

**IUPAC – Division 1 Committee****Minutes of the Off-Year Meeting 2008**

The 2008 meeting was held at Villars-sur-Ollon (Switzerland) 12-13 April 2008.

Present: Michel J. Rossi (President)

Jim McQuillan (Vice-President)

Christopher Brett (Past President)

Ruth Lynden-Bell (Secretary)

Kaoru Yamanouchi (TM)

John Dymond(TM)

Roberto Marquardt (TM and Chair Commission 1.1)

Jianguo Hou (TM)

**1. Introduction, welcome and apologies.**

Michel Rossi welcomed the new members. Apologies had been received from Brian Sykes and Albert Goldbeter.

**2. Agenda.**

The agenda was approved unanimously.

**3. Minutes of Previous Meeting.**

The minutes of the 2007 meeting were accepted.

**4. Progress reports on Current Projects.** Project Monitors shown in brackets.

120/15/95 Thermochemistry - A new document is expected

150/24/05 Spectroscopy under extreme conditions - A new document is expected soon

2000-026 Marsh (Dymond) - Vapour-Liquid critical properties - Part 11 is in preparation; Part 12 is to be an update of earlier data. A no-cost extension until 31/12/09 should be sought.

2001-015- Stanbury (Brett) - Potentials of radicals - A no-cost extension until 30/6/09 should be sought- CB is to suggest a follow-up project for organic radicals.

2001-028 - Stoynov (Brett)- Impedance spectroscopy - The draft report is improved. It was noted that only 50% of the money had been spent.

2001-030 - Schwartz (Weir)- Titration Calorimetry - All is proceeding well

2002-005 - Marsh (RMLB) - Thermodynamics of Ionic Liquids - A no-cost extension until 31/12/08 should be sought. Some money remains.

2003-024 - Ruscic (Rossi)- Thermodynamics of free radicals- 1 publication has appeared and 2/3 of the radicals have been done. Possibly this work is slowing.

2003-036 - Corti (Prini) - Criteria for Phase Diagrams - He should be asked where the work is to be published and whether he wants a no cost extension to 31/12/08.

2004-010 - Ruzicka (Weir) - Heat Capacity of Liquids - this project is well in hand.

2004-026 - Arunan (McQuillan\*) - Hydrogen Bonds - It has proved controversial and it may not be possible to have a straightforward report because of the lack of scientific consensus among the task group members. It was thought that this project needs to be concluded and that a report giving different definitions would be useful.

2004-036 - Tennyson (Yamanouchi) - The water database is said to be available at [www.chaos.chem.elte.hu](http://www.chaos.chem.elte.hu). A paper is about to be submitted and a meeting of the task force is scheduled for Sept 08. A no-cost extension until 31/12/08 should be sought

2004-046 - Majer (Dymond) - Thermodynamics of hydration of Organics - Majer has now moved. We may have to write this one off, but John Dymond will investigate whether anything can be rescued.

2005-044 - Cox (Rossi) - This project is finished.

2006-021 - Rouquerol (Marquardt\*) - Characteristics of porous media.

2006-023 - Alberty (Weir) - Biochemical Thermodynamics. This recommendation is in review. 10 names need to be submitted; Goldbeter and Friedler were suggested. A no-cost extension until 31/12/08 should be sought

2006-050 - McQuillan (McQuillan) - This year will be crucial for satisfactory progress; the task group met in Sept 2007 and will meet in 2009. A one year extension may be needed.

2007-002 - Grolier (Dymond\*) - MTDSC (Calorimetry)

2007-001 - Cox (Rossi\*) extension

2007-015 - Letcher - Sustainable Energy - RMLB\* to enquire whether completed

2007 - 024 - De Loos (Dymond\*)- Reporting phase equilibria

2007-032 - Marquardt - Green book - abridged

2007- 048 - Ramasami (Marquardt\*) - Theoretical methods for reaction rates.

2007-055 Yamanouchi - Ultrafast Laser Chemistry

2007-059 - Letcher - (Dymond\*) - Heat Capacities

New project monitors are shown with asterisks in the above list.

## 6. New proposals

S.Cook and A.Wilson have withdrawn their project. R. Marquardt\* agreed to contact the authors to encourage revision and re-submission.

2008-006 Sun (Hou\*) - Hydrogen storage materials. This proposal is being revised; A fuel cell expert is needed for the task force; we could commit up to \$9000 and seek further support from the project committee. Jianguo Hou agreed to be monitor if it is approved.

2008-014- Jan Sengers has submitted a no-cost project concerning applied thermodynamics of fluids. It was agreed to support this and John Dymond was appointed to be monitor.

Roberto Marquardt is seeking funding for a workshop on the preparation of the green book for translation and hopes to get Chinese and Spanish participation.

Jianguo Hou\* agreed to contact Katherine Holt with a view for a joint project in the area of local probe microscopies.

## 6b Future Strategy.

It was noted that **projects** tended to fall into 2 classes - ongoing traditional projects (often databases) and small finite projects. In future we might hope for more multidisciplinary projects which may well be joint projects with other divisions. When reviewing projects one should always ask 'Why IUPAC?'

A discussion of **Databases** was held. It was agreed that they could not be kept up for ever and that 10 years was probably a typical time span. Eventually some databases could be handed over to some other body, and it would be possible for IUPAC to retain ownership and to grant a licence. It was noted that critical evaluation and international consensus was the key IUPAC contribution.

**Ideas** for future projects include (a) a database of kinetic constants for reactions of environmental importance in the condensed phase and at interfaces; (b) Combustion database for the WWW.; (c) publications of glossaries and acronyms eg for density functional calculations.; (d) protocols for new techniques in surface science.

## Action items

\* RMLB to send K.Holt's e-mail to J. Huo.

\* CB to send Rouquerol's proposal to J. Huo to give an idea of what is required.

\* RMLB to sound out colleagues about a DFT glossary.

## 7. Biophysical Chemistry.

We have been trying to find projects in this field since 2001, with mixed success despite our efforts. Currently we have 2 members in the field, Goldbeter (resigning) and Friedler. It is clear that other organisations cater for Biophysics, but

that there may still be projects that are appropriate for IUPAC. Assaf Friedler is thinking of projects and will consult Goldbeter. It was suggested that he look at the members of the advisory committee for possible task group members.

### **8. Elections**

The committee is made up of 10TMs, 6AMs and up to 10 NRs (as agreed by Council). The period of membership is up to 4 consecutive years for members (as opposed to officers). TMs are elected for 4 years while AMs and NRs are elected for 2 years but may be renewed once.

Christopher Brett was confirmed as Chairman of the Nomination Committee. Jianguo Hou agreed to be the other member from the Division I committee, Names of candidates for the three other places were discussed and will be contacted by the Nomination Committee Chair. [Note added after the meeting. Prof. Anne-Marie Cazabat (Paris), Prof. Don McNaughton (Monash, Australia) and Prof. Hanna Reisler (Los Angeles) have agreed to serve.]

K. Yamanouchi and A. Goldbeter reach the end of their tenure as TMs, R. Lynden-Bell (secretary) and C. Brett (past president) reach the end of their tenure as officers.

### **Officers**

It was agreed that the following would serve as officers for the biennium 2010-2011

President: J. McQuillan

Vice President: K. Yamanouchi

Past President: M. Rossi

Secretary (4 years): R. Marquardt (*agreed by e-mail after the meeting*)

### **Titular Members**

3 new TMs will be needed.

The areas that will be lost are electrochemistry, computational chemistry and biophysics.

Electrochemistry needs to be covered in the new committee, but one biophysics representative may be sufficient.

Assaf Friedler (currently a NR) might be proposed as a TM.

### **Associate Members**

It was noted that Prestidge, Wilson and Kim cannot be renewed as AMs. The AMs will need to be selected in January after the results of the election for TMs are known. Unsuccessful candidates for TMs could be appointed as AMs.

### **National Representatives**

It was noted that Chalaris, Friedler, Stolen and Riazuddin come to the end of their terms and cannot be renewed.

At present we do not have e-mail addresses for Akhtar or Mamchenko. \*RMLB agreed to write to them.

### **Commission 1.1**

Members are nominated by the Commission and appointed by the Secretariat.

### **Advisory Sub-Committee.**

The membership needs to be considered with proposals coming to the Glasgow Committee meeting. M.Rossi agreed to write to Advisory Committee members as incoming president.

### **9. IUPAC Representatives on Other Bodies.**

Robert Schoonheydt wishes to retire from being IUPAC representative on IACS. RMLB agreed to contact John Jost about the procedure for replacing him and Schoonheydt for suggestion for a successor and details about the activities.

### **10. Interdivisional Activity.**

We have some joint projects (see list). \*Liaison with other divisions for joint projects will be

Div 5 - C. Brett; Div 6 - J. Dymond; CPEP - R. Marquardt.

John Dymond, Div I liaison to COCI, has also been involved in ICTNS and has sent an account of Div I activities to COCI.

Jim McQuillan is our representative on CCE. He reported that it holds biennial conferences to promote Chemistry, but their main target is high school rather than tertiary education.

Interdivisional sub-committees.

Materials Chemistry (Div 2) - Ron Weir

Green Chemistry (Div 3) - Chris Brett

Both these representatives will need to be replaced at the Glasgow meeting.

## **11. General Assembly - 2009**

The Bureau meeting will be organised by the Croatian Chemical Society and will be held in April 2009. Our committee meeting will be held in Glasgow on Friday and Saturday July 31st and Aug 1st 2009.

The **Congress** will be held Mon-Fri Aug 3-7 2009. It was noted that there is little divisional input as yet, and it was suggested that members might contact the organisers.

The 2011 GA and Congress will be held in San Juan, Puerto Rico from July 30-Aug 7th 2011.

## **12. Any Other Business**

(a) Committee members were urged to check and update their contact details on the IUPAC website.

(b) The new IUPAC Divisional Discussion board is at <http://iupac-services.fiz-chemie.de/iupacforum/forumdisplay.php?f=4>

It was agreed to review its use in Glasgow.

### **(c) Pure and Applied Chemistry**

This journal has been resurrected by James Bull and now has a respectable impact factor. As well as containing IUPAC reports and recommendations it contains peer-reviewed articles, mainly from IUPAC supported conferences.

### **(d) Division Presidents at the Bureau meeting (April 08).**

Michel Rossi reported that he has raised the problem of the declining worth of the US dollar.

This had been agreed to be a problem because it hampers on-going as well as future Divisional projects.

There has also been considerable discussion about the International Year of Chemistry to be held in 2011. CCE is very involved, and it is expected that the NAOs will become involved. It should also be an opportunity to promote the work of IUPAC and its divisions.