

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

University of Colorado, Boulder, Colorado, Sunday 22 June 2003

0900-1300h

Present at the meeting in the Engineering Department:

Chairman	J.P.-E. Grolier
Secretary	J.H. Dymond
Treasurer	A.R.H. Goodwin
Members	T.W. De Loos K.N. Marsh E. Vogel
Counsellors	M. Frenkel W.A. Wakeham
By invitation:	T. Atake

1. *Preliminary Matters and Announcements.*

The Chairman welcomed those present, and introduced Tooru Atake, who was taking the place of Michio Sorai.

2. *Apologies.*

Apologies were received from Ron Weir, Trevor Letcher, Michio Sorai, Mary Anne White, Manuel Ribeiro da Silva, Natalia Smirnova, Ulrich Deiters, and Haike Yan.

3. *Minutes of the Previous Meeting.*

The Minutes of the Meeting held in Rostock, Germany on 31 July, 2002 were approved, with the minor correction that section 2.3, paragraph 2, should be amended to read that Atake was "encouraged to submit an official proposal before the 2004 meeting".

4. *Matters arising.*

All matters arising were considered under the specific Agenda items below.

5.1 *The Status of IACT.*

The Secretary reminded Members that, with regard to the status of IACT, the situation in Rostock last summer was that we were considering establishment as a Company limited by guarantee. This was the advice of the University of Glasgow legal advisers, following full discussions on the aims and objectives, and possible liabilities of IACT. Subsequently, Bill Wakeham approached his legal advisers at the University of Southampton, who queried the earlier advice on the grounds that, in their opinion, it would lead to an expensive and unnecessarily complicated alternative. They recommended Unincorporated Association status.

Following a consultation of Board Members, there was unanimous agreement that the simpler alternative, namely Unincorporated Association status, was the desirable route for IACT to follow. This result was declared to Board members on 18 December 2002.

At the beginning of 2003, application was made to IUPAC for IACT to be granted Associated Organization status. This has to be approved by the IUPAC Executive Council. John Jost, Executive Director of IUPAC, wrote to the Secretary on 12th May "that at its meeting last month, the IUPAC Executive Committee recommended that the application of the International Association of Chemical Thermodynamics for

Associated Organization status be approved by Council. The Council meets 16-17 August and I will inform you of its decision when it is known".

5.2 *Constitution of IACT*

The Secretary announced that version 6, which had been circulated prior to the meeting, contained minor changes to version 5, in line with previously agreed recommendations. He thanked all those who had contributed to the development of the Constitution. Version 6 was formally approved. It was agreed that this should be publicised on the IACT web page.

5.3 *2004 Elections*

In order to achieve the situation described in the Constitution whereby Directors serve staggered 4-year terms, it was agreed that three Directors should stand down in 2004. From a geographical standpoint, it was suggested that, of these three, two should be from Europe. The Chairman, Secretary and Treasurer were authorised to decide on the three names and, where the Director was willing to put himself forward for re-election, to indicate that this would have the Board members' full support. It was pointed out that this unique nature of the first election would require explanation to the general membership.

6. *Treasurer's report*

The Treasurer reported that an interest bearing account had been opened with the Abbey National Bank in the UK. The current balance was GBP6542.23, made up from USD5000 passed on from the ICCT Conference in Halifax in 2000, and about USD5000 from the Rostock Conference. There had been no withdrawals.

The IACT membership fee for 2004-2006 was fixed at USD20. In most cases this would be paid by those attending the ICCT-2004 who opted to become members of IACT (by ticking the appropriate box on the registration form). The Treasurer agreed to investigate methods for credit payments for others who wished to join IACT. The Secretary agreed to draw up a numbered list of members, which would include all paid members, Board members, the Rossini Lecturer, Plenary Lecturers and Invited Lecturers and Organisers of Workshops at the Rostock Conference.

It was agreed that the USD5000 from the Halifax Conference should be made available to Haike Yan as a float, if so required, to cover initial expenses in connection with ICCT-2004.

It was unanimously agreed to offer a number of prizes to students, based on undergraduate or doctoral work in thermodynamics, which had been carried out in the previous two years. The awards will be made on the basis of abstracts of papers submitted for ICCT's, where the supervisor supports the application for an award. A special slot in the ICCT will be made for the presentation of the award(s) and for the winner(s) to give the paper(s). The prize will take the form of a Certificate for the "IACT Junior Award for Excellence in Thermodynamics". In addition, financial assistance will be provided towards travel costs to attend the ICCT. In the event of a successful approach to a company for funds for these prizes, the company name will be attached to these awards. The number of awards will depend on the standard of the abstracts offered, and the finances available.

The procedure for deciding the award winner(s) will be the same as that for selection of the Rossini Lecturer. (N.B. The Rossini Award is the Senior Award for Excellence in Thermodynamics).

7. *IACT Web page*

Michael Frenkel suggested the possibility that a NIST student might design a web page to specifications put forward by Board members. It was agreed that Ken Marsh and the Secretary should liaise with him over this, and that an estimate of costs should be approved before work commences. The intention was that IACT should take over the web page for maintenance once it had been set up.

It was agreed to have a contest for students to design an IACT logo, with a small cash prize.

8. *Current Projects*

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

In a written report, Josef Barthel reported that Vol. XII part 1h of their Electrolyte Data Collection had been sent to the publisher and will appear in autumn 2003 (560 pages). This part contains solutions of protophilic

aprotic solvents (except amides which were treated in Vol. XII, 1g), e.g. sulfolane, DMSO, 3-methyl-2-oxazolidone, pyridine, hexamethylphosphortriamide, etc.

In addition, there were two parts in preparation: Vol. XII, part 4a, Aqueous solutions of organic acids (about 60 acids of chemical, biotechnological and medical interest) and Vol. XII, part 5a Mixed solvent systems of carbonates (PC, EC with co-solvents, nowadays widely used for HEBs, supercapacitors, etc.).

8.2 *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 he planned to incorporate a few minor suggestions for changes, which he had received, in his text and submit the final version to Pure & Applied Chemistry in September.

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

The Secretary reported that three reviews of this manuscript had been sent to Pino Della Gatta in November 2002. There had been no response to his enquiry about the present status of this manuscript.

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

Ken Marsh reported that the final four items in this project were nearing completion. The paper on organic compounds containing halogen(s), by Ken Marsh, David Morton and Colin Young should be completed in September, as should the paper on organic compounds containing halogen and nitrogen, by Costa Tsionopoulos and Douglas Ambrose. The paper on organic compounds containing nitrogen, by Ken Marsh, David Morton and Colin Young should be completed in November. The final paper will include all those data which have been published since 1985, but which were not included in the previous papers.

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

Bill Wakeham said that the people who had been working on this project had now all left Imperial College. Additional finance, about GBP5000, was required to get this work written up for publication. It was proposed to approach IUPAC and also chemical companies with a specific interest in benzene - Theo de Loos suggested DSM Research in Geleen, The Netherlands - for funding. Bill Wakeham offered to prepare a proposal for IUPAC.

8.6 *Experimental Thermodynamics Volume VI. Measurement of the Thermodynamic Properties of Single Phases* (Editors: A.R.H. Goodwin, K.N. Marsh and W.A. Wakeham)

Tony Goodwin was very pleased to report that this volume had been published and that copies would be sent out to distributors at the end of that week. Advertising literature would be available during the forthcoming 15th. Symposium on Thermophysical Properties. 300 copies of the volume had been ordered already. He briefly summarised the difficulties which had been experienced with the publishers, Elsevier, but was confident that, as a result, Elsevier would liaise more closely with editors of future volumes.

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 they had had some problems with prospective authors and were lacking part of a chapter on vapour pressure and half a chapter on activity coefficients. The book would be typeset as per Volume VI. Ron Weir did not plan to start any editing work until all the copy had been received. Members hoped that this would not result in undue delays.

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

Ken Marsh announced that this had been approved as an IUPAC project. There would be a meeting of the members of the task group during the forthcoming 15th. Symposium on Thermophysical Properties.

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

Trevor Letcher had written to say that he expected publication of this volume in early 2004. The publishers would be the Royal Society of Chemistry.

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

Bill Wakeham said that this had recently been approved as an IUPAC project. There would be a meeting to discuss the project that afternoon, as part of the programme of the International Association of Transport Properties meeting.

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

Michael Frenkel reported that this proposal had been considered by the IUPAC Physical and Biophysical Chemistry Division Committee and the Committee on Printed and Electronic Publications (CPEP). They recognised the importance of the development of an XML data dictionary for thermodynamic properties, and recommended that there should be some co-ordination with IUPAC Project 2002-022-1-024 - Standard XML Data Dictionaries for Chemistry. The database section should be separated out. Michael said that he had had discussions with Steve Stein of NIST, who was a member of CPEP and, with the approval of other task group members, he had submitted a revised proposal. It was expected that a decision on this would be made during the IUPAC General Assembly in Ottawa in August.

9. ICCT's.

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

In view of the significant improvement in the SARS situation in China, Board members had no hesitation in giving their full support to the decision to hold the 18th. ICCT in Beijing. The fact that Haike Yan was unable to attend this meeting because he could not get a visa in time due to earlier problems arising from SARS was unfortunate, but understandable. It was agreed that the Secretary should write to Haike to raise a number of important points:

- it was now a matter of urgency to decide on the conference venue. A single site was preferred, with lecture rooms close together, so that the participants could attend talks from different parallel sessions.
- there must be sufficient rooms for all the parallel sessions, large enough for the expected attendance.
- confirmation was required that symposium and workshop organisers had been formally invited.
- Jan Kwak should be formally invited to be Chairman of Symposium 5, on Surfactants, colloids and interface science
- symposium and workshop organisers should suggest names of invited lecturers, which the Conference Organisers should discuss, and then they should issue the formal invitations.
- the Conference Organisers should seriously consider having a plenary lecture on databases, in view of recent advances in this area.
- it was noted that there were Chinese organisers for each section except section 11 - should one be included here also?
- it was noted that the web page for ICCT-2204 had been set up, but it was felt that it should be compressed to save space.
- it would be helpful to have an idea of the number of participants who would pay a reduced registration fee. Such people would have to pay \$20 to the Treasurer to become general members of IACT.
- a room would be required for an IACT Board meeting before the ICCT, on Monday 16 August 2004, and at a later time during that week (to be arranged) for the new Board.

Haike Yan had offered to come to Europe for a meeting to discuss arrangements for ICCT-2004, and members agreed that this would be most useful. The time and place are to be arranged by the Chairman, Secretary and Haike Yan.

9.2 *The 19th. ICCT, Boulder, Colorado in 2006.*

Michael Frenkel reported on the preliminary arrangements for the 19th. ICCT, which is to be held jointly with the 16th. Symposium on Thermophysical Properties and the Calorimetry Conference, in Boulder, Colorado, 30 July to 4 August 2006. It was intended to have a single name for this gathering, with "World Thermo Forum" the preferred choice.

The structure for the organisation would consist of :

- International Advisory Committee

- Executive Board, with an independent President (Mickey Haynes), two Vice-Presidents (the Chair of the 16th. Symposium on Thermophysical Properties, and the Chair of ICCT-2006 (Michael Frenkel), plus 6 members (3 from each group).

Michael Frenkel announced that there would be a meeting of the Initiative Group of the Organising Committees of the Symposium on Thermophysical Properties-16 and ICCT-19 on the following Wednesday, 09 July 2003 and that he would send the Secretary a report on that meeting.

There would be a plenary lecture for all participants (a joint meeting) each day. These would be the Rossini lecture, the Touloukian lecture and the Hoffmann lecture, plus one plenary lecture nominated by each group.

ICCT would have its own independent, traditional set-up.

9.3 *Future ICCT's*

Spain and Poland were suggested as possible venues for ICCT-2008, with Spain the preferred choice. Jean-Pierre Grolier agreed to pursue this possibility. [Note: Jean-Pierre contacted Josefa Fernández ((Santiago) that afternoon. She will discuss this with colleagues at other Spanish Universities to see if they could organise this meeting, and report back].

Tooru Atake (Tokyo Institute of Technology) agreed to send the Secretary an official proposal to host ICCT-21 in 2010, and to present an outline of his plans to the Board in Beijing in August 2004.

10. New Project Proposals

10.1 *Thermophysical Properties of Polymers: to include D_fH , T_g , glass transition temperatures and thermo-mechanical coefficients over extended temperature and pressure ranges.*

Jean-Pierre Grolier outlined his draft proposal, which will be circulated later to members for comment.

10.2 *Guidelines for Temperature Modulated DSC.*

Jean-Pierre Grolier said that this proposal was being prepared.

10.3 *The critical evaluation of vapour pressure data of low volatile compounds.*

Theo de Loos announced that Cor Peters (Delft) and Roberto Fernández-Prini (Argentina) were preparing a proposal for a project on this topic. Members suggested that the Prague group, Professor Jose (Lyons) and James Chickos (Missouri-St. Louis) should be approached for advice and possible inclusion as task group members.

11. Any other competent business.

Tooru Atake asked if the standard pressure could be redefined as 1 atmosphere (101325 Pa), instead of 10^5 Pa which has been the IUPAC recommendation since 1982, in view of the many objections which had been raised to this recommendation. His comment was noted. [N.B. A definitive answer is given in *Quantities, Units and Symbols*, where it is written that "In principle one may choose any value for the standard pressure.... although the choice must be specified"].

12. Date of next meeting

The next meeting will be held on Monday, 16th. August 2004 in Beijing, China

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

(July 2002 - July 2004)

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Secretary
Treasurer

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J.P.-E. Grolier
J.H. Dymond
A.R.H. Goodwin

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U.K. Deiters
T.M. Letcher
K.N. Marsh
M.A.V. Ribeiro da Silva
M. Sorai
E. Vogel

Counsellors

M. Frenkel
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W.A. Wakeham
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