

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

Institute of Chemistry, Beijing, 16 August 2004

10.20-14.45h

Present at the meeting:

Chairman	J.P.-E. Grolier
Secretary	J.H. Dymond
Members	T.W. De Loos T.M. Letcher K.N. Marsh M. Sorai
Counsellors	M. Frenkel N. Smirnova M.A. White H. Yan
By invitation:	R.D. Chirico (NIST, USA) W.M. Haynes (NIST, USA) M. Thijssen (Elsevier)

1. *Preliminary Matters and Announcements.*

The Chairman welcomed those present.

2. *Apologies.*

Apologies were received from Ron Weir, Manuel Ribeiro da Silva, Ulrich Deiters, Eckhard Vogel, Tony Goodwin and Bill Wakeham.

3. *Minutes of the Boulder Meeting, 2003.*

The Minutes of the Meeting held in Boulder, Colorado, USA on 22 June, 2003 were approved, and signed.

4. *Minutes of the Boulder Meeting, 2003.*

The Minutes of the Special Meeting held in the Athenaeum Club, London, UK on 1 October 2003 were approved, and signed.

5. *Matters arising.*

22 June Meeting:

5.1 *The Status of IACT* IUPAC Council approved the application of IACT for Associated Organisation status at its August 2003 meeting.

5.3 *2004 Elections.* Ulrich Deiters, Manuel Ribeiro da Silva and Michio Sorai agreed to stand down. The first two offered themselves for re-election.

1 October 2003 Meeting:

1c. *Registration and Finance.* Membership of IACT. It was subsequently agreed that participants would be given the option to join IACT on registration for the Beijing ICCT, in which case USD 20 of the fee would go to IACT. The USD 10,000 from the IUPAC Secretariat was transferred direct to the Conference Organisers.

1g. *IACT Junior Awards.* This announcement did not specifically include the deadline for submission of abstracts for application for an award, though the intention was that this should be the same as the deadline

for submission of other abstracts. In case there had been any misunderstanding, the deadline was extended to July 1st. In the event, no additional applications were received in this period.

1h. *Deadline for Abstracts*. This was put back to 30 April to allow more people to submit abstracts.

1i. *General Comments*

- (a) The final number of registrations was close to 400.
- (b) There had been only one minor occurrence of SARS in 2004.

5.1 *Relations with Elsevier*

Michiel Thijssen welcomed closer contact with IACT, and said how pleased Elsevier were to sponsor the IACT Doctorate Awards. It was agreed to set up a sponsor page on the IACT web site to note this sponsorship, and display the Elsevier logo. Michiel suggested the inclusion of a statement about Elsevier, with a <link>, which should be hyperlinked such that it pointed to a sub-page on the IACT web site, giving information on relevant publications in thermodynamics. Details would be the subject of further discussion with the Secretary, Treasurer, Ken Marsh and Michael Frenkel.

Michiel reported that data presented in papers in the Journal of Chemical Thermodynamics could now be transferred to the NIST database. This was optional, and letters describing this transfer were sent out to authors at the time of acceptance of their manuscript for publication. Michael Frenkel pointed out the advantages of this scheme, whereby such data were in open domain, available for access by businesses or academics. Errors in data were detected and corrected before the actual publication, leading to a higher standard. The database itself could not be referenced; users had to refer to the original publication. This scheme was already working successfully with the Journal of Chemical and Engineering Data, where well over 90% of the data were captured. The scheme was being extended to Fluid Phase Equilibria and Thermochemica Acta. These four journals would account for over 80% of all thermodynamic data reported.

Michiel was pleased to report that sales of the volume *Experimental Thermodynamics Volume VI. Measurement of the Thermodynamic Properties of Single Phases* (Editors: A.R.H. Goodwin, K.N. Marsh and W.A. Wakeham) were going well. It was planned to publish *Thermodynamics Volume VII. Measurement of the Thermodynamic Properties of Multiple Phases* (Editors: Th. de Loos and R.D. Weir) in early 2005.

Finally, he asked for further ideas for volumes in this series. The time scale for publication is five months after receiving the diskette. Previous (and related) volumes were:

Calorimetry of Non-Reacting Systems, *Experimental Thermodynamics I*. Eds. J.P. McCullough and D.W. Scott, Butterworths, London, 1968.

Experimental Thermodynamics of Non-Reacting Fluids, *Experimental Thermodynamics II*. Eds. B. LeNeindre and B. Vodar, Butterworths, London, 1975.

Combustion Calorimetry, Ed. S. Sunner and M. Mansson, Pergamon Press, Oxford, 1979.

Measurement of Transport Properties of Fluids. *Experimental Thermodynamics III*, Blackwell Scientific Publications, Oxford 1991, xx + 459pp.

Solution Calorimetry, *Experimental Thermodynamics IV*. Eds. K.N. Marsh and P.A.G. O'Hare, Blackwell Scientific Publications, Oxford 1994, xviii + 331pp.

Transport Properties of Fluids; their correlation, prediction and estimation, Eds. J. Millat, J.H. Dymond and C.A. Nieto de Castro, Cambridge University Press (1996), xiv + 483pp.

Equations of State for Fluids and Fluid Mixtures, *Experimental Thermodynamics V*. Eds. J.V. Sengers, R.F. Kayser, C.J. Peters and H.J. White, Jr., Elsevier, Amsterdam (2000), xix + 928pp.

The Chairman suggested a volume on "Application of Nanotechnologies and Uses of Nanotechniques."

6. *Treasurer's report*

In a written report, the Treasurer noted that, as at 30 April 2004, there was a balance of GBP 5384.17, being the difference between the sums received from previous ICCTs and the expenses in connection with the Special Board Meeting in October 2003. Since then, there had been expenditure on setting up the web site and on the IACT Doctorate Awards

7. *IACT Web Site*

Ken Marsh presented the current contents of the web site, and noted that payment had been made for the web site for 10 years. He highlighted a number of points for consideration, such as the inclusion of links to web sites for individual Board members; links to full papers where titles of publications were given; links to relevant journals; links to other sites of interest; IUPAC books linked to publishers; logo and links to sponsors, where thought must be given to the amount of information that goes in here.

Ken was thanked for all his efforts in setting up the web site, and for the IACT logo. The only suggestion was to lighten the background for the three legs of the pillars in the logo so that the thermodynamic quantities could be more clearly seen.

It was agreed that Michael Frenkel would maintain the site, with the Secretary acting as contact person for news items. The Secretary was asked to contact IUPAC to see if IUPAC recommendations could be put on the IACT web site.

8. Changes to IACT Bylaws: ARTICLE III Membership

The Secretary had circulated Board members on 12 July 2004 with a note that they should consider whether payment of the IACT membership fee should be made compulsory for all ICCT participants (except students), as is the practice with regard to some International Associations at other Conferences. One advantage would be that IACT would then have a good idea of the income and hence be able to plan the number of Doctorate Awards for future years and the level of financial support to IACT-approved projects. There had been the required 2/3rds majority by the Board in favour of this proposal, but questions had arisen concerning invited speakers and others who had their registration fees waived.

After discussion, the following changes to the Bylaws were agreed:

- that Section 2 be changed from
“Payment of the membership subscription will normally be made when registering for the Biennial Conference, but may be made at any time” to
“Payment of the membership subscription will normally be made when registering for the Biennial Conference, as part of the registration fee, and will be paid by all participants, with the exception of (a) those for whom the registration fee is waived, in which case the membership fee is paid by the Conference, and (b) students. Exceptions to this can only be made in advance with the agreement of the Board, at the time that the Conference is awarded. For non-participants at the Biennial Conference, the membership subscription may be made at any time.”
- that Section 4, which becomes redundant, is deleted.
- that Section 5 becomes Section 4.

9. *Current Projects*

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

In a written report, Josef Barthel reported that Vol. XII, part 1h of their Electrolyte Data Collection, Conductivities, Transference Numbers and Limiting Ionic Conductivities of Protophilic H-Bond Donor and Aprotic Solvents. II: Aprotic Solvents, except Amides, had been published in autumn 2003 (560 pages). A volume on conductivities and dissociation constants of aqueous solutions of organic monobasic acids up to C7 will go to the publishers in Autumn 2004. Further volumes on monobasic acids C8 and longer, and on polybasic acids are planned.

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

In a written report, Manuel Ribeiro da Silva noted that the revised version of his manuscript was almost ready to submit to Pure & Applied Chemistry.

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

The Secretary reported that the revised manuscript had been sent to Ron Weir for submission to Pure & Applied Chemistry.

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

Ken Marsh reported on the final four items in this project. The paper on organic compounds containing nitrogen, by Ken Marsh, David Morton and Colin Young was almost ready for submission. The paper on organic compounds containing halogen(s), by Ken Marsh, David Morton and Colin Young was being written up. The paper on multifunctional organic compounds, by Costa Tsonopoulos and Douglas Ambrose, would also include data on miscellaneous compounds, which had been published since the earlier Items in this series. The final paper by Douglas Ambrose and John Dymond will cover inorganic compounds.

9.5 *International Thermodynamic Tables of the Fluid State. Volume 14. Benzene* (Coordinator: W.A. Wakeham)

The necessary calculations had been completed, but there was no possibility of writing up this work. It was therefore recommended that this project be discontinued.

9.6 *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 all manuscripts had been received by May 2004, and a contract had been signed with Elsevier. Publication was expected in early 2005.

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

Ken Marsh announced that the task group members were Ken Seddon, Cor Peters, Andreas Heintz, Joan Brennecke, Joe McGee, Michael Frenkel, Ken Marsh and Luis Rebelo. 1-Hexyl-3-methyl imidazolium bistriflate amide had been selected as the pure ionic fluid, with the objective that different groups would measure different physical properties to resolve disagreements such as the 50% variation in the reported viscosity, and determine the melting point, which was not easy due to glass formation. The presence of water had a marked effect on physical properties, and analysis for water content was essential before and after measurements. Mixture properties to be measured would include gas solubility, LLE, VLE, and γ^∞ .

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

Trevor Letcher circulated a galley copy of this volume. The book was due to be published on September 4th. 2004, by the Royal Society of Chemistry, at a cost of about GBP 60.

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

The Secretary reported that he had been informed that the next task group meeting would be held on October 11th 2004 at NPL, London, UK. It was planned to complete the project in 2005.

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

Michael Frenkel reported that considerable progress had been made, with publication of the framework of ThermoXL, and its validation using the NIST/TRC SOURCE data archival system (J. Chem. Eng. Data **48**, 2-11, 2003), its extension to cover various measures and uncertainties of experimental data (J. Chem. Eng. Data **48**, 1344-2359, 2003), and the incorporation of critically evaluated data, predicted data and equation representation (J. Chem. Eng. Data **49**, 381-393, 2004). A meeting of the Task Group had been held at the offices of ESDU plc, Corsham Street in London in January, a report of which had appeared in *Chemistry International*, **26** (4), 26-27, 2004. Further to that meeting, the "ThermoXL" namespace was now reserved on the IUPAC web site for the standard which was being developed. Further work involved the incorporation of the IUPAC chemical identifiers, the extension of ThermoXL to cover phase equilibria in electrolyte mixtures (where there were problems of standard states), and possible inclusion of data for polymers, where there were problems of identification. ThermoXL had already been established for global data communication through guided data capture. The Journal of Chemical and Engineering Data and the Journal of Chemical Thermodynamics were collaborating, with authors sending their data to NIST for checking and correction, thus leading to a higher standard of presentation of papers. Fluid Phase Equilibria and Thermochimica Acta were going to join the data capture scheme, with editorials in their October issues. The International Journal of Thermophysics would also participate. User groups included Aspen Technology, Virtuals Materials Group, Fiz. Chemie, with NEL, East Kilbride, under development.

A description of this new thermodynamic communication process was planned for submission to Nature in December 2004, with Recommendations for an IUPAC XML-based standard planned for publication in Pure & Applied Chemistry by the end of 2005. A task group meeting would be held during this Conference (Monday 21), with a final meeting probably in the second half of March 2005 (venue to be arranged) to discuss the final draft.

10. *ICCT's.*

10.1 *The 18th. ICCT, Beijing, P.R. China in 2004.*

Members expressed their satisfaction with the accommodation in the Fragrant Hills Hotel, in its beautiful setting, and with the fact that the lecture halls were all part of the hotel, and looked forward to a good

Conference. Haike Yan reported that there would be a total of 408 presentations. There were about 250 overseas participants and 150 from China. The number from China was low, because of the relatively much low salaries in China.

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

Michael Frenkel reported on a meeting, which had been held of the K7 (Thermophysical Properties) and ICCT Board. They were expecting 800-900 participants for this joint Conference, which would therefore have an extensive poster session, in order to reduce the number of parallel oral sessions. There would be four major joint plenaries: one of joint interest; the Touloukian Lecture (Thermophysical Props.); the Rossini Lecture (ICCT), and the Hoffman Lecture (Calorimetry Conf.) in the air-conditioned University Memorial Centre (capacity 1000). Each day would start with one of these plenaries and 2 ICCT plenaries, followed by a breakout session. There would be up to 8 parallel sessions for ICCT, and a total of 13 altogether. Meetings had been held with Sarah Tanner, Conference administrator to discuss room venues.

Michael said that he would be Programme Chair of the Calorimetry Conference, which would help in aligning the programme with ICCT. Participants wishing to join the Calorimetry Conference would be asked, via their Chair, to pay their subscription at their AGM as per normal.

There will be trips for accompanying persons during the week.

There will be a single registration fee, which allows entry to all sessions, 50% of the income going to ICCT (which will then manage its own budget) and 50% to K7. The registration fee will cover a half-day tour and Conference Dinner. The sum to be transferred to IACT as membership fees would be calculated as 50% of the number of participants times USD 20. Those who give oral or poster presentations in ICCT sessions will qualify for IACT membership. It was planned to have the Conference web site up and running in October 2004. Speakers and session chairs would be selected by March 2005.

Regarding accommodation, dorms can accommodate 700, but it was pointed out that nearby hotels offer better facilities at only a slightly higher rate. A list of hotels would therefore be provided, with meal packages available for non-dorm residents.

The Secretary agreed to contact the IUPAC Secretariat to seek IUPAC sponsorship for this Conference.

10.3 *The 20th-ICCT*

An outline proposal had been received from Professors Josefa Fernández and Jose Urieta at the beginning of 2004 to hold the 2008-ICCT in Zaragoza (Saragossa), Spain. This was circulated to Board members for discussion. There was unanimous concern about 3 points: a) the meeting was planned for August, but there was no air-conditioning in the main lecture hall, b) the hotels were not within walking distance of the Conference venue, and c) there was a distinct possibility of EXPO 2008 being held in the same city, which would lead to a large increase in accommodation prices.

The proposers were thanked for their work, and encouraged to consider alternative venues. Professor Fernandez indicated that her group was far too small to consider holding the conference in Santiago de Compostela, and suggested Vigo as a possible venue, with a joint bid from herself and Professor Legido. Unfortunately, it appeared that the Congress Centre in Vigo has only 5 theatres with a capacity above 75 (others will only accommodate 50), and we require a minimum of 6 for parallel sessions. The Secretary and Chairman had discussed this proposal, and agreed that the arrangements would not be suitable. Board members agreed.

A proposal had also been received from Dr. Ivan Cibulka, of the Czech Republic. However, he pointed that it would be necessary to hire the Prague Congress Centre if there were more than 500 participants, and this would act substantially to the cost. As he was still waiting for detailed information, he suggested that we should go ahead with another proposal, if we considered it satisfactory.

Jean-Pierre presented a proposal on behalf of Stanislaw Randzio and Jacek Gregorowicz to host the Conference in Warsaw, at the Gromada Convention Hotel and Exhibition Centre, located 1 km from the international airport in a green environment, and 7 km from down-town Warsaw. There are hotel facilities for 650 persons, (a double room would cost about 22 Euro per person, including breakfast) and a large number of conference halls. The Institute of Physical Chemistry and the Polish Academy of Science fully support this proposal.

Ken Marsh moved acceptance of this proposal, with Michael Frenkel seconding it. Members fully approved, and asked the Chairman to obtain the proposers' agreement on collecting the IACT membership fees as per

the revised Bylaw, and also an estimate of the registration fee. The preferred time would be end-July, beginning August. On receiving a satisfactory response to these points, a letter of acceptance will be sent.

11. *New Project Proposals*

11.1 *Heat Capacity for Liquids*

The Secretary reported that IUPAC had approved the proposal from Vlastimil Ruzicka for a further supplement to the earlier volumes, to cover the period 2002-2004, but encouraged him to find additional collaborators. Board members could not offer any suggestions.

11.2 *Guidelines for Temperature Modulated DSC.*

Jean-Pierre Grolier reported on the comments, which had been received on this proposal. After some discussion, members unanimously agreed that the proposal should be submitted to IUPAC "with IACT approval".

12. *Any other competent business.*

Ken Marsh said that he had been asked to advertise on the IACT website the 15th International Conference on Chemical Thermodynamics, to be held in Moscow, next year. This title would cause confusion with our ICCT's. Natalia pointed out that this should be the Russian Conference and hence "RCCT".

13. *Date of next meeting*

The next meeting, which will be for the new Board, will be held on Friday, 20th. August 2004 in Room 2 of the Fragrant Hills Hotel, Beijing, China.