the PCDC meeting on 7 August and the finances for the Division was discussed. As reserves are available, Ward suggested that the Division could apply for money to cover costs during the present biennium for extra meetings and unforeseen additional cost to finalize project at the IUPAC Thermodynamic Tables Project Centre. The financial situation for IUPAC is good and for the coming biennium the money available will increase somewhat. Money for projects will be allocated in the future directly to the Division Committee and from a pool administered by the Project Committee.

Status of projects

Commission I.1 has one project: preparation of the third edition of the Green Book. Strauss mentioned that the work on the third edition of the Green Book is expected to be completed during autumn 1999. It will be put on the website as soon as the publisher will permit. New projects will be a) updating of the Green Book; b) a simplified version of the Green Book. Bertie expressed a concern about the proposed renaming of the Green Book and Somsen wondered if the name really was a matter only for Commission I.1. Those present agreed that it was a matter for the whole Division. The proposed new title was: "Physical-chemical quantities, units and symbols" and the present title: "Quantities, Units and Symbols in Physical Chemistry". Cvitas suggested that the Division Committee should vote on the matter and a large majority voted for the old title.

Commission I.2. Three projects listed in the IUPAC Handbook have been completed ("Thermodynamics of fast ionic conductors", "Chemical Thermodynamics in the 21st Century" and "Vapour-liquid equilibria and related properties.....") eight more are expected to be completed by 2001. The project on "Critical compilation of activity coefficients ..." has been abandoned and the "Internationally available data bank of recently published transport properties" has ceased. Nine new books and at least eight maybe up to fifteen manuscripts are expected during the coming two years. However, financial support is needed for the work at the IUPAC Thermodynamic Tables Project Centre at Imperial College. The PCDC promised to give additional funding so that volume 14, Benzene, in the series International Thermodynamic Tables of the Fluid State could be completed.

Commission I.3. It is uncertain when the manuscript reporting on the project (jointly with I.7) "Measurements of Redox Potentials of Proteins" can be prepared. The project on "Electrocrystallization: concepts and terminology for theory and experiments" will not be continued. The projects "Electrochemistry for the Environment", "Electrochemistry at the interface between two immiscible electrolyte solutions" and "State of the art of water treatment" will continue to 2001. A new project for organization of workshops "Electrochemistry and interfacial electrochemistry for environmental clean-up and green chemical processes" together with Commission I.6 has been approved by ICSU and will start 2000. Koopal commented that coordination is needed also with bodies outside the Division. A project on "Size effects in electrochemical reactivity" will be proposed. A project on "Micromachining" consisting of a workshop and published proceedings is proposed for the area advanced materials.

Commission I.4: The Commission will continue work on data compilation and evaluation. The project "Evaluated Kinetic Data for Combustion Chemistry" is slated for completion in 2000 (D. Baulch, chairman of subcommittee). The Subcommittee on Gas Kinetic Data Evaluation for Atmospheric Chemistry has published Supplement VI and VII in J. Phys. Chem. Ref. Data and has submitted Supplement VIII to J. Phys. Chem. Ref. Data. All these were dealing with homogeneous (gas phase) reactions and photochemistry. Supplement IX has been submitted and this Supplement deals with heterogeneous chemical reactions of atmospheric interest only. The work of the Subcommittee is a continuing project. The projects on "Aqueous solution kinetics data for atmospheric chemistry" and "Kinetic model data for chemical processes under extreme conditions" will continue to 2001.

Commission I.5. The project on "Practical standards for NMR" is approaching completion but will extend to 2001. The projects on "The computation of experimental structure and..... (150/2/95)", "Spectroscopy under extreme conditions(150/24/95)" and "Quantities, terminology and symbols..... (150/25/98)" will continue to 2001. The project on "Spectroscopic intensities.....150/23/95" is completed but no separate report prepared.

The Subcommittee on Notations and Conventions for Molecular Spectroscopy will prepare 5 documents in all; part 4 will be completed this year while the work on part 5 will extend to 2001. The first part of the project "Guidelines for the presentation of methodological choices in the publication of computational results(155/1/95)" by the Subcommittee on Theoretical Chemistry is completed and published, the second will be ready during 1999 and the third part on molecular mechanics will continue to 2001.

The response of the theoretical chemists to invitations to work with the Subcommittee on Theoretical Chemistry had been disappointing. In order to improve the situation "key persons" in the field should be approached. Mills suggested that a theoretical chemist should become member of the Division Committee. Mills promised to find out if David Buckingham would be interested. If Buckingham would not be interested Mike Rabb or Donald Truhlar were mentioned as possible candidates.

Commission I.6: The project on "Pillared clays and other porous layered structures" will be completed before 2001 and the project on "Nomenclature in zeolites....." will continue to 2001. The project on "Measurement and interpretation of electrokinetic phenomena" is new and will extend beyond 2001. Projects in the form of conferences and published proceedings have been completed on "Interfaces Against Pollution " and "Environmental Protection: Surface, Colloid and Catalytic Aspects". A new project on atomic force microscopy is proposed.

Commission I.7: The projects on "Electrochemical biosensors" and "Recommendations for the measurement and presentation of results on biological substances with scanning calorimetry" are completed. "Terminology in the field of lipid vesicles (liposomes): preparation and essential characterization" is delayed but will be completed soon. It will be published in PAC and in journals publishing papers on liposomes and vesicles. The project "A nomenclature for lipid mesophases" is delayed. The project on "Recommendations for reporting results of computations in biophysical chemistry" should continue but uncertain when it will be completed.

On Tuesday 10 August *Dr Fabienne Meyers* from the IUPAC office visited the PCDC meeting for a discussion about the *Physical Chemistry Division website*. John Bertie has agreed to be the contact person for the website. He will look at the material to see if things need to be changed

/replaced etc and will contact the appropriate person to do the work. Dr. Meyers is responsible for the technical side and will put the material onto the web. Both html and pdf files can be handled but html files are preferred. Dr Meyers commented on the IUPAC site map which can be found in Chemistry International, 1999, 21:4, 112-113.

The possibilities to put the new edition of the "Green Book" on the web was discussed. Koopal wondered how documents available only in printed form could be put on the website. Dr Meyers answered that it is possible to use a scanner to transfer the document. The members of the PCDC expressed the opinion that, if needed, financial resources should be made available to the IUPAC Office to make possible that important reports etc. could be put on the web without undue delay. Dr. Meyers commented that the policy is that material emanating from an IUPAC body (commission, subcommittee, working party etc.) should be on a central computer, that is on the IUPAC website.

Atkins reported from the meeting of the Committee on Teaching of Chemistry, CTC. Among the projects discussed he mentioned a Japanese proposal for a search engine to look for teaching material on the web and the proposed book "The language of chemistry" which would be a shortened version of the "Gold Book".

Elections. Present: Peter Atkins, John Bertie, Chris Brett, Tom Cvitas, Luuk Koopal, Kozo Kuchitsu, Ian Mills, Gerd Olofsson, Waldfried Plieth, Michel Rossi, Gus Somsen, Herbert Strauss, Ron Weir and George Wilson.

Election of officers of the Division Committee: George Wilson was elected president and John Ralston vice-president (13 for, 1 abstention). Tom Cvitas will become past-president and Gerd Olofsson continues as secretary.

Nomination for Associate members of the PCDC: Atkins accepted nomination as associate member of PCDC. He will then continue to be the link to CTC. Cvitas suggested Somsen as associate member. He was supported by Koopal who pointed out how the Division has benefited from having direct information about the reorganization of IUPAC from a member of the Bureau. The new chairman of the Plasma Chemistry Subcommittee, Girschick, will also be an AM. Those present decided that if Buckingham was interested to become involved with IUPAC, Mills should offer him a TM membership in PCDC.

Wilson mentioned that he would like to create a small consultant group with people from the outside for the creation of new project areas and structure of the Division. The consultants would have temporary TM status for the purpose of the PCDC meeting, but would not come to GA in 2001. M. A. El-Sayed has agreed to serve and one or two more will be appointed.

The evaluation and handling of proposed projects was discussed. Rossi pointed out that only good projects should be financed and one should look for matching funds. Somsen commented that criteria for the evaluation of proposals already exist. Rossi argued that it is still not so easy because projects will be of very different categories and difficult to compare. The results of projects need to be well described such as data compilation, recommendations about nomenclature, standardization of methods etc. The size of the "audience" should also be considered. The suggested means of dissemination of the results are important.

Koopal stressed the importance for the PDC to keep in touch with the disciplines (the fields of the former commissions) after the abolishment of the commissions. A representation of the PDC at the important conferences of the different disciplines could be a way to achieve this.

Representation of the Division in other bodies of the Union.

Wilson in the Pure and Applied Chemistry Editorial Advisory Board, PAC-EAB.

Atkins in the Committee on Teaching of Chemistry

Strauss TM and Jeremy Frey AM in the Interdivisional Committee on Nomenclature and Symbols, IDCNS

Brett and Koopal agreed to look after the interest of the Division in interdivisional discussions of projects of environmental relevance and concerning advanced materials, respectively.

Next meeting. The Division Committee will meet early in 2000 to *i.a.* formulate the policy of the Physical Chemistry Division under the new regime and the way the Division Committee will work.