*Off-year Meeting of the Division I of IUPAC (Physical and Biophysical Chemistry)

Glion, Switzerland, April 3 and 4 2004

Present: C. Brett (CB, vice president), M. J. Rossi * (MJR, secretary), W. Baumeister (WB), R. Fernandez-Prini (RFP), R. Lynden-Bell (RLB), Z. Q. Tian (ZT).
Excused: R. Weir (RW, president), G. Atkinson (GA), J. Frey (JF), J. Maier (JM).

1. Introduction.

The Division Committee (DC) was called to order by CB at 9:15 a.m. The vice president (CB) regretted the absence of the president of the Division Committee, Ron Weir (RW), who excused himself a few days prior to the meeting owing to a health problem that prevented him from travelling. The vice president extended a cordial welcome to all, especially to the two new titular members (TM), WB and ZT. Every TM present briefly introduced him/herself for the benefit of the two new TM's who joined the DC for the first time. WB and ZT will represent the broad area of biophysics and materials chemistry, respectively.

2. Approval of Agenda.

RLB proposed to include a discussion of the role of the Div I Advisory Group into the agenda. CB suggested to include this in agenda item no. 6 which met with the approval of the DC. MJR and RLB moved to approve the proposed agenda.

3. Approval of the Minutes of the Ottawa GA.

The draft of the Div I minutes of the Ottawa GA were accepted with minor modifications (typographical errors). MJR will correct the draft copy accordingly and will send a final copy to the Secretariat. On viewing the list of the Advisory Subcommittee of Div I on the IUPAC Website (http://www.iupac.org) the DC suggests to add the names of Professors George Wilson, David Buckingham and Luuk Koopal, an item that had been decided on in Ottawa. Also, the name of Past President John Ralston should be added once his term of National Representative of Australia has ended. MJR will get in touch with the Secretariat on this matter.

4. Finances.

* Version of June 13 2004 sent out by M. J. Rossi, Secretary of Div I.

According to the newest version of the Accounting Sheet sent out by the Secretariat (Project_Expense_20040304.pdf) only one project needs serious follow-up (2000-002-2-100, Yi Hua Ma, Standardization of Methods for the Characterization of Inorganic Membranes) in view of its completion date of 2003 having passed and the fact that apparently no activity has occurred. All others have either been terminated or are in the execution stage. In the case of project 2000-002-2-100 the DC will ask its project monitor, JM, to find out about its status (see also comments by JM made at the GA in Ottawa and to be found in the minutes). The DC decided to wait before removing terminated projects from the accounting sheet whose balance was essentially zero until assurance has been given by the Secretariat that all deliverables have been addressed. Requests for redistribution of positive balances to add-on or similar actions need to wait for approval by the Secretary General. RFP informed the DC that the funds for the new project 2003-036-2-100 (Corti) had been recently released, following a temporary ban resulting from the situation in relation to the project coordinator's NAO.

5. Progress Report on Current Projects

1999-016-3-100 - Recommendation for the use of AFM in the direct measurements of colloidal forces. Project completed by the end of 2003.

1999-037-2-100 - Evaluation of kinetic data for atmospheric chemistry. This project is breaking new ground for IUPAC in that an extensive data base is in the process of being put onto the Web (http://www.iupac-kinetic.ch.cam.ac.uk/). MJR gave a brief progress review over the life of the project from 1999 to 2003. Highlights are: (1) the mirror site located at the IUPAC Secretariat in Research Triangle Park, NC came on-line recently; (2) the interactive data base consisting of a summary sheet of reactions as well as the individual data sheets themselves has been completed to over 50%; (3) the interest in the product remains satisfactory with 2000+ downloads per week and a 300+ e-mail subscription list; (4) parallel updating efforts of parts of the data base in separate IUPAC projects; (5) continuation proposal for the current biennium has been submitted in September 2003. The positive balance of USD 7,563 according to the attached Project Expense file will be used to fund the yearly meeting of the evaluation group for 2004 (meeting planned for June 2004) with the permission of the Secretariat which puts the financial balance essentially to zero. Two new young members have joined the evaluation group (Dr. M. Jenkin (UK), Dr. R. Hynes (Aus)) and are working alongside the established members. MJR stressed the fact that at least for the current biennium both the continuation of the Web project (proposal submitted in September 2003, USD 20k) as well as a separate project for convening the meeting for the updating of the data base (2004 meeting financed out of the positive balance of the current project, 2005 meeting: proposal yet to be submitted) is necessary. Once the data

base has migrated to the Web site updating will be more straightforward from 2006 onwards. An "interim" report written by the project leader, Dr. R. A. Cox, covering details of the initial progress 1999 to 2003 has been circulated at the meeting.

2000-002-2-100 - Standardization of methods for the characterization of inorganic membranes*. See remarks under agenda item 4 (Finances).

2001-015-1-100 - Standard potentials of radicals*. Slated for completion in 2004.

2001-028-1-100 - Electrochemical impedance spectroscopy - terminology, nomenclature and data exchange formats. CB gave a brief overview presentation over this project whose results will both be published in PAC (Pure and Applied Chemistry) as well as in electrochemical journals. A meeting of the working group is planned for May 2004 in Cocoa Beach/FL, USA, where the second draft of the final document will be discussed. The working group will aim at the production of a 15-20 page IUPAC Recommendation. CB informed the DC that this document will be presented to manufacturers of electrochemical instrumentation equipment so that they may heed the proposed recommendations and disseminate them. ZT asked about the viability of including some "example problems" in order to increase the practical aspects of the results. CB concluded that it appears that the working party is approximately one year behind schedule.

2001-030-1-100 - Recommendations on the measurement and analysis of results obtained on biological substances with isothermal titration calorimetry. No further news from project monitor (G. Wilson)

2001-035-1-100 - Measurement and interpretation of electrokinetic phenomena. No further news from project monitor (L. Koopal).

2002-005-1-100 - Thermodynamics of ionic liquids, ionic liquid mixtures, and the development of standardized systems. No further news from the project monitor (RW).

2002-063-1-100 - Chemical thermodynamics in industry. No further news from the project monitor (RW).

2003-005-1-100 - Recommended values of the viscosity of molten iron and aluminum. No further news from the project monitor (RW).

2003-006-1-100 - NMR chemical shifts: updated conventions*. No further news about this multi-Division (I, II, III) project from the project monitor (Sonia Cabral de Menezes).

2003-020-2-100 - Ionic liquids database. RLB made a brief presentation on the progress of the project that seems on track. The initial meeting at Delft University went well. For 2004 an ICCT International Conference including several satellite workshops are planned. A second meeting at Delft in 2005 is planned that RLB would like to attend in order to be able to closely monitor the progress in this interesting subject. In addition to setting up a data base in this rapidly moving and expanding field IUPAC should especially be interested in the fact that ionic liquids do not have CAS numbers so far.

2003-024-1-100 - Selected free radicals and critical intermediates: thermodynamic properties from theory and experiment. MJR is a member of the task group and reports, that work on 27 out of the 36 free radicals of set I is essentially finished, with work on the remaining 9 free radicals on track. A first review paper on 11 free radicals has been submitted to J. Phys. Chem. Ref. Data (JPCRD), and a second review article on 16 free radicals is close to being submitted to JPCRD. Tibor Berces (Hungarian Academy of Sciences) has passed the leadership on to Branko Ruscic (Argonne National Laboratory, US), however, the former will stay involved in the task group. RW is the project monitor.

2003-036-2-100 - Thermodynamics and non-equilibrium criteria for development and application of supplemented phase diagrams. Spending authority has been recently granted (see Finances above). RFP is the project monitor.

* Interdivisional project

OTHER INTERDIVISIONAL PROJECTS

2000-012-1-300 - Single molecule spectroscopy, Divs. I and III. The DC recommends the project be abandoned owing to lack of progress. The completion date is long overdue (2002). In addition, this project does not show any financial activity (Project Expense file). No news from the project monitor (GA).

2001-036-1-300 - Glossary of terms in photocatalysis and radiation catalysis, Divs. I and III. No news from the project monitor (Luuk Koopal).

2002-008-1-300 - Chemical actinometry, Divs. I and III. No news from the project monitor (GA).

2002-024-1-300 - Glossary of terms used in photochemistry (3rd version), Divs. I and III. No news from the project monitor (GA).

2003-056-2-500 - Standard definitions of terms relating to mass spectrometry, Divs. I and V. In view of the recent start of this project there are not yet any news on this project.

PROJECTS NEAR COMPLETION / IN PRESS

110/2/81 - Revision of "Quantities, Units and Symbols in Physical Chemistry" and the Appendices (3rd edition). A long discussion on the history and present state of the new edition of the "Green Book" took place. The completion date of 2002 is long overdue. In view of the absence of the chairman of Commission I.1 (JF) the DC decided to ask MJR to directly approach Martin Quack in relation to the status of the new edition of the Green Book, in order to ensure a speedy resolution of any final problems. Publication of the new edition, an extremely important task of Div.I and very much in the public eye, is long overdue.

No news have been collected on the following projects:

120/15/95 - Thermochemistry of chemical reactions: nomenclature, symbols and experimental methods for bond energies

120/16/97 - New Edition of Experimental Thermodynamics Vol II

121/13/89 - International Thermodynamic Tables of the Fluid State, Volume 14 : Benzene

150/24/95 - Spectroscopy under extreme conditions of temperature and pressure

150/25/98 - Quantities, terminology and symbols in photothermal and related spectroscopies

2000-026-1-100 - Critical compilation of vapour liquid critical properties

6. New Projects and the Future.

It was noted that there is a lack of future projects in the pipeline, and the vice president called upon all TM's and officers of the DC to act as ambassadors for Div I, especially in relation to "raking in" or soliciting new projects. The DC primarily relies on its members as well as on its advisors in order to generate new ideas worthy of pursuit in IUPAC-funded projects.

As of March 18 2004 there is only one project under Review, namely project 2004-0101-1 "Heat capacity of liquids: critical review and recommended values for liquids with data published between 2000 and 2004" by V. Ruzicka (USD 10'000). Another proposal waiting to be funded is the continuation proposal to project 1999-037-2-100 (Evaluation of rate constants for atmospheric chemistry, Dr. R. A. Cox, project monitored by RW) that will be resubmitted in 2004 (USD 20,000). This would be the second half and conclusion of the Web project whose funding should be requested jointly by the Project Committee and the Division. In addition, it was decided that MJR should solicit the resubmission of a proposal by Professor Ernst L. J. Breet of South Africa on the kinetics and spectroscopy of physicochemical systems under extreme conditions. ZT proposed to explore the

feasibility of setting up a working group on recommendation of techniques for the characterisation of the properties of nanomaterials along the following questions: (1) What is a nanomaterial?. It has to be pointed out that the key issue of a nanomaterial is its properties that are in general found to be different from the bulk phase. (2) What are its unique properties? The size effect, surface effect and/or quantum confinement should be emphasized. For example, metals in general change their optical properties when the size is reduced to below several tens of nm, they change their chemical reactivity below ten nm and exhibit quantum confinement effects below approximately three nm. (3) Techniques of synthesis leading to size and shape control. (4) Existing database. At present, it is not possible to compile a comprehensive database for nanomaterials. However, a possible start would be the compilation of data for some of the most commonly used nanomaterials such as TiO_2 and Au. However, such a project would have to be distinctly different from a monograph or a review article.

It remains to be seen whether the present lull in proposal submission activity is the sign of an inherent weakness of the project system or whether it is a manifestation of the random nature of presenting ideas worthy of IUPAC support. A lively discussion ensued on the question of who is able to propose to IUPAC. CB expressed a need for clarification and promised to contact the new Secretary General, Prof. D. Black.

7. Role of Division I in Biophysical Chemistry.

The DC had intense discussion in relation to the strengthening of activities in biophysical chemistry. WB proposed to make a first step in this direction by asking IUPAC for support to hold **IUPAC-sponsored lectures** or series of lectures in a topic of biophysical interest akin to the established AMBO lectures. According to WB, these lectures, depending on the framework, give high visibility to the organizers and would serve to promote IUPAC's willingness to actively search for biophysical or related activities. Two existing frameworks were given by WB: ELSO (European Life Sciences Organization that regularly attracts more than 3000 scientists worldwide), and the European Symposia of the Protein Society, the editor of the scientific magazine Protein Science. The **Advisory Group of Division I** should also be asked for their suggestions. However, it was recognized that the effectiveness to break out into a new field using this approach probably would meet with limited success since the Advisory Group reflects the current composition of the DC. The DC asked WB for names of Advisory Group members in the area of biophysics and biophysical chemistry to add to the roster of competent professionals. Finally, WB made a specific proposal for a timely potential IUPAC project in the biophysical area in relation to the definition of **resolution criteria in biological imaging applications**. MJR proposed a potential project on the definition of the purity of proteins used in laboratory operations. In addition, it was suggested to hold joint meetings with Division IV (Macromolecular) and

V (Analytical) during the next GA in Beijing in order to explore the feasibility of joint projects in the field of biophysical chemistry and the potential interface with life sciences.

With a "surplus" in the operational budget and few committed funds as of date the financial possibilities of Div I should be used to open up new areas of physical chemistry. CB said he would explore the limits of the use of these divisional funds with the Secretary General.

8. Elections (Brett)

The Vice-President, CB, is in charge of organising the elections to the DC for the biennium 2006-7. CB reminded the DC of the election procedures written down by G. Wilson in 2003 and the intended deadline of December 1 2004 in regards to the roster for the 2006/2007 biennium. It is necessary to elect 4 new Titular members, who should, together with the other Committee members, cover as much as possible the areas of physical and biophysical chemistry.

The members of the Nominating Committee, three out of five external to the DC and to current IUPAC activities, should be approved by the Secretary General by September 2004. The following names for the Nominating Committee were agreed upon after discussion. These persons will be contacted in order to ascertain their willingness to serve:

Internal members: CB, RFP; external members: C. Robinson, M. Nakahara, B. Ladanyi.

The importance of having the new members of the DC being able to attend the GA in 2005 was pointed out

An informal discussion regarding the slate of Division I officers for 2006-7, who should come from the members of the Division Committee for the biennium 2004-5, namely the post of future vice president and secretary followed. The proposals agreed on by those present were MJR as vice-president and RLB as division secretary.

9. Inter-divisional Activity.

CB briefly presented the activities on (1) Subcommittee on Green Chemistry and (2) Committee on Chemical Education (CCE), in both of which he is a member as Div. I representative.

The Green Chemistry Subcommittee is planning an International Symposium for 2006, organized by P. Tundo, the subcommittee chairman. The potential support to be given by Div. I to this and other Green Chemistry projects was discussed in the light of the 12 Principles of Green Chemistry. RLB believed that the field is fashionable, and as a consequence that the DC should commit some, but not too many resources, particularly avoiding duplication of efforts. MJR expressed his slightly more optimistic view that Green Chemistry offered an opportunity to study entirely new phenomena such as chemical

reactions of pure components whose kinetics poses a challenge to solution studies. In addition, such a program puts the potential use of ionic liquids into a proper industrial perspective.

In relation to the CCE, CB attended the CCE meeting in the Ottawa GA after the Division I Committee meeting had finished. A number of potential projects and ideas were discussed but no concrete proposals were forthcoming.

See also items discussed under 7 in relation to the plans of the DC of initiating new activities in the field of biophysical chemistry.

10. General Assemblies.

ZT, as a representative of Physical Chemistry of the Chinese Chemical Society, presented the preliminary plan of the Chinese Chemical Society for the 43rd IUPAC and GA in Beijing, P. R. of China that is placed under the motto "Innovation in Chemistry". The program will be organized around 8 central themes, each directed by two co-chairmen. One of these co-chairmen will be nominated by the Chinese Chemical Society (CCS), the other by IUPAC. ZT infomed the DC that the CCS expects the president of Div I to take the co-chairmanship of Theme 5, "Innovation in Traditional Chemistry, Research Methods and Techniques". CB will let RW know as soon as possible as ZT transmitted a sense of urgency of this request. In a lively discussion a name change for Theme 5 was suggested to: "Innovation in Physical and Biophysical Chemistry" as it was felt that the term "Traditional Chemistry" would not attract high calibre invited speakers. ZT proposed that Div I should, through its president, suggest 2 to 3 sub-sessions, at least two of which should be incorporated into Theme 5. He also revealed plans to organize some satellite meetings around the IUPAC Congress, not necessarily in Beijing but at places that may easily be reached by air transport. A possible theme was the role of Chemical Education in Physical Chemistry. A possible workshop may be entitled 'Physical Chemistry Education and Its Challenge'. This satellite meeting may be very helpful for the Chinese colleagues who are teaching physical chemistry at universities. Recently more than twenty Chinese key universities have been requested by the Ministry of Education to teach physical chemistry in English, which is very difficult for both teachers and students. The contact person of the CCS may be reached by e-mail at the following address: qiuxb@iccas.ac.cn.

11. Other Business. See previous discussion. No specific items were discussed under this agenda item.