

Minutes of the off-year Meeting of the Division Committee of the Physical and Biophysical Chemistry Division I (PBPCD) of IUPAC

Morges (Switzerland), 19 - 20 April 2002

Present: G. Atkinson (TM), C. Brett (TM), D. Buckingham (TM), S. Califano (AM), R. Fernandez-Prini (TM), J. Frey (TM), R. Lynden-Bell (TM), L. Koopal (TM), J. Ralston (president, TM), M.J. Rossi (secretary, TM), C. Royer (AM), G. Wilson (past president, TM), R. Weir (TM).

The President, John Ralston, opened the session with a welcome to the new Associate Members (AM's) who joined the Division Committee for the first time. Upon presentation of the meeting agenda it was decided to change the order of discussion to suit the needs of those present.

Divisional Newsletter. This idea originated at the last General Assembly in Brisbane and was designed to keep PBPC members at large informed on the activities within the Division in response to the changeover of IUPAC to a project-oriented organization. However, the Secretariat "vetoed" the initiative as they are concerned that potentially relevant information may not reach them or other Divisions within IUPAC. The Secretariat suggested the use of the columns of "Chemistry International" for communicating important items on a regular basis. The idea of a Newsletter responds to a real need for communication between the Division and the membership at large in the absence of an adequate representation of the membership at large now that the new structure is in place.

This item also prompted a brief discussion of IUPAC's long range goals. Two mainstream ideas emerged after having noted the gap between IUPAC's lofty goals documented in its strategic objectives and the "work in the trenches" dealing with specific work serving the Physical and Biophysical Chemistry community at large: (a) improving the visibility of IUPAC within scientific associations and the community of scientists and government organizations, for example, sponsoring specific symposia on IUPAC topics, (b) strengthening the IUPAC scientific peer review and evaluation process. The need for a pragmatic approach was stressed in order to attract younger chemists, in particular, to IUPAC.

Monitoring of Divisional Projects. The remaining funds of the PBPCD, after deduction of the costs of the off-year meeting, are \$38.5k for the remainder of the current biennium (2001-2002). However, all present agreed with the President that it is justified to expend Division funds to permit direct participation of a broad representative base. Thus two new AMs were invited to participate in the Off-Year Meeting (professors C. Royer and S. Califano). The **project evaluation procedure** within Division I was subsequently discussed. A project may now be submitted to IUPAC by any chemist and is addressed to a Division unless it involves several Divisions in which case it will be

subsequently addressed to the IUPAC Projects Committee. After receipt of the proposal the IUPAC Secretariat sends it out for preliminary evaluation by several DC members in order to decide whether or not to pursue it. Depending on the outcome of this preliminary screen, it may then be sent for external evaluation; this represents a new development for IUPAC. Once the project is completed it will be reviewed by three to four or up to fifteen referees, depending whether it is of a technical nature or whether it proposes IUPAC-sponsored recommendations. The nominated project monitor should propose the names of potential reviewers and should contact them (by electronic mail, if possible) on behalf of the Secretariat, who will do the bulk of the clerical work. The project leader may interact for the duration of the project with the appointed project monitor, who acts independently of any IUPAC directives, much like a scientific journal editor. However, the project leader is wholly responsible for the final product of **their** task group. "The IUPAC Project System" document briefly summarizes the procedure and is attached as **Appendix A** to these minutes. The description of a project at submission should be increased from currently 250 to 500 words in order to better be able to judge the proposal content. Dissemination of results at scientific conferences, workshops and the open scientific literature is an important aspect of a project. It is decided to encourage the re-publication in Pure and Applied Chemistry (PAC) of original IUPAC-sponsored work by seeking the permission from the editor of the original publication.

The following on-going projects were briefly reviewed by the project monitors chosen among the Division Committee members:

DPBPC-02 (1999-016-3-100) Recommendation for the use of AFM in the direct measurements of colloidal forces, monitored by L. Koopal (\$5k): Development of protocols and evaluation of methods. Draft of report in circulation.

DPBPC-06 (1999-037-2-100) Evaluation of kinetic data for atmospheric chemistry, monitored by M.J. Rossi. (\$20k + \$10k coming out of the current Division biennium 2002/03 budget, see below). Detailed presentation of progress of the largest project that Division I is sponsoring. This project aims at putting the whole existing kinetic database representing approximately an estimated 70 man-years of effort on the Web in a user-friendly searchable form. A significant fraction of the database has already been transferred to a Website located at the University of Cambridge (UK) and waits to be transferred to a site under the control of the IUPAC Secretariat once all the available data will have been incorporated. There are currently between 1500 and 2000 visits of the Website per week. At the same time an on-going effort of updating the current database is being undertaken while the subcommittee is still in existence. This also necessitates a recurrent financial need of \$5-6K per year for the next few years and is distinctly different of the one-time nature of putting the existing data base on the Web (project number see below).

Ron Weir reported on the successor organization of the defunct IUPAC subcommittee on Chemical Thermodynamics (I.2) whose needs are similar to the ones outlined for the chemical kinetics database (see above). They have constituted the *International Association of Chemical Thermodynamics*

(IACT). This organization of 400 paying members will organize the biennial International Conference on Chemical Thermodynamics (ICCT) meetings (next meeting 27 Jul – 3 Aug 02 in Rostock, F.R. Germany) in order to ensure the continuity of two former standing subcommittees, chemical thermodynamics and transport properties. The IACT was constituted in 2001 as a legal entity in order to interact with IUPAC on a formal basis.

DPBPC-07 (2000-002-2-100) Standardization of methods for the characterization of inorganic membranes, monitored and reported by L. Koopal (\$6k). A first meeting was held in Montpellier, France, in June, 2001. The first draft, about to be written, seems behind schedule. The project will result in a technical report as a joint project with Division II.

DPBPC-08 (2000-013-1-100) Selected free radicals and critical intermediates: Thermodynamic properties from theory and experiment, monitored by R. Weir (\$15k (Project Committee) + \$7k from current Division biennium, see below). Project is on schedule and will result in datasheets on a set of 35 free radicals. A first meeting took place in Stuttgart, Germany in 2001, next meeting will take place in May 2002 in Lille, France.

DPBPC-14 (2001-015-1-100) Reduction Potentials of radicals, monitored by C. Brett and G. Wilson (\$15k). The project will have its first meeting in May 2002 in Switzerland. As there is no electrochemist currently on the Task Group, the DC will provide input. This is a joint project with Division II.

DPBPC-15 (2001-028-1-100) Electrochemical impedance spectroscopy, terminology, nomenclature and data exchange formats, monitored by C. Brett (\$3.8k). The project is a follow-up of a meeting in Italy on the same subject, started in January 2002.

DPBPC-17 (2001-035-1-100) Measurement and interpretation of electrokinetic phenomena, monitored by L. Koopal (\$5k). The second draft of technical report has been reviewed by the Task Group, and a summer 2002 meeting is scheduled.

DPBPC-16 (2001-30-1) Recommendations/Biological Substances/Titration Calorimetry, monitored by G. Wilson (\$10k). Reviewers made many constructive comments on the proposal. Project was approved by the DC and will be forwarded to the Secretariat with a recommendation by the President. Samples to be sent out to different labs for Round Robin experiments.

DPBPC-06 (2001-51-1) Atmospheric Chemistry June 2002 Meeting, monitored by M. J. Rossi (\$5k). This meeting will allow the annual update of part of the chemical kinetics database discussed above. Expenditure of Division funds for this project was approved.

Interdivisional projects:

DPBPC-19 (2000-012-1-300) Single molecule spectroscopy, monitored by D. Buckingham. Project with Division III on a feasibility study. Query the Secretariat or the Secretary of Division III, funding level uncertain (\$3-4k).

DPBPC-18 (2001-036-1-300) Glossary of terms in photocatalysis and radiation catalysis, monitored by L. Koopal (\$5k). There is an urgent need to bring the two coordinators of this project (V. Parmon,

Div. I and N. Seirpone, Div. III) together to decide on the overall objective of this project so that it can either be abandoned or completed in a timely way.

New projects:

Chemical Actinometry proposed by S. Braslavsky got excellent reviews. Intended as a joint project between Div I and III although former has not yet been approached in a formal way.

Data exchange standard for NIR spectroscopy proposed by G. Downey, proposal has been sent to Division I for comments. Proposal originated from Div. V (Analytical Chemistry) and obtained excellent reviews.

Prof. Corish intends to set up a proper **Materials Chemistry Division** within IUPAC that is an effort originated at the IUPAC General Assembly in Geneva in 1997. J. Maier is proposed as the liaison. This new Division is expected to have strong horizontal components within Divisions I, II (Inorganic Chemistry), III and IV. J. Ralston recommends closely watching the developments and documenting our interests as Division I is certainly a strong component of any materials science initiative. Together with J. Maier R. Weir will act as liaison and/or project monitors for a proposal that we will be happy to support.

Various projects near completion and/or in press have been discussed. The new edition of the "Green Book" (Subcommittee on Nomenclature, I.1) is close to ready but is presently being held back by M. Quack who has put the majority of resources into the production of the new edition. Six to 12 months after the appearance of the printed edition parts or all of the Green Book will be put on the Web for various segments of the market (undergraduates and/or graduate students). People are standing by to translate it into foreign languages.

For up-to-date information one should consult the regular update on IUPAC-wide project submissions and project status on the Web set up and administered by F. Meyers of the IUPAC Secretariat.

New Projects and Initiatives. The President reminded those present that everybody leaves this meeting with an assigned task as a project monitor and/or intent on bringing in new projects.

- In order to obtain a higher degree of dissemination of IUPAC standards and more publicity for IUPAC's *green book* one should distribute it to editors of scientific magazines and journals.

- It is to understand that QUILL (Queen University [Belfast] Ionic Liquid Laboratory) plans to set up a database on ionic liquids. Division I members to inquire whether this *planned data base* could be constructed under IUPAC sponsorship and collaboration. Industry participation in this effort may be envisaged.

- Bring order into the field of Biophysical Chemistry. The emerging needs in the life sciences should be considered from the point of the value of physical chemistry to the newly emerging field. Everywhere in life sciences chemists are doing most of the work at the interface between Biophysics and Biology but are not identified as such. There seems to be no immediate need for a protein data base as it is already in the process of being set up. Other examples may be fluorescence spectroscopy for *in vivo* cell applications, protein stability data bases, CD spectra of biological systems, other

spectroscopies, fluorescence spectroscopy. There is a lesser need for NMR- and X-Ray crystallography data bases as they are already well supported.

- Bring research advances to industry rapidly. *Industry* should be regularly consulted as to their *needs*, all the more that the chemical industry financially supports IUPAC activities. IUPAC should assume stewardship but needs proper focus and/or specific examples of successful intervention by IUPAC for others to follow. One of the roles of IUPAC could be to point out new developments of technological significance to industry as an “early warning” sign of technological change: horizon technologies.

- Standards/Databases and IUPAC Authority/International Links. Any *data base* of significant extent should have the *backing of IUPAC* or other international organization of authority to be of use, much like a stamp of approval, especially for things that IUPAC does well (free unbiased consulting). The example of the Water and Steam Properties data base is given which is the guiding light for steam turbine manufacturers. The ISO Standards was given as another example: IUPAC could play a leading role to feed certified information into ISO. Another area is the role IUPAC can take up projects in or for Third world countries by making them benefit these countries in terms of helping them to be productive in contrast to typical UNESCO projects. The specific example of a low-cost instrumentation initiative and/or an educational project were cited which may be located within Div I. The first step may be a low-cost instrumentation show and demonstration. Such efforts may also alleviate the intellectual isolation of many research groups in third world countries as the motivation for undertaking certain research projects are often not clear. This leads to increasing isolation of the research groups in the developing world. IUPAC currently does not have a charter with specific third world implications. Active links with those countries seem highly desirable in order to identify problems and commit resources. Perhaps graduate students from those countries should be approached.

- Endorsements and recommendations may be a source of income for the organization, especially when bolstered by credibility and past track records.

This discussion ended with all agreeing to a roadmap for Division I from which a catalog with the following seven items emerged:

- 1) Commitment to data base maintenance and management. In addition to maintaining the existing thermodynamics (100 man-years of work) and kinetics (70 man-years) data base there is now a growing demand for further databases, for example one in ionic liquid properties. Database maintenance is seen to be a crucial part of Division I action. The Division President will take swift action and will get in touch with the President of IUPAC, professor Pieter Steyn, in order to get a rapid and sensible policy decision mandated from the top of the organization.
- 2) Standards/Databases/IUPAC Authority. IUPAC as an organization need to connect to the national societies of chemistry. Practically speaking the members of Division I are there as

facilitators of this contact as many are well-connected and willing to help. Before this action can begin one needs a policy decision outlined under 1).

- 3) Expansion of activities into Biophysical Chemistry. In view of its importance to chemistry and to chemists already working in this field a roadmap of projected activities is needed. The personnel committed to set it up is: C. Royer (Chair), J. Ralston, G. Wilson, G. Atkinson and R. Weir. Ron will also tap ICCT members who are interested in this field. A two page document is expected wherein research areas, directions, potential applications including thermodynamic applications are outlined. This document should be circulated to all TM/AM/NR's. Molecular medicine, bioavailability and therapeutic stem cells are heavily dependent upon advances in physical chemistry and may be potential areas of importance in the near future. The setting up of an advisory group in Biophysical chemistry was discussed.
- 4) Confront industry rapidly to emerging advances in science and technology that are potentially important to them. This is a two way street and necessitates listening to industry needs. Stress scientific credibility of IUPAC members ready to take action on behalf of industry. See also 2).
- 5) The role of the Green Book should be a means to promote the goals of Division I. A Web version will be published 6 or 12 months after publication of the hard copy. Different versions (student editions) are planned thereafter depending on the needs of the community. The Green Book should be referenced in the Instruction to Authors Section of scientific journals to ensure broad dissemination. C&E news, Chemistry International and other broadly available publications as well as various national and international education committees are to be reached.
- 6) Roadmap for the future operation and prospects of Division I. Part of the President's report will address this item. Input is expected from advisory committee members (see below) and from NR's in September 2002 at the latest. The discussion of IUPAC Strategic Priorities by the chairman followed the existing official template that did not lead to much discussion.
- 7) Participation of Division I in activities located in or implying the Developing World. The point is to propose and test experiments of modest economic value but of great impact and relevance as a teaching aid. The sequel to the Rio 92 Conference taking place in September in Johannesburg would be an appropriate platform for dissemination of information. The President will contact IUPC President Prof. P. Steyn in regards to putting a paragraph on the agenda of the Johannesburg meeting in relation to the general contribution of IUPAC to the needs of Third World countries.

The role of the Advisory Committee of Division I. The primary tasks of advisory committee members of Division I are:

- Project identification and/or project appraisal
- Nomination or assigning of project coordinators or team members

- Identification/nomination of PBCDC members

Their term of office is two years and is renewable. It is highly desirable to have nominations for the Advisory Committee from industry. The PBCDC will make their names known inside and out of IUPAC. The Advisory Committee members should receive both a letter from the Division as acknowledgement of their participation in the group as well as from the IUPAC Secretariat stating that they are a part of a much larger group of advisors whose mission it is to oversee the quality control of work performed within the Division as well as to solicit a steady stream of high quality proposals. Chairman is going to send a letter asking them if they are willing to let IUPAC publicize their names identifying their role in the PBCDC. Committee members must forward their Advisory Group nominees to the President by June 30, if they have not already done so.

Budget for the remainder of the biennium. There are \$38.5k left for this biennium out of a total allocation of \$65.3k for Division I. It has the following commitments for the remainder of the current biennium:

\$10k DPBC-06 (*1999-037-2-100*, Evaluation of kinetic data for atmospheric chemistry, Cox)

\$7k DPBC-08 (*2000-013-1-100*, Properties of selected free radicals, Berces).

\$5k DPBC-18 (*2001-51-1*, Atmospheric chemistry meeting June 2002, Cox). The Division Committee has agreed to this project as it enables the continuation of the updating process of the atmospheric chemistry kinetics database.

The DC also solicits a proposal from the chairman of the Commission I.1 for the completion of the Green Book. It is clarified that the budget to run Commission I.1 will have to come out of the divisional budget.

The transparency of the financial situation for IUPAC as a whole is desirable. The President will ask proper confirmation of project cost in relation to total budget on the basis of these minutes. The average project cost now is between 10 and \$20k. Any proposal amounting to more than 25% of the Division budget is to be submitted either to Projects Committee of IUPAC for cost sharing or to another Division if it is a joint project.

Division Publicity: It is desirable to have available a series of IUPAC slides on “What is IUPAC? Mission of IUPAC? Strategic Goals of IUPAC?” etc. Existing documentation material on IUPAC will be made available by the Division President. Another question put to the Secretariat: what to do with the archival material from the Commissions? Much of the material is still in private hands. Is there an IUPAC-archive or repository of documents?

Election Issues: The electorate for Division I are the 12 titular (regular 10) members of the DC including the President, Vice-President, Past President, Secretary, and Chairman of the Commission on Physicochemical Symbols, Terminology and Symbols, I.1. The 12 TM’s currently making up the DC of Division I enable an even representation of the different fields of physical chemistry.

Elections 2003: The extension of the Division I electorate has not yet been approved by the Bureau and will be proposed at the meeting in September 2002. The presently approved electorate is 12 (TM) + 6(AM) + 6(NR) + chairs of task groups whose projects have been approved (approx. 10 persons). The Nominating Committee nominates new TM's and AM's and should be made up of three external members with two internal members already nominated (Professors Buckingham and Wilson, with Prof. Wilson serving as Chairman). The three external members have yet to be nominated and approved by the Secretariat. Thus at present the electorate consists of 27 + task group chairmen. The electorate for the DC is believed to be too small, a possibility would be to include the members of the Advisory Subcommittee (6-12 advisory panel members proposed by each DC member for a total somewhat in excess of 100). The by-laws of IUPAC relating to elections will be discussed in September 2002 at the Bureau meeting and it is hoped that the proposed electorate will be accepted. A potential problem might be the definition of the Task Group leader: Proposal approved, funded, submitted? It is the intention of the DC to reduce the tally of 12 to 10 TM's in order to get some flexibility within the Division. Professors Atkinson, Lynden-Bell, Fernandez-Prini, Rossi and Maier have already been elected for 4-year terms each. This means that one TM will be elected for the next biennium to bring the total number to 10 TM's. The candidates for President and Vice-President for the next biennium 2004/5 are Chris Brett and Ron Weir with the order to be decided this fall. Elections, conducted by the Secretariat will be held in the fall of 2002 so that the new members of the DC may attend the GA in Ottawa in 2003.