IUPAC – Division 1 Committee

Minutes of the off-year meeting 2006

The 2006 Off year meeting was held at Coimbra, Portugal on 8-9April.

Present: Christopher Brett (President)
Ron Weir (Past President)
Michel J. Rossi (Vice President)
Ruth Lynden-Bell (Secretary)
Wolfgang Baumeister (TM)
Jim McQuillan (TM)
Zhong Qun Tian (TM)
John Dymond (AM)
Bryan Henry (IUPAC President)

1.Introduction, welcome and apologies.
Christopher Brett welcomed Bryan Henry and the committee members. Apologies had been received from the other members (TMs and AMs). He invited Bryan Henry to address the meeting.

Bryan Henry said that, as part of his IUPAC Vice President's Review carried out during the 2004-5 biennium, he had addressed the question as to how well the project system was going. Following meetings with most Divisions at their Off-Year Meetings and in Beijing he had found that the system was proceeding well, but that there was a lack of contact between IUPAC officers and divisions. For this reason, he had recommended that officers should visit about 1/3 of the off-year committee meetings.

2. Agenda
The agenda was approved without changes.

3. Minutes of Beijing Meeting
The proposal by Ron Weir, seconded by Ruth Lynden-Bell that these should be accepted was approved.

4. Review of Current Projects

(1) Cox – Database for Atmospheric Chemistry (Monitor Rossi). Transfer of the database to the web was almost complete and data sheets are being updated. It was planned to publish a snapshot (in portions) in 'Atmospheric Chemistry and Physics'. This part of the project is to be finished by the end of 2006.
The task force had agreed to continue for 1-2 years and to submit a new project in 2007.
Bryan Henry stated that IUPAC is committed to such databases and will set up an ad hoc committee to examine how they should be managed. This is a long-

standing problem that has been mentioned as early as 1999 when the ideas of a Web-based project regarding kinetic data emerged within the IUPAC subcommittee.

John Dymond remarked that the 'ThermoML' database had been adopted by 5 journals and that authors entered data when submitting papers. They then had free access to the database.
Michel Rossi remarked that there were problems in citing "old" data when it is eventually superseded by new, more accurate data.

(2) Stanbury - Standard Potentials of Radicals (Monitor Brett). The first technical report is in press and the project should be completed by December 2006.
(3) Stoynov - Electrochemical Impedance Spectroscopy (Monitor Brett) – A final draft of recommendations should be complete by summer 2006.
(4) Schwarz/Heinz - Isothermal Titration Calorimetry (Monitor Weir). No further information.
(5) Marsh - Thermodynamics of Ionic Liquids (Monitor Lynden-Bell). No further information.

.

(6) Harris-NMR Chemical Shifts (Monitor Lynden-Bell). A final draft of recommendations should be complete by June 2006.
(7) Seddon- Ionic Liquids Database (Monitor Lynden-Bell) – Good progress – Database was launched at the March ACS meeting.
(8) Ruscic-Thermodynamics of Free Radicals (Monitor Rossi) – Part I has eventually come out (JPC Ref Data **2005**, 34(2), 573-656) and Parts II and III are ready. The project is 75% complete and needs a 'no cost' extension and a meeting to give momentum. Set II (more exotic radicals) may be a new project.
(10) Corti – Supplemented Phase Diagrams (Monitor Prini – with Brett to liaise). Good progress, should be finished by the end of 2006.
(11) Ruzicka- Heat Capacity of Liquids-(Monitor Weir). A manuscript should go to ICTNS by September 2006.
(12) Arunan – Hydrogen Bond (Monitor McQuillan) - A workshop has been held in Italy – The project is going well.
(13) Tennyson- H_2O Spectral Line Database (Monitor Yamanouchi). (C. Brett to ask Yamanouchi).
(14) Majer – Thermodynamics of Hydration of Organics (Monitor Dymond).
(15) Letcher – Solubility (Monitor McQuillan) – satisfactory progress.
(16) Letcher –Solubility and Thermodynamic Properties Related to the Environment (Monitor McQuillan) – funding just confirmed.

Joint projects
There are joint projects with Divisions 3 and 5.
Contact persons for joint projects
Div 3. 1-2005-042-7-300 – Baumeister
other Div 3 projects – Tian
Div 5 - Brett

Projects near completion or in press
120/15/95 Bond energies - R. Weir to check status.
150/24/95 Spectroscopy under extreme conditions – C. Brett to check status.
2000-026-1-100 Vapour Liquid Critical Properties (John Dymond) Several publications have come out or are in press. The task force is still working on Miscellaneous and Inorganic publications.

Green Book (3rd Edition)
IUPAC has received an electronic version which has just finished the period of public review on 31st March 2006 and is with referees.
It is hoped that a final version should be ready by the end of May 2006, Index by July 2006 and the manuscript should be with the publishers by the end of September 2006.

Report from Commission 1.1
This report was tabled and discussed. It is attached to these minutes as an appendix.

Item 5. It was agreed that the Division should support a further meeting of the commission, but that the sum informally proposed was too large.
Items 7-10 The Commission should be encouraged to submit projects under these items (Web version; student version; 4th edition). Bryan Henry noted that ICSU has no money to support projects. Christopher Brett will speak to the Chairman of the commission (Jeremy Frey) to discuss these issues and to find out how he will deal will comments on the draft green book.

Project evaluation
Ron Weir explained that he chairs the new Project Evaluation Committee which has been asked to (a) provide criteria for retrospective evaluation of projects; (b) monitor for completion of original aims and (c) assess the impact of projects on the chemical community.
The committee has discussed (a) and has devised a simple form to be sent to project leaders when projects are completed.
It was noted that only small amounts of money are involved and most work is voluntary. Evaluation must not be onerous and must be kept in proportion to the effort. It was suggested that one should concentrate on evaluating what is relatively easy to assess (e.g. bibliometric measures under item (c)) .

5. Financial Report

Ruth Lynden-Bell reported that the budget for the 2006/7 biennium was USD 65,300 which was the same as the previous year. This can be split 25:75 between operations and projects. Brian Henry said that up to 30% can be spent on operations. So far USD 8,500 has been committed to 2 new projects and further projects are needed.

6. Future Strategy

Project proposals
A proposal was expected from Zhong Qun Tian and Jim McQuillan soon and would be circulated for unofficial comments.

Christopher Brett will e-mail the advisory committee seeking ideas for projects and areas where projects might be useful.

Bryan Henry remarked that some divisions establish a subcommittee for feasibility studies and use IUPAC sponsored conferences to generate proposals. Small workshops could be useful. He also said that in the next biennium (2008-9) the divisional reserve fund would be replaced by a strategic goals fund of about USD 120,000.

Christopher Brett agreed to liaise with chairmen of IUPAC-sponsored conferences linked to the PBCD to ensure that the IUPAC representative talks about projects and solicit ideas for project areas.

7. Biophysical Chemistry
Wolfgang Baumeister led a discussion of about the possible contribution that we might make. He pointed out that there were other national and international bodies in the biological field and that IUPAC is very weakly connected to the community. Good databases already exist.

In the discussion it was agreed that we did not wish to move into territory that is already well-covered, but that we should look for areas where there were openings for chemical input. Possibly an IUPAC sponsored session at a Biological symposium or conference would be useful.

Wolfgang Baumeister agreed to look out for further openings and to contact Albert Goldbeter and Clive Prestidge to explore this together.

8. Elections for the next biennium (2008/9)

The committee comprises up to 10 titular members (including officers), up to 6 associate members, and up to 6 national representatives.

The tenure of members is:

Overall maximum service of any member is 12 consecutive years

Officers: President – max 4 years
Vice President – max 4 years
Past President – 2 years
Secretary- 4 years (max 8 years)

TM – max 4 years consecutive
AM – 2+2 years
NR – 2+2 years

It was noted that Wolfgang Baumeister, Zhong-Qun Tian, Jeremy Frey and Ron Weir reach the end of their terms at the end of 2007.

The usual pattern of officers in this Division is 2 years as vice-president, 2 years as president and 2 years as past president, which has worked well, and it was agreed that this scheme should therefore continue.

Wolfgang Baumeister agreed to continue on the Committee as an AM in 2008-9, but Zhong-Qun Tian wishes to leave the committee at the end of his tenure as a TM. Jeremy Frey will be replaced by the new chairman of Commission I.1.

Jim McQuillan provisionally agreed to become the next vice-president.

Nominating Committee
This is the committee which prepares the slate of candidates. It was agreed that Ron Weir and Z. Tian would be the Division Committee TM representatives with Ron Weir in the chair. Suggestions for the three outside members were discussed.

9 Interdivisonal activity

Green Chemistry sub-committee. Chris Brett reported that this committee is organising the 1st IUPAC conference on Green and Sustainable Chemistry in Dresden on 10-15 September 2006.

CCE sub committee. Jim McQuillan reported that he had attended his first meeting during the Beijing GA. There will be an ICCE conference in August in Seoul where the draft code of practice for teaching in English drawn up by Chris Brett and Natalia Tarasova will be discussed.

In the discussion, Zhong-Qun Tian emphasised the importance of the WWW in the lives of modern students and it was suggested that IUPAC might have a role in approving e-learning lessons and web sites. However it is unclear where there is a role for IUPAC in addition to initiatives from other bodies.

Chemistry International It was agreed to try to contribute two short articles (750 or 350 words) to a series on 'the Tools of the Trade' on the Atmospheric Chemistry database (Michel Rossi) and the Ionic Liquids database (Seddon – Lynden-Bell to contact)

Chemistry Olympiad Bryan Henry will attend the next one (in Seoul, South Korea 2006). Tian commented that the material was too similar to first year undergraduate material which was a problem for ex-olympiad students at University.

10. General Assemblies – Torino 4-12 Aug 2007; Glasgow 2009.
Chris Brett will contact the organisers of the 2007 IUPAC congress in Torino to see whether they want any further input from the Division, apart from the names of division representatives that were already suggested.

11. AOB
Bryan Henry thanked the Division for hospitality and Chris Brett thanked Bryan for his useful input.

Elections Bryan Henry noted that the rules will be changed and should be much clearer. It was unclear whether the commission and advisory sub-committee should be included in the electorate. Chris Brett argued for flexibility and will write to David Black with his opinion.

Appendix

Report of Commission I.1 for IUPAC Division I April 7 & 8 2006

Jeremy G. Frey
School of Chemistry
University of Southampton

1. The Commission I.1 met in Beijing to discuss the Green Book and consolidate the amendments generated within the group and make editorial changes known to be needed at that point. The resulting draft edition of the Green Book was then reviewed by at least 3 IUPAC agreed referees who did a magnificent job in reviewing the document rapidly. Following this the draft was made available by IUPAC for public review. This period has just finished (31 March 2006) and we have a collection of corrections and suggestions. Typographic corrections have already been made and we have about 200 comments that the group will consider, via email during April. The final version will be completed in May, an index produced in July, and the document sent to the Publishers (The RSC).

2. Due to a misunderstanding the note sent out via IUPAC indicated that old fundamental constants and masses were in the GB, this was not the case, the most recent numbers were used in the draft. This did lead to some confusion, which has now been resolved.

3. Jurgen Stohner has done a major job in bringing together all these issues for the Green Book and I would like Div I to note that his time, a considerable amount of time, has been funded by Martin Quack, along with secretarial support. IUPAC funds were not available for this at the time the revision of the GB was started.

4. In Beijing we agreed the new members of commission I.1 and the details are now available on the IUPAC web site. We also have a plan for succession, which should take us smoothly through the next few years.

5. It would be ideal to have a final 3rd Ed Green Book meeting to draw together the experience and information generated so far and plan the future. This does not fit well with IUPAC project system and I would like to request limited funds from Div I (from for example the savings from the fact that I was not able to attend Beijing) to support such a final meeting. We then plan to request Project funding as detailed below, but to be finalised at the meeting. *Request for funds from Div I*

6. Possible Project 1: Publicity for the Green Book. Experience with the 2nd Ed indicated that there is a considerable market for the GB, in for example the USA, which was not exploited. We will clearly undertake any publicity effort in collaboration with the RSC and with their support. I plan to request funds to send

copies of the GB to book and journal editors, to high profile academics and industrial research leaders, and to ensure that the GB is highlighted at several international Chemistry Conferences.

7. Possible Project 2: A fully interactive Web version of the GB. Pdf versions of the GB will be made available by the RSC over a 6-12 month period. We would like a much more interactive and helpful version to be created. This would make use of the newer e-science aspects of computer representation of chemical information.

8. Possible Project 3: A reduced version of the GB suitable for undergraduate and possibly school students. We already plan to bring out a replacement for the 4 page laminated summary produced from the last edition. A more in depth discussion with the Analytical Division over the treatment of uncertainty is warranted and from this a useful introductory summary would be prepared.

9. Possible Project 4: We will wish to set in place procedures for collecting information for the next version of the GB to avoid the delays encountered this time. We will set a time horizon for the 4th edition and work backwards. Given the changes in IUPAC the consultative methods used to check GB issues in different chemistry areas will clearly be different now.

10. I have now made contact with IUPAP's equivalent committee SUNAMCO and hope to have interactions with them in the future. I hope that a joint IUPAC/IUPAP application for funding from ICSU will be possible to support GB like activities, and indeed increase the scope of them.

Other Areas of interest to Division I

1. I think that the whole area of the impact of computers and software on supporting laboratory science is one worth considering. It is crucial that information recorded in electronic laboratory notebooks (ELNs) meets standards if the aim of wider dissemination of the essential raw data is to be achieved. I believe IUPAC can play an important international role here.

2. IUPAC and Div I should take as active a role as possible in promoting exciting physical chemistry to ensure that the supply of interested students is at least maintained. We must make greater efforts to publicize our interesting work and engage the community. If we can think of community activities that involve physical chemistry it would be ideal to try and promote these. I am trying to fund a project to get the public to measure the pH of rainwater throughout the UK. They would use the mobile phone cameras to record the colour of the pH paper (and a calibration chart) and send this in to a central automated computer processing system, which would know the location of the measurement as this can

be provided from the mobile phone companies (once we have their agreement for this).

3. In my research group we are preparing a units ontology suitable for the Semantic Web (known as WWW2 in some areas) to help with unit translation. We hope to extend this to more chemical areas and more derived units soon.

Jeremy G. Frey, Chair IUPAC Commission I.1
School of Chemistry
University of Southampton
Southampton SO17 1BJ

Email j.g.frey@soton.ac.uk