

**Minutes of the Meeting of the Board of Directors
of the
International Association of Chemical Thermodynamics (IACT)**
Chemistry Building, Campus des Cézeaux, Université Blaise Pascal, Aubière
Wednesday 30 May 2007 from 09.30 to 12.45 and 14.00 to 16.00

Present at the meeting:

Chairman	Prof. J.-P. E. Grolier
Secretary	Dr. J.H. Dymond
Members	Prof. T. Atake Prof. U.K. Deiters Prof. T.W. De Loos Prof. M. Frenkel Prof. T.M. Letcher Prof. M.A.V. Ribeiro da Silva
Counsellors	Prof. S. Randzio Prof. Li-Xian Sun

1. **Preliminary Matters and Announcements.**

The Chairman welcomed those present, especially Professors Stanislaw Randzio and Li-Xian Sun who had been appointed as Counsellors from 2006-2010 since the previous meeting, and who were attending their first Board meeting. He noted that Prof. Alexey Victorov from St. Petersburg, who had also been appointed as a Counsellor, was unfortunately unable to be present.

2. **Apologies.**

Apologies were received from Dr. A.R.H. Goodwin (Treasurer), Prof. A. Victorov, Prof. E. Vogel, Prof. W.A. Wakeham, Prof. M.A. White and Prof. R. Weir.

3. **Minutes of the Boulder, Colorado, Meetings, 2006.**

The Minutes of the Meetings held in Boulder CO, U.S.A. on 30 July and 4 August 2006 were approved, and signed.

4. **Matters arising from the Beijing Minutes.**

4.1 *Publicity*

Good publicity had resulted from having an IACT stand at ICCT 2006, where the IACT banner had been on display and A5-size flyers with information on IACT had been distributed. It was agreed to up-date the flyer and have copies available for the Thermodynamics 2007 Conference, which will be held at IFP, in Rueil-Malmaison, France from 26-28 September. **Action JD,**

AG

4.2 *IACT Logo*

It was agreed that the Secretary would circulate the IACT logo, which should be widely used on presentational material (power-point presentations etc.), on letterheads and notices on doors at meetings. The web address www.iactweb.org should also be advertised widely. **Action JD**

4.3 *Membership Cards*

It was agreed that the Secretary should send out IACT Membership cards electronically. **Action JD**

4.4 *Doctorate Awards*

In view of the small number of applicants for IACT Doctorate Awards for ICCT 2006, it was decided to send out details to everyone on the mailing list for ICCT 2008. **Action JD, SR**

5. **Secretary's Business**

5.1 *Arrangements for the 2008 elections to the Board*

Dr. Dymond noted that Professor Grolier will retire as Chairman in 2008, and become Past Chair in place of Prof. Weir. Dr. Goodwin will become Chair for the period 2008-2012. Dr. Dymond will continue as Secretary to 2010. A new Treasurer is required to take over from Dr. Goodwin (see Para. 6)

Elected members:

Prof. T. Atake	his first term ends in 2008 – eligible for a further 4-year term
Prof. U.K. Deiters	his second term ends in 2008 (6 years)
Prof. T.W. De Loos	appointed to 2010 [second term]
Dr. M. Frenkel	appointed to 2010 [first term]
Prof. T.M. Letcher	appointed to 2010 [second term]
Prof. M.A.V. Ribeiro da Silva	his second term ends in 2008 (6 years)
Prof E. Vogel	appointed to 2010 [second term]

Counsellors

Prof. S. Randzio	appointed to 2010 [first term]
Prof. Li-Xian Sun	appointed to 2010 [first term]
Prof. A. Victorov	appointed to 2010 [first term]
Prof. W.A. Wakeham	appointed to 2008 (6 years)
Prof. M.A. White	appointed to 2010 [second term]

6. **Treasurer's Report.**

The financial statement, which had been sent by the Treasurer, showed that, as at April 28th 2006, the Abbey bank balance stood at £3143.69. Since then, on the debit side, £794.07 was paid to the Keynote speaker at Thermo International 2006 on Sept 1st, and 4 sums were paid to the IACT Doctorate Award winners: on Sept. 4th two payments were made of £290.07; on 3rd Oct. there was one payment of £288.29 and on 24th Oct. there was a payment of £291.65. These were each for \$500, but vary according to the exchange rate. They include wire transfer charges.

On 24th April this year, the sum of £460.23 was paid to Prof. T. Letcher for attendance at the Seminar on European Energy policy, held by the European Association of Chemical and Molecular Sciences (see Item 15).

On the credit side, there was interest added £32.33, a payment of £31.95 (from 3 \$20 subscriptions) and a cheque from NIST of £4667.55 which is made up of \$1500 reimbursement for the payment to the Keynote Speaker, plus subscriptions from 400 participating IACT members.

The balance at April 28th 2007 is £5461.14. Our present commitments are sponsorship of two Conferences this year (see Item 14), which will cost from USD 950 to USD 1250. The total assets, including cash in hand, are £5840.64

USD 9000 which Prof. Frenkel had paid to the Plenary Lecturers at ICCT 2006 was very gratefully acknowledged.

Professor Theo de Loos was nominated as Treasurer by Prof. Michael Frenkel, to serve from now until 2010. He agreed to serve and his appointment was unanimously approved. The Secretary will arrange for transfer of all the documentation. **Action JD**

7. **Membership 2006-2008**

After Thermo International 2006, Prof. Frenkel provided the Secretary with a list of participants at the meetings of the 19th ICCT and the joint meetings with the 16th Symposium on Thermophysical Properties. This constitutes our membership list for the period 2006-2008.

8. **Life Membership**

It was agreed that there would be complications arising if an individual person was permitted to take out a Life Membership of IACT. Instead, it was decided that Life Membership would be bestowed as an honour in appreciation of life-long work.

9. **IACT Website**

Prof. Frenkel was thanked for arranging for the recent update of the website. He said that he would maintain the website for the foreseeable future, and that NIST would cover the necessary fee.

10. **Relations with Elsevier**

It was noted that Michiel Thijssen is no longer the contact person at Elsevier. Dr. Goodwin had discussions with Karel Nederveen who agreed that Elsevier would continue to sponsor the IACT Doctorate Awards, with a payment of USD 1000 for this year.

11. Current Projects

11.1 *Electrolyte Solution Data*

This is an on-going project with Prof. J. Barthel as editor. Part 5 with several volumes is in preparation. It will contain data of electrolytes in binary organic liquid mixtures of technical interest. The first volume should appear end 2007/2008.

11.2 *Thermochemistry of Chemical Reactions: Nomenclature, Symbols and Experimental Methods for Bond Energies*

Prof. Manuel Ribeiro da Silva plans to complete the final changes to the text in August 2007 for publication in two parts in *Pure and Applied Chemistry*. **Action MdaS**

11.3 *Vapour-Liquid Critical Properties*

Part 10. Organic Compounds containing Halogens. A draft manuscript on this extensive set of compounds has been sent out for final review, with submission to the Journal of Chemical and Engineering Data planned for next month.

Part 11. Multifunctional Organic Compounds, and Miscellaneous Compounds for which Data have been published since the earlier Items in this Series. Work on this is well advanced, with recent assistance from Alan Abramson, who has a very comprehensive collection of critical property data, and who was not previously involved.

The proposed Part 12, on Inorganic Compounds and Elements, has not progressed for some time as Douglas Ambrose, who was working on this, has been in poor health and has now decided that he cannot continue. Tables and references up to 1995 have been prepared, and Alan Abramson will be approached to see if he can assist in the completion of this Item.

11.4 *Ionic Liquids*

There have been many publications on the measurement of various properties of these liquids as part of this project, and a summary report will follow later. The database set up at NIST has the url ilthermo.boulder.nist.gov. Prof. Atake reported that a large Conference on Ionic Liquids would be held in Yokohama, Japan from 5-10 August 2007.

11.5 *Heat Capacities of Liquids: Critical Review and Recommended Values for Liquids with Data Published between 2000 and 2004*

Progress with this project has been a little slower than expected, but it is hoped to finish it by the end of 2007.

11.6 *Establishing Recommended Data on Thermodynamic Properties of Hydration for Selected Organic Solutes*

Roberto Fernandez-Prini and his group in Buenos Aires have produced a report on one part of the project, entitled "The $DG_2^{\infty}(T)$ for ambient temperature ($T < 333$ K) for binary systems of non-reactive gases dissolved in water".

Unfortunately, Vladimir Mayer who, since December 2006 has been the Representative of CNRS for Russia and the NIS, and will spend 2-4 years in Moscow, is unable to continue his scientific work. It is therefore necessary to find a successor for him as Project Leader. Vladimir could not suggest any possible candidates, but will contact other task group members to find the best way forward.

11.7 *Developments and Applications in Solubility*

Prof. Letcher was congratulated on the publication of this book by the Royal Society of Chemistry in February 2007.

11.8 *Thermodynamics, Solubility and Environmental Issues*

Prof. Letcher was congratulated on the publication of this book by Elsevier on 2 April 2007. It was noted that the IACT logo should appear on the cover of such books in future.

12. New Project Proposals

12.1 *Guidelines for Modulated-Temperature Differential Scanning Calorimetry*

This project has received IUPAC approval and will start immediately, though only USD 6000 had been granted instead of the USD 10,000 requested. It was hoped that the balance would be made available later. Prof. Grolier noted that Prof. Toda replaces Prof. Hata in the task group.

12.2 *Guidelines for Reporting of Phase Equilibria Measurements*

This proposal by Prof. de Loos was approved by the 14 Board members who had responded. It will be submitted to IUPAC with a note that it has the support of the IACT Board. It is proposed that publication will be in *Pure and Applied Chemistry*, with the intention to put it on a website.

Action JD

12.3 *Thermodynamic Study on Hydrogen Storage Materials*

Prof. Li-Xian Sun reported that many groups and large companies were active in the search for hydrogen storage materials with lighter mass, for which thermodynamic data were required. He was encouraged to discuss this further with Profs. J.-P. E. Grolier and S. Randzio, and for them to undertake a feasibility study.

Action L-X S/J-P G/SR

12.4 *XML-based IUPAC standard for Thermodynamic Property Data Capture and Storage*

Prof. Frenkel said that within two months he would produce a project proposal for the expansion of ThermML to include biomolecular materials.

MF

Action

12.5 *Volume on Green Chemistry Thermodynamics*

Prof. Grolier pointed out that the adjective “green” in this context referred to compounds coming from plants. There was a need for such a volume, which would cover mainly experimental aspects. He was encouraged to discuss this further with Prof. Letcher and to undertake a feasibility study.

Action J-P G/TL

12.6 *Heat Capacities*

Prof. Letcher reported that Prof. Wilhelm had suggested a project on heat capacities to produce two volumes, one on Theory and the second on Applications – to include food chemistry; solar cells; buildings; biochemistry; cement etc. They were encouraged to pursue this, bearing in mind the section on theory in the earlier project on critical compilation of heat capacities of liquids, and to undertake a feasibility study.

Action

TL/EW

12.7 *Future Energy*

Prof. Letcher reported that he would be editing a volume on Future Energy, to be published by Elsevier in the summer of 2008. Although not a book on Thermodynamics, the proposal will be sent round to Board members for comment.

Action TL/JD

12.8 *Vapour Pressure of Low-Volatility Compounds*

Prof. Deiters pointed out that much of the published data was incorrect, often by orders of magnitude. This was often as a result of impurities, but there were complications arising from phase transitions in the solid. Computational methods were now available. Prof. Frenkel offered to extract all such vapour pressure data, which have defined uncertainties, from his database. Profs. Ribeiro da Silva, Deiters and Frenkel agreed to undertake a feasibility study.

Action RdaS/UD/MF

12.9 *pH-sensitive Nanostructured Copolymer Gels*

This was referred back to Prof. Victorov for further information.

Action

JD

13. **ICCT's.**

13.1 *The 20th-ICCT in Warsaw, Poland, 3-8 August, 2008.*

Prof. Randzio reported on the arrangements for the 20th ICCT. Board members approved the list of plenary and invited lecturers. Formal letters of invitation will be sent out following this meeting, with replies expected within two to three weeks. An application will then be sent to IUPAC for sponsorship of this Conference. [It was noted that in three instances the speakers came from the same institute as one of the session organisers. Even when the recommendation came from the co-organiser, it was agreed that this situation should be avoided in future, as far as possible.]

Action SR/JD

The registration fee will be in the range 400 – 450 euro, with an expectation of 350 fully-paid registrants. This fee is inclusive of the Conference dinner, a Chopin Concert and a transport pass for the week. It was noted that there is a 22% tax on the registration fee. There will be a reduced fee for students. The organisers were seeking funds from the Government to assist people from developing countries. It was noted that, for the previous joint ICCT and Symposium on Thermophysical Properties, 25 persons had been given some financial support.

13.2 *The 21st-ICCT in Tsukuba, Japan, 1-6 August 2010.*

Prof. Atake announced that the conference would take place at Epochal, Tsukuba. The number of expected participants was 700-800. Accommodation would cost about USD 90 per person per night, with dormitory accommodation available about 10 minutes by bus from the Conference centre. The registration fee would be about USD 400. It was agreed that there should be a special session in honour of Profs. Seki and Suga.

13.3 *The 22nd-ICCT, 2012.*

Possible venues are Calgary, Alberta, Canada and Brazil, where Prof. Frenkel will make an informal approach, and Greece, where Dr. Dymond will contact Prof. Panayiotou. **Action MF/JD**

14. **Sponsorship and awards**

14.1 *RCCT 2007.*

IACT is sponsoring this Conference, which is being held in Suzdal, Russia from 1 - 6 July, 2007, by the award of a minimum of three, and a maximum of five, poster prizes. A selection committee was set up under the Past-Chair Prof. R. Weir as Chairman, the other members being Profs. Letcher and Randzio. They have ranked the 22 applications in order of merit as a guide to Prof. Victorov who will make the final decision at the Conference itself. **Action AV**

14.2 *Thermodynamics 2007.*

IACT offered to sponsor this conference, which is being held at IFP, in Rueil-Malmaison (near Paris), France, from 26 to 28 September 2007, by presenting poster prizes, paying for refreshments at a poster session, or making a cash donation. The organisers preferred the last of these, and it has been agreed that IACT will pay \$500 to the conference. In return:

- IACT will have its logo printed with the other sponsors' logos on the documents distributed to the participants on site.
- IACT will display a poster in the exhibition area, setting out the objective of the association and its activities.

14.3 *Rossini Lectureship Award 2008.*

The vote for this award had been in two stages. The first vote was undertaken to produce a short list of four candidates from the original 9 nominations. The second vote identified the top three candidates and ranked these in order. In what was an extremely close final vote, Prof. Jürgen Gmehling of the University of Oldenburg, Germany was the winner. He has agreed to present the 2008 Rossini lecture.

It was agreed that it should be made clear in future that self-nominations would not be accepted. Those who were pioneering new frontiers should not be nominated, but only those who have been active in such a way throughout their career.

15. **Report on EuCheMS Seminar and Workshop**

This Seminar and Workshop on "Europe's Energy Policy – the role of Chemistry" was held in the West Midlands European Centre in Brussels on 18 April 2007. It was attended by Prof. Letcher on behalf of IACT. The morning session consisted of presentations designed to stimulate thinking on the issues under consideration, and the afternoon was a Workshop, led by Richard Pike, to consider a) what delegates would like to see in 25 years time, b) what barriers there were to achieving this (political/economic; social/educational; technical; and resource), and c) ways of overcoming these different barriers. Key scientific fundamentals which were identified were a) measurement of key thermodynamic and kinetic properties of materials and b) better understanding (teaching) of electrochemistry. As a follow-up, the Royal Society of Chemistry will redraft the 6-page EuCheMS energy summary, and undertake a prioritisation exercise to highlight key policy messages.

16. **Any Other Business**

16.1 *Book out of print*

The volume *Equation of State for Fluids and Fluid Mixtures*, edited by Prof. J. Sengers and published in 2000, is out of print and the publishers Elsevier have indicated that sales in recent years do not justify a reprint. The matter has been drawn to the attention of the IUPAC Secretariat. Significant changes would be necessary to up-date this volume.

16.2 *European Federation of Chemical Engineering (EFCE)*.

This organisation has set up a working party on Thermodynamics and Transport Properties that is intending to organise a biennial conference. IACT, through Prof. Wakeham, is in correspondence with the EFCE President to seek collaboration with this organisation, with the possibility of sending an IACT observer to their meetings.

17. **Date of next Meeting**

There will be a meeting of the outgoing committee on the afternoon or evening of Sunday 3 August 2008 in Warsaw. After the election at the Business Meeting, there will be a meeting of the new Committee on the afternoon of Friday 8 August 2008 (provided the Conference ends at lunch-time on that day).

ADDENDA

Publications since the meeting in Boulder, 2006:

New Global Communication Process in Thermodynamics: Impact on Quality of Published Experimental Data. M.Frenkel, R.D. Chirico, V. Diky, C. Muzny, Q. Dong, K.N. Marsh, J.H. Dymond, W.A. Wakeham, S.E. Stein, E. Königsberger, A.R.H. Goodwin, J.W. Magee, M. Thijssen, W.M. Haynes, S. Watanasiri, M. Satyro, M. Schmidt, A.I. Johns and G.R. Hardin, J. Chem. Inf. Model., 46, 2487-2493, 2006.

Developments and Applications in Solubility, Ed. T. Letcher, The Royal Society of Chemistry, (2007) 414 pp.

Thermodynamics, Solubility and Environmental Issues, Ed. T. Letcher, Elsevier, (2007) 470 pp.

Chemistry International : Making an impact

XML-based IUPAC standard for experimental, predicted, and critically evaluated thermodynamic property data storage and capture (ThermoML), M. Frenkel et al, Chem. Int., Vol. 28, 22 (2006).
Letters in support of the ThermoML standard, M. Thijssen and J. Magee *ibid*.

Standards, calibration and guidelines in microcalorimetry. Part 2. Calibration standards for differential scanning calorimetry. G. Della Gatta, Chem. Int., Vol. 28, 27 (2006)

Chemistry International : The Project Place

Solubility and thermodynamic issues related to environmental issues, T.Letcher, Chem. Int., Vol. 28, 23 (2006)

Developments and applications in solubility, T.Letcher, Chem. Int., Vol. 29, 27 (2007)

Chemistry International : Conference Call

ThermoML: New IUPAC standard for thermodynamic data communications, M.Frenkel, Chem. Int., Vol. 28, 38 (2006).

The 19th International Conference on Chemical Thermodynamics, J.H. Dymond and M. Frenkel, Chem. Int., Vol. 29, 24 (2007).

Signed.....

Date.....

IACT Chairman

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