



International Association of Chemical Thermodynamics
IACT

Minutes of the Meeting of the Board of Directors

in the

Business Room of the Organising Committee, Hotel Gromada, Warsaw, Poland

Sunday August 3rd 2008 from 16.00 to 18.00

Present at the meeting:

Chairman	Prof. J.-P. E. Grolier
Past Chair	Prof. R.D. Weir
Secretary	Dr. J.H. Dymond
Treasurer	Prof. T.W. De Loos
Members	Prof. T. Atake Prof. U.K. Deiters Dr. A.R.H. Goodwin Prof. T.M. Letcher Prof. M.A.V. Ribeiro da Silva Prof. E. Vogel
Counsellors	Prof. S. Randzio

1. **Preliminary Matters, and any Announcements**

The Chairman welcomed those present.

2. **Apologies**

Apologies were received from Prof. M. Frenkel, Prof. Li-Xian Sun, Prof. A. Victorov, Prof. W.A. Wakeham and Professor Mary Anne White

3. **Minutes of the Clermont-Ferrand Meeting, 2007**

The Minutes of the Meeting held in Clermont-Ferrand, France on 30 May 2007 were approved and signed.

4. **Secretary's Business**

4.1 *IACT Publicity at 20th. ICCT*

Arrangements had been made to display the IACT banner and hand out up-dated A5-size flyers, with information on IACT, at a stand at this Conference. A rota was drawn up for Board members to man this stand during the coffee breaks.

4.2 *IACT Awards 2008*

The Rossini Lectureship: The 2008 Rossini Award winner is Prof. Jürgen Gmehling, University of Oldenburg, Germany. His certificate will be presented to him by Professor Grolier, just before his lecture on Wednesday at 9 a.m.

Junior Awards: There were 28 applications for the so-called Doctorate Awards this year. Now that Michiel Thijssen has moved on from his position in Elsevier, we have reverted to our

preferred name of “Junior Awards” this year. A committee was set up under Ron Weir to review these applications – other members were John Dymond and Trevor Letcher. They independently drew up a Merit List of 8 candidates in order, and by awarding 8 points for a first choice, 7 for second etc, scores were obtained for each candidate. The top 5 were granted awards. In alphabetical order, they are:

Dr. R.M. Bogel-Lukasik, Department of Chemistry, Universidade Nova de Lisboa, Portugal. (Polish).

Dr. L.M. Casás, Department of Applied Physics, University of Vigo, Spain (Spanish).

Mr. O. Elizalde-Solis, Thermodynamics Laboratory, Instituto Politécnico Nacional, México D.F. (Mexican).

Dr. F. Lovell, Department of Chemical Engineering, Imperial College, London, UK (Spanish).

Dr. A.F.L.O. M. Santos, Department of Chemistry, University of Porto, Portugal. (Portugese).

It is to be noted that they represent 4 different countries; there are three male and two female winners.

These certificates will be presented by Dr Goodwin during the Cocktail Party before the Concert of Chopin Music.

Note added: All certificates were signed by the Chairman and Secretary after this meeting. Prof. Randzio undertook to have them framed, at IACT’s expense.

4.3 *Arrangements for the IACT Business Meeting*

As per last time, slides had been prepared in PowerPoint for this meeting.

The following papers had been emailed to all IACT members:

- Agenda
- Minutes of the Boulder meeting
- Election notification
- Resumés of candidates
- Financial statement
- Project list 2008

4.4 *Arrangements for the Election to the Board*

It was agreed that voting for Directors should take place at the beginning of the meeting to allow time for the tellers (Prof. Weir and Prof. Ribeiro da Silva) to count the votes and declare the result before the end of the meeting. Voting slips would therefore be handed out at the door.

Dr. Dymond noted that Prof. Weir was retiring as Past-Chair. Prof. Grolier was retiring as Chairman, and will become Past-Chair for 2008-2012. Prof. Deiter and Prof. Ribeiro da Silva will retire, having served two terms, and Prof. Atake had come to the end of his first term. Prof. de Loos, having been appointed Treasurer in 2007 will continue to 2010.

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 Treasurer to 2010 (first term as officer)
Dr. J.H. Dymond	his second term ends in 2010
Dr. M. Frenkel	appointed to 2010 [first term]
Dr. A.R.H. Goodwin	becomes Chair 2008-2012
Prof. J.-P. E. Grolier	becomes Past-Chair 2008-2012
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]
Prof. R. Weir	retires in 2008

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]

As per the Constitution, a Nominating Committee had been set up, under the Chair-Elect. It produced a list of 5 nominees for the four vacancies: Prof. T. Atake (Japan), Prof. J. Boerio-Goates (U.S.A.), Prof. J.P.M. Trusler (UK), Prof. A. Victorov (Russia), Prof. W.A. Wakeham (UK). No additional names were submitted by members.

It was agreed that the unsuccessful candidate and the organiser of the successful bid for ICCT-2012 would be appointed as Counsellors. In order to encourage younger chemists to become involved in IACT, it was decided to invite Dr. Deresh Ramjugernath (South Africa), Prof. Josefa Fernández (Spain), Prof. Luis Galicia-Luna (Mexico), Dr. Rob Chirico (U.S.A.) and Professor Manuel Minas da Piedade (Portugal) along to the meeting of the new Board, immediately after this ICCT, as observers, with a view to their standing for election next time. Prof. Weir agreed to invite them.

5. Treasurer's Report

The Abbey bank balance at April 28th 2007 was GBP 5461.14, and the total assets, including cash in hand, was GBP 5840.64. In the following twelve months, a donation of GBP 490.05 was received from Elsevier, and there was bank interest of GBP 33.27. On the debit side, five poster prizes were made at the Russian Conference on Chemical Thermodynamics in 2007, at a total cost, including wire transfer charges, of GBP 508.94, and a donation of GBP 280.26 was made to Thermodynamics 2007. Our annual subscription to IUPAC was GBP 29.77. The balance at April 28th 2008 was GBP 5165.49. In addition, there is cash in hand of GBP 20.00 and USD 734.09. Dr. Goodwin moved the adoption of the accounts. This was seconded by Prof. Weir and unanimously approved.

It was noted that, since then, bank interest of GBP 146.15 and a single membership fee paid in international stamp vouchers which realised GBP 5.70 have been received, but there are the following outstanding expenses:

- i) 50% of the costs of travel and subsistence for the Rossini Lecturer. (It was recommended in the Report of the IACT Awards Committee in 2006 that IACT and ICCT share these costs.)
- ii) the cost of the 5 Junior awards, at USD 500 each plus the cost of wire transfers.
- iii) £23.80 for the photocopying of 400 flyers for IACT.
- iv) the cost of framing the certificates which were awarded at this Conference.

6. 20th ICCT, 2008, Warsaw, Poland

Professor Randzio reported that there were 325 people from 39 countries registered for the Conference. On-line registration had worked very smoothly, but there had been lots of correspondence from intending participants. Successive reminders to pay the registration fee had resulted in more payments. A number of abstracts had been received for which the authors had not paid the registration fee – these abstracts were not included in the Abstracts Book. Several authors asked to have their abstract in the Book, and were prepared to pay for this, though they were not intending to come to the Conference - this was not accepted.

There had been many problems over visas, especially from Russia, India, Algeria and Iraq, which required different details. However, only one person had been prevented from coming by not having a visa, and he had been too late in applying. The organisers had been unsuccessful in obtaining an official definition of a “developing country”, from whence participants might be charged a reduced fee. In the end, the organisers decided who qualified. There had been sponsorship to a total of 30,000 Zlotys.

Only one speaker, Prof. Wunderlich, had been unable to attend (by injury). His lecture would be presented by Prof. M. Pyda.

IUPAC Poster Prizes: IUPAC has offered 3 Poster Awards to this Conference. The winners will each receive a certificate and a personal copy of the Green Book. Normally the Conference organisers arrange the judges for these prizes but, on this occasion, the IACT Board agreed to take responsibility, with Prof. Weir, Prof. de Loos and Prof. Vogel acting as judges. Presentation of these prizes will be at the Closing Session of the Conference on Friday.

Prof. Randzio reported that there had been a number of financial problems:

- i) the Government had indicated, at the time the budget was drawn up, that they would pay up to 50% of the Conference costs. This was subsequently changed to zero support from Government. It was hoped to claim some money back from Universities.
- ii) each registration fee was subject to 22% VAT, but it was hoped that some of this could be claimed back as the Conference Centre included VAT in its charges.
- iii) prices for meals had increased by 100% since the budget was drawn up.
- iv) variation in exchange rates meant that income from registration fees was lower than expected.

As a result of these budgetary problems, it will be necessary to negotiate the standard payment to IACT of USD 20 per participant.

A vote of thanks was expressed to Prof. Randzio, and to his committee, for all they had done to lay the groundwork for a very successful Conference.

7. Update on Projects

7.1 *Project on Thermochemistry of Chemical Reactions* (M.A.V. Ribeiro da Silva)

Two manuscripts are at present being checked by members of the Physical and Bio-physical Chemistry Division Committee for consistency with the Green Book. A recommendation will then be submitted on behalf of Division I as to the suitability for external review by 15 reviewers.

Professor Ribeiro da Silva drew Members' attention to the IUPAC website which announced, unknown to him, that these manuscripts would be subject to yet another round of reviews. Members expressed their concern at the unacceptably long delays from the IUPAC publication process for these manuscripts.

7.2 *Project on Guidelines for Modulated-Temperature Differential Scanning Calorimetry* (J.-P.E. Grolier)

The Project progresses well. At this ICCT in Warsaw, there will be a Workshop "Modulated and Oscillation Temperature Techniques" (MOTT) dedicated to the Project. Two Invited Lectures will be given by Task Group members (B. Wunderlich, Ch. Schick). The objectives of the project are clearly defined and writing up of guidelines and directives will not be a problem.

A Task Group meeting during the Conference will discuss whether recommendations should be published by scientific journals in the field and/or in a monograph. This might depend on whether the guidelines are restricted to just Differential Scanning Calorimetry (DSC) or extended to any other types of calorimetry/thermal methods where temperature modulation or temperature oscillation are nowadays becoming current practice. The same consideration stands for multifrequency (in fact high frequency) methods applied to thermal techniques.

7.3 *Electrolyte Solution Data* (J. Barthel)

Dr. Dymond reported that Prof. Barthel was working on Part 5 in the Electrolyte Data Collection on Electrolyte Solutions in Mixed Solvents for Applied Research (Part 5a: HEBs).

7.4 *Vapour-Liquid Critical Properties* (K.N. Marsh)

The manuscript for Part 11 on Multifunctional Organic Compounds is ready for submission to J. Chem. Eng. Data. Part 12 will be an up-date of earlier papers. Part 13 on Inorganics has been partly completed by Douglas Ambrose, who has now withdrawn from the Project. Prof. Marsh and Dr. Dymond plan to complete this Item.

7.5 *Ionic Liquids* (K.N. Marsh)

Two draft reports have been prepared. Part 1 has been sent to NIST and has to go through BERB review. Part 2 has been through the NIST BERB review. They will be submitted to Pure and Applied Chemistry. This will complete Project 2002-005-1-100.

7.6 *Heat Capacities of Liquids: Critical Review and Recommended Values for liquids with Data Published between 2000 and 2004* (V. Ruzicka)

Dr. Dymond reported that Project 2004-010-3-100 had been completed with the preparation of a manuscript to be submitted to Dr. Don Burgess, editor of J Phys Chem Ref Data. It would then go for external review. Ron Weir will provide the names of some possible reviewers.

7.7 *Establishing Recommended Data on Thermodynamic Properties of Hydration for Selected Organic Solutes* (V. Majer)

This project has come to an early end as Prof. Majer had moved to a position in Moscow and had no time to take care of the Project. Unfortunately he has been unable to find anybody to take over the lead. A report which was produced by Roberto Fernandez-Prini and his team is due to be published in the Journal of Solution Chemistry this coming October.

7.8 *Guidelines for Reporting of Phase Equilibria Measurements* (T.W. de Loos)

Discussions are taking place on specific points prior to producing a list of recommendations.

7.9 *Future Energy: Improved, Sustainable and Clean Options for our Planet* (T.M. Letcher)

This book will be published by Elsevier on 4 August 2008.

7.10 *Experimental Thermodynamics: Applied Thermodynamics of Fluids* (A.R.H. Goodwin)

This text, which includes 14 chapters, is compiled by an editorial team of A. R. H. Goodwin, J. V. Sengers and C. J. Peters. It will be the eighth in the series *Experimental Thermodynamics* and, published under the auspices of IUPAC (Project Number Project number 2008-014-1-100), by the Royal Society of Chemistry in December 2009.

The intent of *Applied Thermodynamics of Fluids* is to revise and at the same time update *Experimental Thermodynamics, Volume V, Equations of State for Fluids and Fluid Mixtures, Parts I and II*, albeit with a change in emphasis to the application of theory, without recourse to derivations of the constitutive equations, while retaining the fundamental aspects. It will also include topics omitted previously such as *nano* and *meso* scale thermodynamics, associating fluid theory, chemically reacting systems and non-equilibrium thermodynamics. The new volume is intended to address the needs of practitioners within academia, government and industry.

7.11 *Heat Capacities of Liquids, Solutions and Vapours* (T.M. Letcher)

The project is on-going and the book, with 21 chapters, is scheduled to be published by the Royal Society of Chemistry in the latter half of 2009.

7.12 *Extension of ThermoML – the IUPAC Standard for Thermodynamic Data Communications* (M. Frenkel)

The proposal has been discussed on a preliminary basis in August 2006 during Thermo International 2006 in Boulder, Colorado, USA. It was submitted for IACT review in August 2007, and obtained the endorsement from the Board in September, 2007. It was submitted to the IUPAC (Committee on Printed and Electronic Publications) in October, 2007. It has been officially approved by the IUPAC in January, 2008. Subsequently, the Team was organized into 3 subteams (General Review and Implementation Team, Biothermodynamics Team and Speciation

Team). The first meeting of the Team will be held in Warsaw, Poland during ICCT-2008. It is planned to complete the first phase of the project in 2009 (Biothermodynamics), the second one ("Speciation issues") in 2010, and third phase (Recommendations and Report) in 2011.

7.13 *Thermodynamic Study on Hydrogen Storage Materials: Metal Organic Frameworks and Metal or Complex Hydrides* (Li-Xian Sun)

This proposal was approved by the IACT Board in December 2007 and submitted to IUPAC in January 2008. The nine reviews were generally very favourable, but helpful suggestions had been made. These were discussed by Prof. Sun, Prof. Grolier and Prof. Frenkel in Dalian in May, 2008, and a final revision of the proposal would be made at a meeting of Task Group members during this Conference (ICCT-2008).

In the meantime, new metal organic frameworks and nano metal complex hydrides have been synthesized and the corresponding hydrogen storage performance and thermodynamic characteristics measured. Some results were reported at the CATS2008 in Dalian, China.

8. **Membership 2008-2010**

All participants at the 20th ICCT would be IACT members for 2008-2010. It was agreed that Dr. Goodwin would ask Prof. Frenkel if he could produce e-cards for members.

9. **IACT Website**

The website will be up-dated when the draft Minutes of the two Board meetings and the Business Meeting have been prepared. The list of Board Members, completed projects and the publication list will also be brought up to date. **ACTION: JD**

10. **Publications 2006-2008**

A publication list is appended to these Minutes.

11. **Relationship with EFCE**

There was concern that the European Federation of Chemical Engineers was planning to set up a group to discuss Thermodynamics and Transport Properties, without reference to IACT or to the International Association on Transport Properties. Their key projects were i) a survey of how Thermodynamics is taught to Chemical Engineers in Europe, and ii) a survey of the needs of chemical industry for data. It was agreed that we should seek to collaborate with them.

12. **Possible New Projects**

12.1 *Volume on Green Chemistry Thermodynamics*

Prof. Grolier commented that "clean-safe" would be a better description than "green", but said that this was a longer-term project. He suggested that a volume should be written on "Plant and food processing. **Action J-P G**

12.2 *Vapour Pressure of Low-Volatility Compounds*

There had been no progress towards consideration of the feasibility of a project on this topic.

Action RdaS/UD/MF

12.3 *pH-sensitive Nanostructured Copolymer Gels*

This topic is withdrawn for now.

13. **Next Meeting**

There will be meeting of the new Board on Friday, August 8th 2008.

IACT Publications 2006-2008

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. Mode.* 46, 2487-2493 (2006).

Vapour-Liquid Critical Properties of Elements and Compounds. 10. Organic Compounds containing Halogens, K.N. Marsh, A. Abramson, D. Ambrose, D.W. Morton, E. Nitikin, C. Tsonopoulos and C.L. Young, *J. Chem. Eng. Data* 52 1509-1538, 2007.

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

ILThermo: A Free-Access Web Database for Thermodynamic Properties of Ionic Liquids, Q. Dong, C. Muzny, Andrei Kazakov, Vladimir Diky, Joseph Magee, Jason Widegren, Rob Chirico, Kenneth Marsh, Michael Frenkel, *J. Chem. Eng. Data*, 52, 1151-1159 (2007).

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

Ionic liquids database, K.R. Seddon, A.N. Burgess, M. Frenkel, M. Gaune-Escard, A. Heintz, J.W. Magee, K. N. Marsh and R. Sheldon, (ILThermo), <http://ilthermo.boulder.nist.gov>

Papers based on presentations at the 19th IUPAC Conference on Chemical Thermo-dynamics (ICCT-19), 30 July to 4 August 2006, Boulder CO, USA. Ed. J.H. Dymond, *Pure Appl. Chem.* 79, 1345-1462, (2007).

Articles in Chemistry International

Alexandra Navrotsky awarded the 2006 Rossini Lecture, *Chem. Int.* 28, No. 2, 17-18 (2006).

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, No. 3, 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, No. 6, 27 (2006)

ThermoML: New IUPAC standard for thermodynamic data communications, M.Frenkel, *Chem. Int.*, Vol. 28, No. 5, 38 (2006).

Solubility and thermodynamics related to environmental issues, T.Letcher, *Chem. Int.*, Vol. 28, No. 5, 23 (2006)

The 19th Int. Conference on Chemical Thermodynamics, J.H. Dymond and M. Frenkel, *Chem. Int.* 29, No. 2, 24-26 (2007).

Developments and Applications in Solubility, Ed. T. Letcher, The Royal Society of Chemistry, *Chem. Int.* 29, No. 3, 27 (2007).

Jürgen Gmehling awarded the 2008 Rossini Lecture, *Chem. Int.* 29, No. 5, 17-18 (2007).

Guidelines for Modulated-Temperature Differential Scanning Calorimetry, *Chem. Int.* 29, No. 5, 20-21, (2007).

Chemical Thermodynamics, 3-8 August 2008, Warsaw, Poland, *Chem. Int.* 29, No. 5, 31 (2007).

Manuscripts in course of publication:

Thermodynamic and thermophysical properties (including mixtures) of the reference ionic liquid: 1-hexyl-3-methylimidazolium bis[(trifluoromethyl)sulfonyl]amide – Part 1. Experimental methods and results. *Prepared for publication in PAC* by Kenneth N. Marsh, Joan F. Brennecke, Michael Frenkel, Andreas Heintz, Joseph W. Magee, Cor J. Peters, Luis Paulo N. Rebelo, Kenneth R. Seddon.

Thermodynamic and thermophysical properties (including mixtures) of the reference ionic liquid: 1-hexyl-3-methylimidazolium bis[(trifluoromethyl)sulfonyl]amide. Part 2. Critical evaluation and recommended property values. (IUPAC Technical Report 200x), *Prepared for publication in PAC* by Robert D. Chirico, Vladimir Diky, Joseph W. Magee, Michael Frenkel, Kenneth N. Marsh.

Thermochemistry of Chemical Reactions: 1 Terminology and Symbols (IUPAC Recommendations 2008). *Prepared for publication in PAC* by Manuel A. V. Ribeiro da Silva.

Thermochemistry of Chemical Reactions: II. Experimental Methods for the Determination of Bond Energies (IUPAC Technical Report 200x). *Prepared for publication in PAC* by: Manuel A. V. Ribeiro da Silva.