

**\*IUPAC General Assembly of the Division of Physical and Biophysical  
Chemistry (Division I)  
Beijing, P. R. China, 13–14 August 2005**

Present: R. D. Weir (RDW, president), C. Brett (CB, vice president), M. J. Rossi \* (MJR, secretary), R. Lynden-Bell (RLB), J. McQuillan (JMQ), Z. Q. Tian (ZQT), K. Yamanouchi (KY, TM for next biennium).

Young observers: Victoria Cornelius (U Greenwich), Catherine Holt (electrochemist, UC London), Robert Hinde (theoretical chemist, U Tennessee), Nicholas Walker (U of Bristol, on Sunday), Y. Alexander Wang (U of BC Vancouver; from 2:00 p.m.), Angela Wilson (theoretical chemist, U NTexas at Dallas).

**Saturday, 13 August 2005**

The GA was called to order by the president at 9:15 a.m. in the presence of Bryan Henry, president elect of IUPAC who wanted to get a first-hand experience of the work performed within the Divisions.

**1. Introduction.** Everybody present introduced themselves in a few words given the significant number of young observers.

**2. Approval of Agenda.** The agenda at the end of this document was approved unanimously. An additional agenda item dealing with the appointment of a member of the DC to ICTNS (Interdivisional Committee on Terminology, Nomenclature and Symbols) and to the Committee for Chemical Education (CCE) was approved on the occasion of the visit by Peter Atkins (CCE) later in the day (see item 17 below).

**3. Approval of Minutes of the GA Meeting held in Ottawa 9-17 August 2003.** The minutes of the Division I Meeting were already approved at the off-year meeting in Glion (Switzerland), 3–4 April 2004.

**4. Finances.** According to MJR an amount of USD 2800 of the Division I budget was still uncommitted. Bryan Henry pointed out that additional funds were available from the Project

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\* December 14 2005/MJR

Committee through the General Secretary. Two recently approved projects were briefly mentioned: 2003-036-2-100 (H. A. Corti), 2004-026-2-100 (E. Arunan and S. Scheiner). A request was made by MJR to clear the books of completed projects. RDW will attend to this item in one of his next Bureau meetings.

**5. Elections.** The roster of Division I presently includes 10 Titular members (TM) including Division officers and the chairman of Commission I.1, 6 Associate members (AM) and 6 National Representatives (NR). The president (RDW) together with the officers are trying to significantly increase the representation of the biophysical activities of Division I. The Division I Advisory Committee consisting of approximately 60 colleagues should assist in this slow but steady change. The question of a reward on behalf of the members of the Advisory Committee was briefly discussed. It was stated that they receive the publication "Chemistry International" (CI) and are promoted to IUPAC Fellows upon retirement. However, nothing more can be done under the present By-laws since their activity may be understood as part of the normal peer review system. RDW is going to ask Fabienne Meyers to keep the list of the members of the Advisory Committee up to date.

CB briefed the Division about the Nominating Committee consisting of 2 TM's plus 3 external members. The present roster is composed of Chris Brett and Roberto Fernandez-Prini for the TM's, Masahiro Nakahara (Japan), Branka Ladanyi (US) and Carol Robinson (UK) as external members. CB emphasized his efforts to pay attention to geographical and gender distribution as well as scientific expertise in different areas of physical chemistry. The elections of June 2005 were a bit disappointing from the point of view of electorate participation, which amounted to 31% of the electorate of 47 members within Div I. It was pointed out that Division I still has a very restricted electorate that consists of all TM's, AM's, NR's as well as the coordinators of all active projects within Division I. The members of the Advisory Committee are not part of the Div I electorate. Bryan Henry was openly questioning the legitimacy of this restricted electorate and was of the opinion that the possibility of more flexibility in the election procedure should be examined for the future.

As a result of the 2005 elections, whose results have been communicated in June 2005 by CB, the new TM's are Albert Goldbeter (Belgium), Kauru Yamanouchi (Japan) and James McQuillan (NZ) (presently Div.1 AM), the latter two having been present in the Division Committee during this GA. These new TM's replace George Atkinson (USA), Roberto Fernandez-Prini (Argentina) and Joachim Maier (Germany) whose terms on the Division Committee finish at the end of 2005.

Jeremy Frey was elected president of Commission I.1 by the commission members for the next biennium 2006-7 and was therefore re-elected as TM. RDW pointed out that this *ex officio* TM membership is counted as part of the Division I roster of 10 slots.

All six slots for Associate members have to be renewed, since AM's are only elected for 2-year periods, renewable once. RDW and CB pointed out how the pool of eligible candidates for AM was set up: present AM's whose term can be renewed, unsuccessful candidates from the TM elections, nominees from NAO's who had not been included in the TM elections and other candidates suggested by members of the Division Committee.

Out of the present AM's, Sonia Cabral-Menezes (Brazil) is to be asked to continue as AM for the next biennium leaving five further positions available. The three unsuccessful TM candidates would be asked to serve as AM's, leaving two further slots to fill.

TM's and AM's of Argentina and Chile are currently not eligible owing to arrears of financial contributions to IUPAC from those countries whereas the suspension on Brazil has been recently lifted.

**6. Report for the biennium 2004-2005.** An extensive report written by the president (RDW) on behalf of the Bureau has been sent out to the members of the Division Committee whose members acknowledged the extensive documentation, which will form a solid basis for the management of Division I on behalf of the next generation of Division officers. MJR will submit a brief report to Chemistry International on the satellite meeting "PCEC - Physical Chemistry: Education and Challenges" held on 9-11 August 2005 in Xi'An and organized jointly by professors Fu Yang and Z. Q. Tian (ZQT) under the auspices of IUPAC.

**7. Progress Report on Current Projects.** In the general discussion RDW observed that the members of the Advisory Committee are not tasked sufficiently as far as the input to data projects is concerned. One of the lingering questions discussed was that of the required periodic update of databases such as the one on atmospheric chemistry (1999-037-2-100), which was identified as a long-term issue (ZQT). It was suggested to treat data base projects separately in their own right. Bryan Henry asked who should manage the database in the future: Should IUPAC hire a resource person for special computer needs? Given the limited human resources of IUPAC it was expected that it would be very difficult to maintain and keep up to date such a database (see project 11 below). RLB pointed out that the ionic liquids data base (project 11) will be put up on NIST computer facilities. Angela Wilson expects that such a kind of database will significantly expand in the near future. The National Science Foundation of the US, more specifically the supercomputer

facilities managed by Tom Dunning, may be of help in this respect. No recommendations for nomenclature and standards do yet exist in the biophysical chemistry area. This is seen both as a serious deficiency as well as a growth area for new projects within Division I.

Specifically, the following projects were briefly mentioned (numbering taken from the recent report of the president to the bureau):

1999-037-2-100 - Evaluation of kinetic data for atmospheric chemistry. MJR notifies the Division that a request for a no-cost extension of this project is to be expected. It is anticipated that the last data sheets will be entered into the data base by mid 2006 on or before the next subcommittee Meeting in June 2006.

Regarding projects 2001-028-1-100 - Electrochemical impedance spectroscopy - terminology, nomenclature and data exchange formats and 2001-030-1-100 - Recommendations on the measurement and analysis of results obtained on biological substances with isothermal titration calorimetry RDW voiced some concern as these two have been essentially completed for a certain time and are awaiting final publication that is in various stages of completion. The last progress reports date back a few years.

2001-035-1-100 - Measurement and interpretation of electrokinetic phenomena has recently been completed.

Project 150/24/95 - Spectroscopy under extreme conditions of temperature and pressure will be dropped for lack of activity and interest.

Project 2002-005-1-100 - Thermodynamics of ionic liquids, ionic liquid mixtures, and the development of standardized systems is a promising and emerging data project accompanied by RLB who requested that IUPAC be visible and represented by officers at the highest level at the ACS March Meeting in 2006 in order to present the scope and the goals of this project. RDW would ask Bryan Henry to attend the ACS Meeting in order to generate some publicity for this project and lobby for support. Bryan Henry subsequently agreed to this mission.

Progress on project 2003-024-1-100 - Selected free radicals and critical intermediates: thermodynamic properties from theory and experiment has been held up by more than a year by a long delay of its first publication in J. Phys. Chem. Ref. Data. A request for a no-cost extension by one year is to be expected as communicated by MJR.

**8. Green Book.** It was deplored that no progress has taken place since the GA in Brisbane in 2001. Unfortunately, Jeremy Frey cancelled his trip to this GA on a short notice. However, e-mail messages have been sent instead. On behalf of the DC, CB and MJR will attend a meeting on the Green Book on Thursday, August 18, convened by Roberto Marquardt who will communicate

the latest status on the Green Book. It seems, however, that a corrected LATEX version of the second edition is close to completion. A draft in printed form is circulating.

**9. Future Projects.** To this date Division I has USD 2,800 of uncommitted funds left for this biennium as communicated by MJR. It later turned out that this information was inaccurate as there were USD 3,300 still uncommitted. David Stanbury, the coordinator of project 2001-015-1-100 - Standard potentials of radicals has submitted or will shortly submit an extension proposal in the amount of USD 3,500 in view of the significant progress of this data project, RDW as well as a majority of the DC agreed to this extension. JMQ as well as ZQT both intend to submit new proposals in the next biennium. The subject matter pursued by JMQ will be the use of modern spectroscopy and applications whereas ZQT will file a proposal dealing with the reform of the physical chemistry (PC) curriculum in China as well as aspects of bilingual teaching of PC. RDW will contact the Div I Advisory Committee to solicit large proposals, especially in the biophysical chemistry area.

**10. Inter-divisional Activity.** There are a total of 8 interdivisional projects underway, 7 are well established, one has recently been approved (2005-016-1- Solubility for Industry). The status of project 2001-036-1-300 - Glossary of terms in photocatalysis and radiation catalysis is not clear as Division III does not carry it in its books. RDW will inquire with Division III. It turns out that John Bolton, Nick Serpone and Valentin Parmon are the contacts of Division III. However, RDW will find out if Div I has made financial contributions or commitments to this project in the past.

**11. Chemical Education Committee (CCE).** CB as an associate member of the standing committee informed the DC of the agenda of last year's ICCE Congress in Turkey. ZQT reported on the highly successful PCEC – Physical Chemistry Education and Challenges Satellite Meeting held in Xi'An the week before the GA (see also point 6 above). MJR will provide a report on this meeting for CI (see item 6). Concerning PC teaching, the lead should be taken by Div I, whereas aspects of bilingual teaching in PC should be the realm of the CE Committee. This subtle distinction represents a fine line between tasks undertaken by the two bodies. Concerning PC education Catherine Holt proposed to work on options for carrying out demonstration experiments with limited funding. This documentation could be of use to teachers in many geographic areas and situations. JMQ was asked to be the liaison with the CCE and thereby becomes an associate member. JMQ wants to promote PC emphasizing spectroscopic techniques for the solution of practical problems.

Peter Atkins (PWA) announced that Peter MacAfee will take over the chairmanship of the CCE in the next biennium. ZQT proposes work on visualization videos for teaching purposes. However, PWA thinks that this proposal is already being pursued by commercial publishers. He claims that the subject of e-books and animation in science will become important subjects in the years to come. PWA sees his activity within CCE as someone planting seeds that ultimately will grow to be picked by members of the Divisions.

**12. Off year Meeting.** The criterion for the selection of the venue must be cost. There are currently 6 European and 4 non-European TM's which nudges the choice towards a European location, preferably before Easter, thereby taking advantage of the low air fares. Coimbra/Portugal (CB) as well as Geneva/Switzerland (MJR) are potential candidates. CB and MJR will each estimate the cost for their location and communicate the results in due time. Taking advantage of low weekend airfares the meeting will take place during a weekend with travel on Friday and Monday before and after the weekend, respectively.

**13. Advisory Committee list.** RDW feels that the members of the Div I Advisory Committee are not tasked sufficiently, some members have retired since their recruitment. Members should serve four years with a possibility to extend their mandate by two years and should be thanked in some form at retirement. Retired TM's of Div I should be asked to serve on the Committee. The initial size of the Committee (about 60 members) is judged too large by RDW, 40 members seems about right. This question will be addressed further after the GA.

**14. Divisional Committee-member responsibilities.** It was decided that in the future the major divisional responsibilities will be further shared between the officers of the Division, as has been the recent trend, and advice on specific cases will be sought from other members of the Division Committee, according to their scientific expertise. Evaluation of project proposals will be carried out by members of the Committee, on request from the President, as well as by members of the Advisory Subcommittee, whose advice will be actively sought regarding future developments of the Division. At present, each approved project will be monitored by a member of the Committee, selected according to his/her affinity with the subject matter of the project. The coordination of these activities will be through the president.

**15. 44<sup>th</sup> General Assembly, Torino, Italy, 4-12 August 07.** RDW calls for early cooperation with the organizing committee that is represented at this GA.

**Sunday, 14 August 2005**

**16. Other Business.** According to a letter sent out by Ian Mills on 12 July 2003 a proposal for refining the base units kg, A, K, mole and reducing the associated uncertainties is being circulated. The new definition of the kg is based on either Avogadro's number  $N_A$  or Planck's constant  $h$ . The new definition of K makes use of the triple point of H<sub>2</sub>O that will fix Boltzmann's constant  $k$ . The new definition of the mole will imply fixing Avogadro's constant. As a result  $h$ ,  $e$ ,  $k$  and the mole will be defined with increased accuracy.

**17. ICTNS.** The representative of Division I has been Jeremy Frey. RDW is volunteering to serve as Div I representative starting with the next biennium, which was unanimously accepted by the Division Committee.

**18. Addendum to Elections and Roster of the Division Committee.**

Division I has 10 TM's, 6 AM's, 6 NR's (the NR's cannot hail from countries of origin of TM's and AM's). The final roster of Division I for the biennium 2006-2007 is as follows:

Titular members (TM):

Chris Brett, president, electrochemistry, environmental chemistry, Portugal

Ron Weir, past president, thermodynamics, materials, Canada

Michel J. Rossi, vice president, chemical kinetics and atmospheric chemistry, Switzerland

Ruth Lynden-Bell, Secretary, theoretical chemistry, simulation, Great Britain

Wolfgang Baumeister, biophysics, Germany

Jeremy Frey (chairman of Commission I.1) spectroscopy and structure, Great Britain

Albert Goldbeter, biophysical chemistry, Belgium

A. James McQuillan, surface chemistry, spectroscopy, New Zealand

Zhongqun Tian, interfacial spectroscopy, China

Kaoru Yamanouchi, molecular and laser spectroscopy, Japan

Associate members (AM):

Sonia Cabral-Menezes, NMR spectroscopy, Brazil

John Dymond, thermodynamics, fluids, viscosity, Great Britain

Bruce Kay, reaction dynamics, USA

Sung-Jin Kim, solid state chemistry, Korea

Clive Prestidge, biophysical chemistry, Australia

Angela Wilson, theoretical chemistry, USA

National representatives (NR):

Sergei Aldoshin, solid state chemistry, Russia

Michalis Chalaris, molecular liquids, Greece

Assaf Friedler, protein biophysics, Israel

Mika Oivanen, physical organic chemistry, Finland

S. Riaduzzin, molecular biology and applications, Pakistan

Svein Stolen, solid-state chemistry, thermodynamics, Norway

Two young observers from the US, Angela Wilson and Robert Hinde, asked to serve on the Division Committee for the next biennium. It was suggested that Angela would become AM and Robert NR on Commission I.1.

The delay of the publication of the Second Edition of the Green Book led to intense discussions as to the future of the Commission on Physicochemical Symbols, Terminology and Units of Division I (I.1) whose roster was discussed at length. It is currently composed of 3 TM's and 7 AM's. The current chairman, Jeremy G. Frey, has been re-elected for 2006-2007 (item 5). Two out of three TM's (Martin Quack, Switzerland, Herbert L. Strauss, US) have reached their term limit with the end of the current biennium. RDW and CB should contact Martin Quack and Herbert Strauss to seek advice concerning the appointment of two TM's and the future of Commission I.1. The election of Jeremy Frey is hopefully providing some continuity to Committee I.1 regarding the resolution of the Green Book project and provide guidance to new members. CB suggested two candidates for TM of I.1: Roberto Marquardt (France) and Franco Pavese (Italia). Four names have been suggested for NR's: Yunk Yong Ha (Korea), Alexander Milchev (Bulgaria), Mohammed Iqbal Choudary (Pakistan) and Robert Hinde (USA). In addition, the search will go on for three further NR's of I.1.

It is suggested that John Jost will have to check the current status of the publishing contract with the RSC concerning the publication and production of the second edition of the Green Book.

The following posters related to projects of Division I were on display during the GA and the IUPAC Congress at

**IUPAC Project Place**

Beijing International Convention Centre

13 to 21 August 2005

Evaluated kinetic data for atmospheric chemistry (#1999-037-2-100)  
**R. A. Cox**, R. Atkinson, J.N. Crowley, R.F. Hampson, R.G. Hynes, M.E. Jenkin, M. J. Rossi, and J. Troe.

The thermochemistry of free radicals of importance to combustion and the atmosphere. (#2003-024-1-100)

**Branko Ruscic**, Tibor Bérces, J. E. Boggs, A. Burcat, A. Császár, J. Demaison, R. Janoschek, J.M.L. Martin, M. J. Rossi, J. Stanton, P. Szalay, P.R. Westmoreland, and F. Zabel.

Standard potentials of radicals (#2001-015-1-100)

**David M. Stanbury**, D. Armstrong, J. Butler, R. E. Huie, W.H. Koppenol, Sergei V. Lymar, G. Merényi, Pedi Neta, S. Steenken, and P. Wardman.

At the end of the GA the Division officers on behalf of the Division Committee thanked the president of Division I, Ron D. Weir, for his dedication and efforts throughout his tenure as TM and president during the last two years. He is leaving behind a healthy Division oriented towards new horizons in that he substantially strengthened the biophysical aspects. He took over the Division in a difficult and changing time without the help and advice of a past president and provided a report that will be of great help for the following generation of Div I officers.

## DIVISION OF PHYSICAL AND BIOPHYSICAL CHEMISTRY

### Approved Division Committee Agenda

Meetings scheduled during the IUPAC General Assembly 13-14 August 2005, Beijing, P.R.China

1. Introduction (RDW)
2. Approval of Agenda (RDW)
3. Approval of Minutes of the Division held at the GA Ottawa 9-17 Aug 03 (CB)
4. Finances (RDW/MR)
5. Elections (CB)
6. Report for the Biennium 2004-05 (RDW)
7. Progress Report on Current Projects (RDW)
8. Green Book (RDW)
9. Future Projects (RDW)
10. Inter-divisional Activity (RDW)
11. Chemical Education Committee (CB)
12. Off year meeting spring 2006 (CB)
13. Advisory Committee List (RDW)
14. Divisional Committee – member responsibility
15. 44th General Assembly, Torino, Italy 4-12 Aug 07
16. Other Business