

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

Chautauqua Meadow Conference Centre, Boulder Outlook Hotel, Boulder, Colorado, USA

on 4 August 2006 from 13.00-15.00 h

Present at the meeting:

Chairman	Prof. J.-P. E. Grolier
Secretary	Dr. J.H. Dymond
Treasurer	Dr. A.R.H. Goodwin
Members	Prof. T. Atake Prof. T.W. De Loos Dr. M. Frenkel Prof. M.A.V. Ribeiro da Silva Prof. E. Vogel
Counsellors	Prof. W.A. Wakeham

1. *Preliminary Matters and Announcements.*

The Chairman welcomed those present.

2. *Apologies.*

Apologies were received from Prof. U.K. Deiters, Prof. T.M. Letcher, Prof. R.D. Weir, Prof. M.A. White and Prof. H. Yan.

3. *Secretary's Business.*

3.1 *Election of Chair-Elect*

The Secretary reported that he had received just one nomination, that of Dr. A.R.H. Goodwin, for Chair-Elect. This nomination was unanimously approved by Board members.

3.2 *Appointment of Treasurer*

The appointment of the Treasurer to Chair-Elect leaves a vacancy as Treasurer. There were no offers from the Directors present to take on this role, and the Secretary will contact the other Directors.

3.3 *Appointment of Counsellors*

It was noted that the following have reached the end of their 4-year term: Prof. Mary Anne White (Halifax, Canada), Prof. Natalia Smirnova (St. Petersburg, Russia), and Prof. Hai-Ke Yan (Beijing, China). Prof. White was re-appointed for 2006-2010. Prof. Smirnova had indicated her willingness to step down to make way for a younger person, and Prof. Alexey Victorov (St. Petersburg, Russia) was proposed in her place. Other names which were considered were Prof. Weiguo Shen (Lanzhou University, PR China) and Prof. Jingtao Wu (Xi'an Jiaotong University, PR China), Prof. Martin Trusler (Imperial College, London, UK) and Prof. David Remeta (Rutgers University, USA). No decision was made, and it was agreed that the Secretary should write to all elected Board members to seek their views.

4. *Treasurer's Report*

The Treasurer pointed out that there would be additional expenditure from the ICCT in regard to the awards, with \$ 2000 for the Doctorate Award winners still to be paid. In addition, there would be around \$ 500 as the shared costs (with ICCT) for the Rossini Lecturer. He thanked NIST for waiving the registration fee for the Doctorate Award winners, and for making payment to the Plenary Lecturers.

5. *ICCTs*

5.1 *ICCT 2006*

Professor Grolier congratulated Dr. Frenkel, and the other organisers for the excellent organisation, which had led to the success of ThermoInternational 2006. Great care had been taken to group together talks on similar themes in the same venue to minimise the need to change venues.

Some reservations were expressed about the content and delivery of this year's Rossini Lecture. It was agreed that the selection process in future should include written comments from each Director as to the ability of each nominee to give a good, exciting lecture and to determine how widely they were known.

It had been reported that the Gordon Research Conference on Water and Aqueous Solutions had been held at exactly the same time as ICCT-2006. In order to avoid possible overlap with other conferences in future, early advertising of the ICCTs is recommended.

## 5.2 ICCT 2008

At the Closing Ceremony of ThermoInternational 2006, Professor Grolier had used a CD prepared by the organisers of ICCT-2008 to illustrate the Conference facilities, and accommodation for this meeting in Warsaw, which will be held from August 3 to 8, 2008.

## 5.3 ICCT 2010

Professor Atake said that he was actively seeking financial support for this meeting, which would be held in Tsukuba, Japan from August 1 to 6, 2010. Details of the venue, Tsukuba Congress Centre, can be found from the website: <http://www.epochal.or.jp/english/index.html>

## 5.4 ICCT 2012

Professor Grolier asked members to consider possible venues for this Conference. In line with the pattern of recent meetings, we might think in terms of North or South America, but applications from other countries would be very welcome, especially if no ICCT had been previously held there.

## 6. IACT Business Meeting

The Business Meeting was deemed to have been successful. There had been 43 attendees. Profs. Theo W. de Loos, T.M. Letcher and E. Vogel had been re-elected as Directors for a further 4-year period, and Dr. M. Frenkel had been appointed for 2006-2010.

## 7. IACT Projects

### 7.1 Electrolyte Solution Data

This is an on-going project with Prof. J. Barthel as editor. The latest publication was in the DECHEMA Data Series, Volume XII, Part 4b: Electrolyte Conductivities, Ionic Conductivities and Dissociation Constants of Aqueous Solutions of Organic Monobasic Acids 2005, ISBN 3-89746-067-X, 523 pages

### 7.2 Project on Thermochemistry of Chemical Reactions

Prof. Ribeiro da Silva reported that he had sent his revised manuscript to Prof. J. Lorimer in June of this year.

### 7.3 Standards, Calibration and Guidelines in Micro-Calorimetry

This project was completed with the publication : Della Gatta, G., M.J. Richardson, S.M. Sarge and S. Stølen, Temperature scanning (micro)calorimetry. *Pure Appl. Chem.* **78**, No. 7, 1455-1476, 2006. Publication in the Journal of Chemical Thermodynamics is being negotiated with possible publication in *Thermochimica Acta* and the Journal of Chemical Analysis and Calorimetry. Alternatively, a one-page description with reference to the on-line version of the IUPAC recommendations will be considered.

### 7.4 Vapour-Liquid Critical Properties

This project is nearing completion, with Part 9 recently published: Vapour-liquid critical properties of elements and compounds. Part 9. Organic compounds containing nitrogen, K.N. Marsh, C.L. Young, D.W. Morton, D. Ambrose, C. Tsonopoulos, *J. Chem. Eng. Data*, **51**, 305-314, 2006. The next part, on organic compounds containing halogen, should be ready for publication later this year. That will leave a publication covering multifunctional organic compounds, and miscellaneous compounds for which data had been published since the earlier Items in this series. There will also be a part on inorganic compounds and elements.

### 7.5 Experimental Thermodynamics. Vol. VII. Measurement of the Properties of Multiple Phases

This volume, edited by Profs. Th. de Loos and R.D. Weir, was published by Elsevier in 2005.

## 7.6 Ionic Liquids

A report on this project, which was presented at ICCT-2006 by Professor Marsh, described the steps taken to establish reference quality data for ionic liquids and ionic liquid mixtures. Reliable handling techniques and operating procedures had been devised. The compound 1-hexyl-3-methylimidazolium bistriflate amide had been selected as reference material, and a stock prepared with known water content. This had been circulated to all participants in the project. The properties measured included heat capacity, viscosity, density, thermal conductivity, electrical conductivity, speed of sound, relative permittivity, TGA (in nitrogen and air), DSC and melting point. Mixture properties included gas solubility, LLE, VLE, infinite dilution activity coefficients, enthalpy of dilution, speed of sound, density and excess volumes. A summary was given of the measurements made.

## 7.7 Ionic Liquids Database

This project was completed with the first public release of the IUPAC Ionic Liquids Database (IL Thermo) liquids, which took place during the Ionic Liquids session of ICCT-2006. This database contains numerical data and metadata, including their synthesis, structure, properties and uses, for 206 ions and 315 ionic liquids. The experimental data include that for phase transitions, transport, volumetric and thermal properties as well as electrical conductivity, refractive index, speed of sound, vapour pressure, and activity coefficients. At present, there are 17958 data points. The database, which is available at <http://ilthermo.boulder.nist.gov/ILThermo/mainmenu.uix>, is freely accessible, and will be regularly up-dated by authors providing their data to the Thermodynamics Research Centre at the National Institute of Standards and Technology in Boulder CO, USA in the form of files prepared using the TRC Guided Data Capture software.

## 7.8 Viscosity of Molten Iron and Aluminium

The project was completed with the publication:

Recommended values for the viscosity of molten iron and aluminium. M.J. Assael, K. Kakosimos, R.M. Banish, J. Brillo and I. Egry, R. Brooks, P.N. Quedstedt, K.C. Mills, A. Nagashima, Y. Sato, and W.A. Wakeham, *J. Phys. Chem. Ref. Data* **35**, 285-300, 2006.

## 7.9 XML-based IUPAC Standard for Thermodynamic Property Data Capture and Storage

The project was completed with the adoption by IUPAC of ThermoML as an IUPAC Standard for thermodynamic property data storage and capture. This was fully described in the publication:

XML-based IUPAC standard for experimental, predicted, and critically evaluated thermodynamic property data storage and capture (ThermoML), M. Frenkel, K.N. Marsh, W.A. Wakeham, J.H. Dymond, S.E. Stein and E. Koenigsberger, *Pure Appl. Chemistry*, **78**, No. 3, pp. 541–612, 2006.

ThermoML will continue to have a positive impact on data activities, including scientific publishing, where it is already used by 5 major journals. This is described in a forthcoming publication:

New global communication process in thermodynamics: impact on quality of published experimental data, M. Frenkel, R. D. Chirico, 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, in *J. Chem. Information and Modeling*.

## 7.10 Heat Capacities of Liquids: Critical Review and Recommended Values for liquids with Data Published between 2000 and 2004 [V. Ruzicka]

A written report from Prof. Ruzicka noted that the literature for this period had been fully reviewed and all correlations and assessments were completed. It was expected that the manuscript would be ready by September this year for sending to ICTNS (Interdivisional Committee on Terminology, Nomenclature and Symbols).

## 7.11 Establishing Recommended Data on Thermodynamic Properties of Hydration for Selected Organic Solutes

The Secretary reported that Dr. Majer had visited all the participating groups in 2005 to establish the roles that each would take in this project. As a first step, it had been agreed that they would consider 30 solutes, selected to represent different groups of organic compound for which there were extensive sets of reliable hydration data. A workshop had been held as part of ICCT-2006, consisting of one invited lecture (Majer), 5 oral communications (Chirico-Boulder, Dohnal-Prague, Sedlbauer-Liberec, Fernandez-Prini-B.A., Costa Gomes- Clermont), 3 posters and a panel discussion.

## 7.12 Developments and Applications in Solubility

Proofs were being sent to Prof. Letcher to await his return, and publication was expected later this year.

### 7.13 *Solubility and Thermodynamic Properties Related to Environmental Issues*

Prof. Letcher expected manuscripts for this volume to be with him by September this year, with publication of this volume by Elsevier next year.

## 8. *New Project Proposals*

### 8.1 *Guidelines for Temperature Modulated DSC.*

Jean-Pierre Grolier presented a revised proposal, which was approved by the Directors for submission to IUPAC "with the approval of the Board of Directors of IACT".

### 8.2 *Recommendations for Literature Communication on Phase Equilibria*

Prof. de Loos (editor of Fluid Phase Equilibria), Prof. K. N. Marsh (editor of the Journal of Chemical and Engineering Data), and Prof. M. Trusler (editor of the Journal of Chemical Thermodynamics) all had concerns about the shortcomings in the literature on reported phase equilibria measurements. This was shared by Dr. R. Chirico (NIST, expert in interpreting VLE data files) and Drs. S. Gupta and Dr. J. Olson (Dow, industry experts). Lack of crucial information has frequently reduced the value of such published work. There was clearly a need to offer guidance in reporting sample purity, the experimental technique used, the validation process and the estimation of uncertainties so that the reader had sufficient information to judge the quality of the data. Calculation of additional properties would be demonstrated and the use of modelling, and thermodynamic relationships between different properties, in data quality evaluation described.

It was agreed that this was a worthwhile project. Prof. de Loos was invited to complete an IUPAC project proposal form and send it to the Secretary, who would forward copies to Board members for comment.

### 8.3 *Data Capture and Storage in Biothermodynamics*

Dr. Frenkel said that he was considering the extension of the ThermoML schema to Biothermodynamics.

### 8.4 *Experimental Thermodynamics VIII*

Dr. Goodwin reported that Michiel Thijssen from Elsevier had suggested that IACT should consider producing a volume on the thermodynamic aspects of Green Chemistry. There was discussion as to whether this related to natural products or to green solvents. However, it was agreed that there was no new thermodynamics involved with such materials, and the idea was rejected.

### 8.5 *Clean Energy*

Prof. Wakeham suggested that IACT should consider a project, which carefully analysed the many current proposals for alternative forms of energy, some of which were driven by political arguments whereas in fact they did not make sense thermodynamically. It was agreed to discuss this further and bring it up at the next meeting.

### 8.6 *Thermodynamic Properties (Heat Capacities) of Polymers*

It was reported that Dr. M. Pyda, recently the Director of the ATHAS Laboratory, University of Tennessee at Knoxville had a large database on heat capacities of polymers, which required conversion from its current format to become more accessible. The possibility of helping him in this work will be examined.

### 8.7 *Education of the Third World in the Use of Energy*

It was suggested that this topic might be considered.

## 9. *Date of next meeting.*

The next Meeting of the present Board will be held in 2007. The proposed venue is Clermont-Ferrand, France on May 30-31.