

**Minutes of the Meeting of the Board of Directors
of the
International Association of Chemical Thermodynamics (IACT)**

Sesimbra Room, Hotel do Mar, Sesimbra, Portugal, 8th April 2005

13.30-16.15 h

Present at the meeting:

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| Chairman | J.P.-E. Grolier |
| Secretary | J.H. Dymond |
| Treasurer | A.R.H. Goodwin |
| Members | T. Atake U.K. Deiters T.W. De Loos T.M. Letcher K.N. Marsh M.A.V. Ribeiro da Silva |
| Counsellors | M. Frenkel W.A. Wakeham |
| By invitation: | J. Magee (NIST, USA) M. Thijssen (Elsevier) |

1. *Preliminary Matters and Announcements.*

The Chairman welcomed those present.

2. *Apologies.*

Apologies were received from R.D. Weir, N. Smirnova, E. Vogel, M.A. White, and H. Yan..

3. *Minutes of the Beijing Meetings, 2004.*

The Minutes of the Meetings held in Beijing, China on 16 August and 20 August 2004 were approved, and signed.

4. *Matters arising from the Beijing Minutes.*

A Report of the 2004 Beijing ICCT was published in *Chemistry International*, Vol. 27, 34-35 (2005).

5. *Treasurer's Report and Audit Preparation.*

The Treasurer presented his financial statement, which showed that, as at 25 March 2005, there was a balance of GBP 3708.51 in the interest bearing Abbey Bank account. The previously agreed change to just one signatory for this account had been implemented. In addition, IACT has USD 253.88 and GBP 20 in cash.

Problems with payment of membership subscriptions by wire transfer, or by USD cheque, into the Abbey account, which involved high costs, were discussed. The Treasurer reported that the only way to open a USD account was to register as a not-for-profit association. He was embarking on the process to do this.

IACT membership currently stands at 65, but membership numbers would increase at the Boulder Conference, with an estimated income of USD 8000.

It had been agreed to audit the accounts prior to the Boulder meeting, so that audited accounts could be presented at that time. The following IACT members were proposed for the Audit Committee: Ron Weir, Joe Magee, Cor Peters and Kazuya Saito, to be invited by the Secretary.

6. *IACT Website*

Ken Marsh reported that the website had been updated after the Conference in Beijing. The Minutes of the current meeting would be added. It was agreed to advertise post-doctoral positions, and also to list the names of those in the final year of their Ph.D. degree, with the title of their research and a link to their resumé. The Secretary will check with IUPAC to see if relevant recommendations can be placed on the website.

7. *Relations with Elsevier*

Michiel Thijssen welcomed closer contact with IACT, and confirmed that Elsevier would be pleased to sponsor the IACT Doctorate Awards by an annual donation of \$1000 for each of the next two years. He approved the decision to make two awards at the Conference in Russia this year, and asked to be informed of the names of the award winners. He agreed that, as requested by Board members, in future, the donation in one year could be held over till the following year. As a result, an increased number of awards can be given at the International Conferences on Chemical Thermodynamics.

Michiel said that Elsevier was very pleased with the high quality of Experimental Thermodynamics Volume VI, which was selling well. He was keen that Elsevier should continue to publish volumes in the experimental Thermodynamics series and invited suggestions for possible future titles. Trevor Letcher reported that he had 23 potential authors for a book on Solubility. Although members of the IUPAC Solubility Committee were involved, he was probably going to be the sole editor, but would check as to whether it would become an IUPAC or IACT volume. The Royal Society of Chemistry was an alternative publisher.

8. *Current Projects*

8.1 *Electrolyte Solution Data* (Co-ordinator: J. Barthel).

In a written report, Josef Barthel reported that Vol. XII, part 4a of their Electrolyte Data Collection, Electrolyte conductivities, ionic conductivities and dissociation constants of aqueous solutions of organic monobasic acids $\text{CH}_2\text{O}_2\text{-C}_7\text{H}_{14}\text{O}_3$ was published in 2004. Part 4b with monobasic acids higher than C8 will be sent to the publisher soon.

8.2 *Thermochemistry of Chemical Reactions: Nomenclature, Symbols and Experimental Methods for Bond Energies* (Co-ordinator: M. Ribeiro da Silva).

Manuel Ribeiro da Silva described the problems that had arisen with this manuscript since its approval by IUPAC Commission I.2 in 1999. First, Ian Mills had wanted a number of changes, which had been incorporated. The revised version was approved in 2000, and sent as a "Technical Report" to IUPAC in May 2001. IUPAC then said that it should be a "Recommendation", with 15 reviewers. Comments were sought in *Chemistry International* in May 2002, with a closing date of September 2002. Further changes were required, but in 2004, Manuel had been informed that the manuscript should be divided into two parts: Part 1 a "Recommendation" and Part 2 a "Technical Report". Manuel said that he proposed to complete the necessary changes by end-2005. The question arose as to whether Part 1 would have to go through the review process again.

Members were unanimous in voicing their disquiet with the decision of ICTNS (the Interdivisional Committee on Terminology, Nomenclature and Symbols) to change its recommendation on the way this work should be presented, with subsequent significant additional editorial work to be carried out by Manuel. They recommended that the Chairman should write to let John Lorimer, Chairman of ICTNS, know their feelings on this matter, and point out that such action would inevitably lead to a decision not to publish in IUPAC publications if this happened in future.

8.3 *Standards, Calibrations and Guidelines in Micro-Calorimetry* (Co-ordinator: G. Della Gatta).

The Secretary reported that there had been a problem to resolve over benzoic acid data, and additional changes to make before submitting this to PAC.

8.4 *Critical Compilation of Vapour-Liquid Critical Properties* (Co-ordinator: K.N. Marsh).

Ken Marsh reported on the final items in this project. The paper on organic compounds containing nitrogen, by Douglas Ambrose, Ken Marsh, David Morton, Costa Tsonopoulos and Colin Young had been circulated and comments received. The paper on organic compounds containing halogen(s), by the same authors required a bit more work before it was sent for review. Papers by Costa Tsonopoulos and Douglas Ambrose would cover multifunctional organic compounds, and miscellaneous compounds, for which data had been published since the earlier Items in this series. The final paper by Douglas Ambrose and John Dymond will cover inorganic compounds.

8.5 *Experimental Thermodynamics Volume VII. Measurement of the Thermodynamic Properties of Multiple Phases* (Editors: Th. de Loos and R.D. Weir)

Theo de Loos said that the 16 chapters had been sent to Elsevier. Publication was planned for end-2005.

8.6 *Thermodynamics of Ionic Liquids, Ionic Liquid Mixtures, and the Development of Standardized Systems* (Co-ordinator: K.N. Marsh).

Ken Marsh reported that samples of the fluids for investigation had been sent out to group members for measurements of the specified properties by end-July. One person per group was responsible for collating the results, and passing on the recommended values together with a note of the experimental technique. The project should be completed by July 2006, and a report presented in Boulder.

8.7 *Chemical Thermodynamics in Industry* (Co-ordinator: T.M. Letcher).

The book was published in 2004, by the Royal Society of Chemistry.

8.8 *Recommended Values of the Viscosity of Molten Iron and Aluminium* (Co-ordinator: W.A. Wakeham)

Bill Wakeham drew attention to the literature on this subject, in which measurements from all known sources were included in small graphs, with no indication of possible uncertainties. Some data sets differed by a factor of 4. They were aiming to give recommended values with an uncertainty of $\pm 10\%$ for aluminium, and a slightly lower uncertainty for iron. To this end, a round robin was being undertaken on iron, involving groups in the U.S.A., the UK and Japan. The results would be published in the *International Journal of Thermophysics*.

8.9 *XML-based IUPAC Standard for Experimental and Critically-Evaluated Thermodynamic Property Data Storage and Capture* (Co-ordinator: M. Frenkel)

Michael Frenkel reported that the project was close to completion. A Task Group meeting would be held after this Board meeting to produce a draft of final recommendations. This manuscript would be sent to Tony Davies, Secretary of the IUPAC Committee on Printed and Electronic Publications, who would send it to ML experts for comment, and subject it to the IUPAC process for Recommendations. A note would appear in *Chemistry International*, there would be a six-month period for comments, with publication in *Pure and Applied Chemistry* expected by end-2005.

8.10 *Ionic Liquids Database* (Co-ordinator: Ken Sneddon)

Ken Marsh reported that the pure liquid section was complete, and that work was proceeding on mixtures. It was the intention to launch the database by end-2005 at the latest (possibly by end-July). This will be freely accessible from TRC-NIST.

8.11 *Heat Capacity for Liquids : Critical Review and Recommended Values for Liquids with Data Published between 2000 and 2004* (Co-ordinator: Vlastimil Ruzicka)

John Dymond reported that this project had been approved by IUPAC. The other Task Group members were Eugene Domalski, Zdenka Kolská and Milan Zábanský. The search for additional collaborators had proved unsuccessful, but Milan Zábanský would be able to devote more time to the project.

8.12 *Establishing Recommended Data on Thermophysical Properties of Hydration for selected Organic Solutes.* (Co-ordinator Vladimir Majer)

John Dymond reported that this project, with a large Task Group under Vladimir Majer, had been approved by IUPAC

9. *New Project Proposals*

9.1 *Guidelines for Temperature Modulated DSC.*

Jean-Pierre Grolier confirmed that he would be submitting his proposal to IUPAC.

9.2 *Vapour Pressure for Compounds with Low Vapour Pressure*

The Secretary said that he would contact Cor Peters about the possibility of a project on this topic. Other likely Task Group members would be Roberto Fernandez-Prini, Josefa Fernandez and Vlastimil Ruzicka.

10. *2006 Rossini Lectureship Award*

Professor Alexandra Navrotsky has been elected as the Rossini Lecturer for 2006. The vote had been close, but it was noted that she also had more first place choices than the next candidate. Members asked for details of the ballot, and it was agreed that these would be circulated to Board members only, in strict confidence.

11. *RCCT-2005, and IACT Awards.*

A Committee of Ron Weir (Chairman), Ken Marsh and John Dymond had been set up to review the applications for the two RCCT-2005 IACT Doctorate awards. It was decided that, in future, these awards would only be made at ICCT's.

12. *ICCT's.*

12.1 *The 19th. ICCT, 16th. Symposium on Thermophysical Properties and Calorimetry Conference, Boulder Colorado, 30 July to 4 August 2006.*

Michael Frenkel reported on arrangements for this meeting, which would be held in conjunction with the 61st Calorimetry Conference, and the 16th Symposium on Thermophysical Properties. There would be four joint Symposia: Ionic Liquids; Molecular Modelling, including Simulation; Databases, Data Systems, Software Applications and Correlations: Thermodynamics and Properties in the Biological, Medical, Pharmaceutical, Agricultural, and Food Sectors. In addition, there would be a joint Workshop on Properties and Processes for a Hydrogen-Based Economy. They were in the process of identifying a speaker for the Keynote Address, Plenary and Invited Speakers, and Symposium Chairs. In discussion, a dead-line of end-June 2005 was agreed in order to submit the application for IUPAC sponsorship for this Conference. The International Advisory Board would consist of IACT Board members plus three calorimetry people. It was suggested that addition of other industrial chemists would be helpful for the IUPAC application. The Secretary agreed to liaise with the organisers in applying for IUPAC funding to support people from developing countries.

12.2 *The 20th-ICCT in Warsaw, Poland.*

As a result of a satisfactory response to the points which had been raised at the Board meeting on 20 August 2004, Jean-Pierre reported that he had written a letter on behalf of the Board to Stanislaw Randzio and Jacek Gregorowicz accepting their offer to host the Conference in Warsaw, at the Gromada Convention Hotel and Exhibition Centre. The proposed dates were 3-8 August, 2008.

12.3 *The 21st-ICCT.*

Tooru Atake presented his proposal to host the 2010-ICCT in Japan, referring to a well-produced brochure which set out the suitability of Tokyo as a venue. However, he said that, in his opinion, there were better sites (including Yokohama), and he would appreciate an early decision from the Board members to give him the maximum time to pursue these ideas. The Board agreed in principle to award ICCT-2010 to Japan. [Note added: As a result of further information provided by Tooru, the Chairman will send a formal letter of acceptance of Tooru's offer].

13. *2006 Election of Board Members.*

The Secretary noted that the following Members would be standing down in 2006: Theo de Loos, Trevor Letcher, Ken Marsh and Eckhard Vogel. They are all eligible for re-election. For continuity, it was agreed that the Secretary and the Treasurer should serve a second term (2006-2010). In order that all three officers should not stand down in the same year, it was agreed that the Chairman should continue to 2008.

14. *Sponsorship.*

Further sponsors are needed, at about the USD 1000 level, for example for the Rossini Lectureship. Jean-Pierre said that he would approach Setaram. Other possible companies include Schlumberger and Unilever.

13. *Dates of next meetings.*

A Meeting of the present Board will be held immediately before the ICCT in Boulder, end-July 2006, with a meeting of the new Board at the end of that Conference. A Business Meeting for all members will be arranged during the ICCT.