

## IUPAC Division I Committee

### Minutes of the General Assembly Meeting 2009

The 2009 meeting was held during the IUPAC General Assembly at Glasgow, UK, July 31 and August 1st.

Present: Michel Rossi (President)  
Chris Brett (Past President)  
Jim McQuillan (Vice President)  
Ruth Lynden-Bell (Secretary)  
Kaoru Yamanouchi (TM)  
John Dymond (TM)  
Roberto Marquardt (TM)  
Jiang Guo Hou (TM)  
Angela Wilson (AM)  
Assaf Friedler (NR and YO)  
Anders Thor (NR)

Observers: Maria Zaharescu (Romania - Fri am)

Young Observers (YO):

Charles Sykes (USA)  
Shuqing Sun (China)  
Pierangelo Metrangolo (Italy)  
Jon Schwantes (USA)

IUPAC Officer: Bryan Henry (Past President) (Fri)

#### **1. Introduction, Welcome and apologies**

The President welcomed the committee members and the Young Observers. He conveyed apologies from Brian Sykes (TM).

#### **2. Agenda**

The agenda was approved.

#### **3. Minutes of past meetings**

The minutes of the Division meeting held at the GA in Torino in 2007 were approved.

The minutes of the Off-Year meeting in 2008 were approved.

In connection with the latter, the secretary reported that she had written to the two NRs (Akhtar and Mamchenko) for whom we had no e-mail addresses and had had no reply.

#### **4. Finances**

The Secretary reported that there was still about \$23K available for projects this biennium. The proportion spent on operations is 24% of the budget - well within the guideline of 30%.

The President reported that the IUPAC finances are in good order and that the budget for the next biennium will be much the same. However the Project Committee is more or less out of money for this biennium.

#### **5. President's report to the Council.**

This will be available on the IUPAC web site soon after the GA.

He reported that we had 24 projects on the books during the biennium. 8 had been completed and 7 were interdivisional.

He had drawn attention to the necessity of an IUPAC policy on databases and their upkeep.

## 6. Review of Current Projects.

**120/15/95** Da Silva: Thermochemistry of chemical reactions: nomenclature, symbols and experimental methods for bond energies . There is disagreement with internal reviewers of IUPAC and ICTNS about the form of the final report/recommendations.

It was agreed that Marquardt, Rossi and Dymond (possibly with Weir) should meet to make detailed suggestions.

**150/24/95** Heyns: Spectroscopy under extreme conditions of temperature and pressure . A report has been submitted to PAC. The project will be completed when it is accepted.

**2000-26** Marsh: Vapour-Liquid equilibria (monitor: Dymond). The final section should be ready shortly. Request no cost extension until 12/09.

**2001/15** Stanbury: Potentials of Radicals (monitor: Brett). There are problems with the value of the superoxide potential. No cost extension until 12/10.

**2001/28** Stoynov: Impedance spectroscopy (monitor: Brett). The document (recommendations or possibly technical report) should be ready in time for comments at an international conference on the subject in June 2010. No cost extension until 9/10.

**2003/24** Ruscic: Thermodynamics of Radicals (monitor: Rossi). There is a delay in the production of the second part. Angela Wilson emphasised the importance of access to the data. Rossi (monitor) agreed to ask for a final report including the data and to suggest that a new project might be initiated.

**2003/36** Corti: Criteria for Phase Diagrams (monitor: Prini). The second report is expected to be submitted to PAC shortly. No cost extension to end 09.

**2004/10** Ruzicka: Heat Capacity of Liquids (monitor: Weir). This project is completed with a technical report in press in J. Phys. Ref. Data.

**2004/26** Arunan: Modern Definition of the Hydrogen bond (monitor: McQuillan). A draft manuscript is nearly ready. It is not clear whether this will be a technical report, recommendation or a review. No cost extension to 12/09.

**2004/35** Tennyson: Database of water transitions (monitor: Yamanouchi). This project is nearing completion with two or three more papers in the pipeline. They plan to seek funding for a further phase. No cost extension until 12/09.

**2004/36** Sedlbauer: Thermodynamics of hydration of organics (monitor: Dymond). Progress seems on track after initial delays owing to the change of the task group chairman (from Majer to Sedlbauer).

**2006/21** Rouquerol: Characterisation of porous materials (monitor: Marquardt). Draft of technical report has been prepared.

**2006/23** Alberty: recommendations for biochemical thermodynamics (monitor: Weir). There have been problems with the quality of the submitted technical report and recommendations. Goldberg has agreed to take over and Ron

Weir agreed to convene a small group from Div I to recommend how to proceed.

**2006/50** McQuillan: Wet surface spectroscopy experiments (monitor: McQuillan). This is making progress albeit slowly.

**2007/1** Cox: Atmospheric Chemistry database (monitor: Rossi). This project has been completed. Many and an increasing number of hits (approximately 1000 a week as of June 2009) are made on the website showing that it is useful. A new group under the leadership of Tim Wallington will seek project funding for continuation and updating.

**2007/2** Grolier: Guidelines for temperature modulated DSC (monitor: Dymond). There will be a task group meeting at a calorimetry conference in June. No cost extension until 12/2009.

**2007/24** De Loos: Guidelines for reporting phase equilibria measurements (monitor: Dymond). A draft paper has been circulated to the Task Group.

**2007/32** Marquardt: Abridged Green Book (monitor: Marquardt). This is proceeding but abridgement is difficult. A web version would be a separate project.

**2007/48** Ramasami: Reactions involved in global warming (monitor: Marquardt). This project is proceeding and the technical report should be ready by the end of 2009.

**2007/55**: Yamanouchi: Ultrafast laser Chemistry (monitor: Yamanouchi). This project is proceeding satisfactorily.

**2007/59**: Letcher: Heat capacity book (monitor: Dymond).. This project is now completed as the book is with the publisher.

**2008/6**: Sun: Hydrogen storage materials (monitor: Hou). A good start has been made with four papers being produced.

**2008/45**: Assael: Viscosity and density of Cu/Sn. Dymond was appointed to be monitor of this new project.

## **7. International Year of Chemistry. IYC2011.**

This will start with an event in January 2011 at UNESCO headquarters in Paris and will end with an event in December 2011 in Brussels. There will be many local activities sponsored by NAOs, but ideas were being sought for global IUPAC activities. There was considerable discussion with some specific ideas. Michel Rossi agreed to summarise our ideas and convey them to CCE and the IUPAC IYC2011 committee.

## **8 Future Projects.**

The Division President said that he expected several projects to be submitted before the end of the year: (a) Axel Griesbeck (Photochemical processes for industry); (b) Pierangelo Metrangolo (who gave a short presentation on halogen bonding); (c) Tim Wallington (extension of atmospheric chemistry database). He urged all members to seek new proposals and said that officers and members of the committee are always ready to give advice.

## **9 Interdivisional activity.**

There are several joint projects with other divisions.. Visits were received from members of CCE, COCI, Chemistry International

editorial team and Div V (Analytical Chemistry). The latter is looking for further cooperative projects with Div I.

Materials Chemistry interdivisional subcommittee. At present it is embedded in Div II, but is exploring options to become either a new Division or a stand-alone interdivisional committee. The involvement of Div I is essential. Michel Rossi and Angela Wilson agreed to be our representatives.

Green Chemistry subcommittee. This is in a similar situation being embedded in Div III. It is proposed to organize it as a stand-alone Interdivisional Committee under the leadership of Div III. J.G. Hou will be the new Division representative from January 2010, to replace C. Brett.

#### **10 Internet notice board.**

Brian Pearson from the IUPAC secretariat attended to illustrate its use. We can post items such as minutes and agenda. E-mail messages would automatically be sent to committee members.

#### **11. CCE**

It is currently concerned with plans for IYC2011. It was decided that Assaf Friedler will represent Division I at CCE.

#### **12. Elections**

The nominating committee was C. Brett (Division Past President), J.G. Hou (TM), with three outside members: A.M. Cazabat, D. McNaughton and H. Reissler. The areas identified were electrochemistry, biophysics and computational chemistry-statistical mechanics. An election was held with two nominees for TMs in each category. A. Friedler, R. Guidelli and A. Wilson were elected. Unsuccessful candidates were nominated as Ams or NRs. The Division committee for the biennium 2010-2011 will be:

President: Jim McQuillan

Vice President: Kaoru Yamanouchi

Past President: Michel J. Rossi

Secretary: Roberto Marquardt

TMs: J. Dymond, A. Friedler, R. Guidelli, J.G. Hou, B.D. Sykes and A.K. Wilson.

AMs: V. Barone, K. Bartik, A.R. Goodwin, V. Miskovic-Stankovic, G.R. Moore and M. Rico. NRs (nominated by NAOs) : K. Bhattacharyya (India), S.J. Kim (Korea), V.Yu. Kukushkin (Russia), A.J. Mahmood (Bangladesh), O.V. Mamchenko (Ukraine), F.H. Quina (Brazil), A.W.M. Rodriguez (Uruguay), N. Soon (Malaysia), V. Tsakova (Bulgaria) and M. Witko (Poland).

#### **13. Representatives on other bodies.**

IUPAC committees:

Materials: M.J. Rossi and A. Wilson

ICTNS: J. Dymond

CCE: A. Friedler

Green Chemistry: J.G. Hou

COCI: J. Dymond

The secretary has informed these committees of our representatives.

Non-IUPAC bodies. The secretary reported that as R.A. Schoonheydt did not wish to continue as representative of IUPAC on IACS – the international Association of Catalysis Societies, she had contacted R. Prins of ETH Zurich. However the IUPAC secretariat had not yet asked for names.

Note: Oct 2009. The following have agreed to be IUPAC representatives on outside bodies as listed. Paul LeClair has been informed.

IACS – Prof Roel Prins – ETH

SUNAMCO – Prof Jeremy Frey

CCU, and ISO/TC 12 – Prof Ian Mills

#### **14. Off year meeting**

This will be held in the Spring of 2010 - probably in Zurich in early April. Roberto Marquardt will make arrangements.

#### **15. Advisory Subcommittee.**

This provides a pool of referees, but has proved less useful for obtaining new proposals or nominations. In order to get some turnover we need to retire about 20 people and replace with new nominees. Former TMs are added automatically.

The secretary undertook to provide a list of current members of the advisory committee with their areas of expertise and to circulate to TMs suggesting

(1) old TMs to suggest about 5 people to be retired,

(2) new TMs to suggest about 3 names to be added and to identify current members (of IUPAC or colleagues at large?) who would be useful.

Those suggested should NOT be contacted at this stage.

The policy for getting turnover needs to be reviewed in future.

#### **16. 46th General Assembly**

The 46th general assembly will be held at the end of July and beginning of August 2011 in Puerto Rico. Future meetings will be in Turkey (2013) and Seoul (2015).

It is hoped to have Division I participation in the program. Angela Wilson is on the Scientific Program Committee.

#### **17. Any Other business**

(a) Michel Rossi agreed to provide a short report on the Division Committee Meeting for Chemistry International.

(b) Concern was expressed about the current lack of divisional oversight of edited books published with projects funded by the division. It was agreed that in the future the task chairman would be informed at the time of the project announcement that completed chapters should be reviewed by people nominated by the division; the division should be kept informed about the choice of publishers and IUPAC should be credited. Bryan Henry had informed the officers that this was in line with IUPAC policy as noted in the Bratislava 2009 minutes.

(c) The President undertook to write to the IUPAC officers asking them to review general policy concerning electronic databases. While it is appropriate for task groups to provide critical evaluation of data, there is a need for the provision and maintenance of the web sites on which the data is mounted. Money may be available from bodies such as the US National Science Foundation to support this. There may also need to be a mechanism for the closing down of websites which are superseded and no longer used.

(d) The president thanked the retiring TMs - Christopher Brett (Past President) and Ruth Lynden-Bell (secretary).