

Minutes of Meetings of IUPAC Commission I.2 on Thermodynamics

Brisbane, Australia, 30 June and 1 July 2001

0900-1300h and 0900-1800h

Present at the meetings at Queensland University of Technology, Australia:

Chair	R.D. Weir
Secretary	J.H. Dymond
Titular Members	J.P.-E. Grolier T.M. Letcher M.A.V. Ribeiro da Silva E. Vogel
Associate Members	A.R.H. Goodwin
National Representatives	Hai-Ke Yan
Observers	J.M.G. Barthel

Also present during the meeting: G. Della Gatta
K.N. Marsh

1. Preliminary Matters and Announcements

Opening of Meeting at 0900h, Saturday 30 June 2001.

The Chair welcomed those present and noted that the following were unable to attend: T.W. De Loos, U.K. Deiters; J.A.R. Cheda, V.A. Durov, K. Murphy, A. Schiraldi, M. Sorai, S. Stølen, M.A. White; C. Airoidi, T. Boublik, G. Kaptay, J.L. Laynez, H. Pak, and I. Wadsö.

Customary brief introductions were made.

1.05 The Agenda was accepted as written.

1.1 The Halifax (2000) Minutes were approved without change. All business arising is covered by the Agenda item 1.05.

2. Substantive Business

2.1 Electrolyte Solution Data.

Reporter: Barthel.

Barthel reported that the project was proceeding well. He presented an up-dated list of his publications in the Chemistry Data Series, Vol. XII Electrolyte Data Collection, and circulated the latest two volumes. These were parts 1e. *Conductivities, Transference Numbers and Limiting Conductivities of Solutions of Aprotic, Protophobic Solvents, III, Ketones, Esters and Nitrohydrocarbons (C1-C4)*, and 1f. IV. *Ketones, Esters and Nitrohydrocarbons (C5-C8)*, by J. Barthel and R. Neueder. Part 1g *Conductivities, Transference Numbers and Limiting Conductivities of Solutions of Protophilic H-bond Donor and Aprotic Solvents I. Amides* was in preparation and should be ready for the Rostock ICCT. The present series would run to 25-30 volumes. Future work would be on enthalpy of dilution and mixed solvent systems. The database at Regensburg contained some 700,000 data sets for electrolyte and non-electrolyte solutions, including much data from Eastern Countries. A subsequent series was expected to produce about 20 volumes. The group

welcomed collaboration, but in the meantime would continue to work through DECHEMA as before.

Commission I.2 congratulated Professor Barthel and his group for their impressive output.

- 2.2 Recommendations regarding Legendre Transforms in Chemical Thermodynamics Reporter: Weir

Weir reported that this manuscript was in the process of being reviewed by IDCNS for publication in *Pure and Applied Chemistry* and, subsequently, in the *Journal of Chemical Thermodynamics*.

- 2.3 Theory of Equations of State for Fluids and Fluid Mixtures. Reporter: Weir.

This was published as two volumes by Elsevier (928 pp.) in October 2000.

- 2.4 Project on the Thermochemistry of Chemical Reactions. Reporter: Ribeiro da Silva

Weir reported that this manuscript was at present undergoing a review by IDCNS for publication in *Pure and Applied Chemistry* and, subsequently, in the *Journal of Chemical Thermodynamics*.

- 2.5 Subcommittee on Thermodynamic Data. Reporter: Dymond

The current state of the projects is as follows:

- a. Vapour Liquid Critical Properties of Elements and Compounds.

The latest papers in the series are Part 7. Oxygen Compounds other than Alkanols and Cycloalkanols, by A.P. Kudchadker, D. Ambrose and C. Tsonopoulos, *Journal of Chemical and Engineering Data*, **46** 457-479 (2001), and Part 8. Organic, Sulfur, Silicon and Tin Compounds, by D. Ambrose and C. Tsonopoulos, *Journal of Chemical and Engineering Data*, Vol. **46** 480-485 (2001). Completion of this project with Part 9 Nitrogen-containing compounds, Part 10 Halogenated compounds, and Part 11 Polyfunctional compounds is planned for late 2001. This final part of the work was approved by the Physical Chemistry Division Committee as project number 2000-026-1-100.

- b. International Thermodynamic Tables of the Fluid State. Benzene.

The necessary calculations for this project had been completed, but time is required to write up this work for publication. Although Mrs. M. de Reuck has retired, she fully intends to complete this project.

- c. International Tables of the Fluid State. Carbon Dioxide.

This project had to be abandoned as Dr. Span (Bochum), who had carried out this work, had now taken up a position in industry, and neither he nor Professor Wagner would have the time to complete this work.

- d. Thermochemical, Thermodynamic and Transport Properties of Halogenated Alkanes and their Mixtures

The second workshop of this project was very successfully organised by Professor Richon in Paris from 9-11 April, 2001. There were about 120 participants, with 11 invited lectures, 27 oral and 60 poster presentations. The meeting was structured with 4 main themes: i) environmental constraints and regulations, ii) new products, iii) new measurements, and iv) fundamentals and simulation, with a concluding round-table discussion. 30 manuscripts had been submitted for publication later this year in a special issue of *Fluid Phase Equilibria*, with Dymond and Richon as Guest Editors.

A follow-up workshop will be held as part of the IUPAC Conference on Chemical Thermodynamics in Rostock in 2002. This will be organised by U.K. Deiters and M.A. Assael.

[Note added: Assael will not attend the ICCT 2002 in Rostock. Therefore, A. Laesecke will take over the task].

- e. Heintz had indicated by letter that it was still his intention to start a new project on Ionic Liquids (low temperature organic molten salts), with a workshop to be chaired by Ken Marsh as part of the 17th. ICCT in Rostock in 2002.

Dymond will liaise with Heintz and Marsh and complete a New Project Submission Form.

Members of Commission I.2 thanked Prof. Deiters and the members of the Subcommittee (in their absence) and the other volunteers for all their work.

2.6 Subcommittee on Transport Properties.

Reporter: Dymond

122/1/83 Definitive correlation of transport properties of fluids

Publication since the last report:

- Reference correlation for the viscosity of liquid toluene from 213 to 373 K at pressures to 250 MPa, M.J. Assael, H.M.T. Avelino, N.K. Dalaouti, J.M.N.A. Fareleira, and K.R. Harris, *Int. J. Thermophys.*, **22**, 789-799 (2001).

The following projects are continuing:

- Correlation of the Thermal Conductivity of R134a, R. Perkins, A. Laesecke, & J.V. Sengers.
- Transport Properties of Methane + Ethane, S. Will, A. Leipertz, E. Vogel, V. Vesovic, & W.A. Wakeham.
- Thermal Conductivity of *n*-Butane, R. Perkins, J.V. Sengers, & C.A. Nieto de Castro.
- Viscosity of Alkali Chlorides, H. Oye & C.A. Nieto de Castro.
- Viscosity and Thermal Conductivity of Water & Steam, M.J. Assael, J. Millat, A. Nagashima, D. Friend, & J.V. Sengers.
- Viscosity and Thermal Conductivity of D₂O, M.J. Assael & A. Nagashima.
- Viscosity of *n*-Pentane, A. Laesecke, E. Vogel, & M.J. Assael.
- Viscosity of Cyclopentane, N. Dalaouti, M.J. Assael, J.M.N.A. Fareleira, H. Bauer, & K. Harris.
- Feasibility Study for a Book on The Properties of Water, Air and Sea Water, A. Nagashima, M.J. Assael, & J. Millat.
- Thermal Conductivity of Iso-Butane, R. Perkins, K. Marsh, & C.A. Nieto de Castro.

122/3/85 Standards of viscosity and thermal conductivity.

- A first draft on Viscosity of Toluene at Atmospheric Pressure in Wide Ranges of Temperature. F.J.V. Santos, C.A. Nieto de Castro (Portugal), J.H. Dymond (UK), N. Dalaouti, M.J. Assael (Greece), A. Nagashima (Japan) has been prepared.
- The project: Viscosity of Liquid Water, W.A. Wakeham, J.H. Dymond (UK), H.A. Oye (Norway) has been stopped due to lack of funds.
- Work is continuing on Investigation of a New High-Viscosity Standard, J.M.N.A. Fareleira, M.J. Assael, H. Bauer.

122/4/91 Transport properties of fluids - theory and representation

Work in this area is in progress.

Future Meetings:

The next meeting of the subcommittee will be held in Possidi, Greece on 8-9 September 2001.

[Note added: At this meeting, the group decided to maintain association with the residual body of the Commission on Thermodynamics. It was felt that a new name was needed for the subcommittee on Transport Properties, and the title "International Association for Transport Properties (IATP)" was agreed by consensus. For the time being, W.A. Wakeham and M.J. Assael would continue as Chairman and Secretary, respectively.]

The 2002 meeting will take place in London (UK) in September 2002 prior to the European Thermophysical Properties Conference.

The 2003 meeting will take place in Boulder (USA) in June 2003 prior to the 15th Symposium on Thermophysical Properties.

The subcommittee was congratulated on its continued progress and high productivity.

2.7 New Edition of Experimental Thermodynamics Vol II.

Reporters: Goodwin & Weir

Volume VI. *Measurement of the Thermodynamic Properties of Single Phases* : Editors: Goodwin, Marsh

and Wakeham.

After some discussion over the terms, a contract has now been signed with Elsevier. They require all material to be with them by 15 September 2001. It was agreed that they will typeset the material, at IUPAC's expense. Some money (\$3000) was available from the Secretariat for reimbursement of secretarial expenses. The publisher will supply 16 copies free of charge, and IUPAC will purchase additional complimentary copies for the authors.

Volume VII. *Measurement of the Properties of Multiple Phases*: Editors: de Loos and Weir.
The contract with Elsevier was expected shortly, with the same deadline for material.

2.8 16th ICCT, 7-11 Aug 2000, Halifax, Canada. Reporter: Weir

Weir thanked White (in her absence) for the highly successful Conference. An excellent report on this appeared in *Chemistry International*, **23**, 49-51 (2001).

2.9 17th. ICCT, 28 July to 2 August, 2002, Rostock, Germany Reporters: Vogel

Vogel reported that they had started to prepare in 1998. The experiences of the Halifax meeting had been most helpful, especially a computer programme to facilitate registration. The problem of reaching people by eMail was noted. For the Halifax meeting, messages to some 1000 out of 6000 addresses did not reach the intended persons. Full use would be made of the homepage for the Rostock meeting.

They were planning for 400 to 600 participants. There was sufficient hotel space but not in the hotels originally planned. Alternative accommodation was available at 50 to 70 euro (middle category) and 70 to 90 meuro (upper category) (together up to 450 places) and at 20 to 30 euro (150 rooms).

The City Hall had been booked to accommodate the plenary lectures and most of the parallel sessions. It comprised 5 lecture halls, but one is too large for parallel sessions. The City Hall was ideal for staging posters, and for book and equipment exhibitors. It is necessary to use four further lecture halls of the University for parallel sessions. These are seven minutes walk from the City Hall.

Lunch would be provided by the City Hall caterer for about 7 euro. Tickets would be sold for the whole week.

A reception was planned for Sunday, with a Concert on Tuesday, an excursion on the Wednesday afternoon and the Banquet on Thursday.

The registration fee would be about 350 euro, of which 20 euro was agreed in discussion to be the two-year membership fee for the proposed International Committee on Chemical Thermodynamics.

The International Advisory Committee and the Committees for individual workshops had suggested plenary lecturers - of which there will be seven, in addition to the Rossini Lecturer John Prausnitz. Two of these are from the U.S.A., two from Japan, and one each from the UK, Germany and Sweden. Formal invitations had been sent out the previous week. The 26 invited lecturers come from a total of 12 countries. It was intended to close the meeting with two Plenary lectures and the Closing Ceremony.

For accompanying persons, the Tourist Travel Office would have whole day and half-day excursions.

Publications:

It was agreed to organise the publication of papers from this Conference as follows:

- Rossini lecture : J. Chem. Thermodynamics
- Plenary lectures (7): Pure & Applied Chemistry
- Weir will talk to 5-10 authors whose papers he would like to publish in J. Chem. Thermodynamics
- Papers on ionic fluids : Barthel will look after these papers (~15) for J. Mol. Liquids
- Thermochemistry papers : della Gatta will arrange publication in Thermochemica Acta
- Halon workshop papers : Deiters and Assael will arrange publication in Fluid Phase Equilibria.

[Subsequently, de Loos enquired about publishing papers from Symposia 1 and 2 in Fluid Phase Equilibria. This was agreed subject to Weir having first refusal on papers from Symposium 2 for publication in J. Chem. Thermodynamics.]

[Note added: the 2nd circular was sent to 6000 e-mail addresses on 12 October 2001].

2.10 The 18th. ICCT, Beijing, P.R. China in 2004. Reporter: Hai-Ke Yan

The paperwork for IUPAC Sponsorship would be sent in to the IUPAC Secretariat by October 2001.

The Conference would be organised by the Chinese Chemical Society, with funding from the Chinese Academy of Sciences and companies. No final decision had been made on the location; they were considering different Universities. Accommodation would be available for \$15 for students, with availability from \$15 upwards for staff. It was suggested that the period 20-25 August 2004 would be the best time in Beijing, and that the conference should certainly take place before 1 September. It was noted that the ICTAC meeting would be taking place in Sardinia in 2004, probably in mid-September.

Post-Conference tours would be arranged. Each province has a branch of the Chinese Chemical Society which can arrange these.

2.11 Guidebook for Organisers of IUPAC ICCTs. Reporter: Weir

In Halifax, White and Kusalik met with Heintz and Vogel to discuss the working of their programme for registration and their list of eMail addresses. This will be updated and passed on to future organisers.

[Note added: White has produced a very comprehensive 52-page report on Guidelines for the Organisation of IUPAC International Conferences on Chemical Thermodynamics, based on her experience in organising the Halifax meeting. This will be invaluable for the Chairs of future ICCT's.]

2.12 Forthcoming change in IUPAC operation Reporter: Weir

It was reported that the Commission on Nomenclature, Symbols and Units would continue past 2001, but all other Commissions would cease at 31 December 2001.

At a meeting with George Wilson (President) and John Ralston (Vice-President) of the Physical Chemistry Division Committee, it was pointed out that Commission I.2 had 29 publications in the Divisional list of 57 publications from all the Commissions.

Our proposal for funding for \$5000 (submitted in September 2000 to IUPAC), to help set up the International Committee on Chemical Thermodynamics in place of Commission I.2 (as agreed at our Halifax meeting), and seek industrial links, had been rejected by Ted Becker, IUPAC Secretary General, on the grounds that it was not a real project. However, the Division members were keen to see that ICCT should be supported and, after Weir had addressed an earlier meeting of the Division Committee, had agreed to pay this sum out of their discretionary funds. The conditions were i) that this was a one-off request, ii) that the new organisation should become an Associated Organisation of IUPAC (cf Statute 11 of IUPAC Bye-Laws), iii) that we should continue to submit proposals for projects, iv) that we should report on the use to which the money would be put.

The committee was keen to see how we were going to go about seeking industrial links. [see 5.03]

There was discussion about the best method to incorporate the new organisation. Weir said that he would obtain a copy of the Constitution of the Calorimetry Conference, which he and Dymond would rewrite to form a first draft for circulation to all Commission members. Goodwin offered to assist, in order to incorporate it in the U.S.A., and to act as Treasurer initially for the purposes of setting up a bank account. There was further discussion over the use of "Committee" in the title, with "Confederation" and "Conference" being alternative suggestions. After initial costs had been met (to be taken from the IUPAC grant), funding for on-going expenses for running the ICCT would be met from the membership fee paid as part of the total sum collected at registration at the Thermodynamics Conferences. This would grant membership for two years. The Conference attendance list would be the membership list.

As previously agreed, it is necessary to write into the constitution:

- that the main role of this Committee would be to act as an Advisory Board for the biennial International Conference on Chemical Thermodynamics.
- that the ICCT would engage in project-based activities. Committee meetings would provide an opportunity for discussion of on-going projects, of feasibility studies of other proposed projects, and of ideas for new projects.
- that the Committee would assume responsibility for and co-ordinate the activities of the two existing subcommittees of Commission I.2, viz. Thermodynamic Data and Transport Properties.
- that the Committee should actively seek to offer its expertise to science and technology. The intention is to approach industry to inform them about the activities of the Committee and to seek funding from

companies so that the Committee can be financially independent.

- that the membership of the Committee for the period until the 17th. ICCT in Rostock, August 2002, should be the present members of Commission I.2 with Professor Ron Weir as Chairman and Dr. John Dymond as Secretary.

Barthel suggested that the Conferences on Solution Chemistry, which take place in the in-between years of the Thermodynamics Conferences, should also come under the umbrella of the new organisation.

A website would be set up to advertise previous and current work of the organisation, with a view also to getting ideas for new projects.

The first meeting of the new organisation would be immediately before the Rostock International Conference on Chemical Thermodynamics, with a meeting in 2003 possibly at the Solution Chemistry Conference.

- 2.13 Guidelines for Publication of Equations of State II. Mixtures Reporter: Dymond
Dymond will contact Deiters about a possible proposal for this project.

- 2.14 Global Phase Diagrams of Fluid Mixtures Reporter: Dymond
Dymond will contact Deiters about a possible proposal for this project.

- 2.15 The Journal of Chemical Thermodynamics. Reporter: Weir
Statistics for the past four years were as follows:

	Papers submitted	Papers accepted	Printed pages	Time from receipt to Acceptance (days)	Acceptance to appearance (days)
1997	170	146	1554	109	
1998	167	138	1631	126	
1999	187	141	1654	116	147
2000	192	138	1718	111	175
2001	(176)	(142)			

The scope had been widened to include surfaces and DSC. There was an increased number of pages, and the question was asked whether more information could be put on each page.

The delay in some papers after acceptance was noted. It was suggested that the Journal be asked if a scheme could be introduced for authors to find out the status of their m/s with regard to refereeing, proof stage etc, as per *Thermochimica Acta*, which gives a password for this purpose.

It was reported that the Impact Factor of the Journal was 1.1 (cf. *Thermochimica Acta* 0.7).

Goodwin had started as an Editor and is relieving the workload on O'Hare.

- 2.16 Standards, Calibration and Guidelines in MicroCalorimetry Reporter: Weir

The manuscript entitled "Standards in Isothermal Microcalorimetry", by I. Wadsö, A.E. Beezer, R.N. Goldberg, G. Olofsson, K. Murphy, J. Rouquerol, and J. Sipowska was going through the IUPAC publication process, and would appear in *Pure & Applied Chemistry*. Weir would also arrange for publication in the *Journal of Chemical Thermodynamics*, *Thermochimica Acta* and *Calorimetry and Thermal Analysis*.

A revised draft on "Standards for Differential Scanning Calorimetry", by G. Della Gatta, M.J. Richardson, S.M. Sarge and S. Stølen was presented, and minor corrections pointed out. A footnote was required to link to the other part, and an acknowledgement added. Della Gatta agreed to make the corrections, and send a diskette to Weir for processing as per part 1.

It had previously been agreed that copies of the final document, or at least a reference to the published paper, should be sent to manufacturers so that users of their calorimeters can be advised.

- 2.17 Thermochemical, Thermodynamic and Transport Properties of Halogenated Alkanes and their Mixtures
This item was dealt with under 2.5.
- 2.18 Heat Capacity of Liquids: Supplement Reporter : Weir
The supplement to the two volumes on Heat Capacity of Liquids, published as *Journal of Physical and Chemical Reference Data* Monograph 6, in 1996, is going through the publication procedure for that journal, having received IUPAC approval.
- 2.19 Ionic Liquids Reporter: Vogel
A workshop was to be held as part of the ICCT in Rostock in 2002. There are many interested groups in Germany from the preparation, purification and application aspects, and representatives from these as well as thermodynamic groups are likely to attend. Heintz and Marsh would submit a proposal for an IUPAC project for two workshops (the other in Beijing).
- 3.0 Finances of the I.2 Commission. Reporter: Weir
Weir reported that there was no money left in Commission funds. However, he said that Division President Wilson had agreed \$2000 for project 120/18/97, for expenses of members of Della Gatta's group in connection with their meetings.
- 4.0 Membership Reporter: Weir
There were no changes to the membership as the Commission ceases to exist on 31 December 2001.
The list of the current members of Commission I.2, with addresses, telephone and FAX numbers has been up-dated, and is attached at Annex A.
- 5.0 Other business
- 5.01 Links to industry
It was suggested that industrial support should be sought for:
i) international workshops, which could carry the name of the company, and might be held close to where the company was based. Examples were: separation science, colloid and surface science and environmental science.
ii) projects, particularly data projects, where the results would be of benefit to the company, or companies. This was becoming increasingly important as many companies were giving up their research facilities. Possible areas which were quoted were ionic fluids (U.S.A. and Japan), separation science (South Africa) and the environment (Canada, U.S.A. and Sweden). French polymer and oil companies were seeking partners, for example, with experience with blowing agents, asphaltenes and nanoparticles.
- 5.02 IUCOSPED Reporter: Grolier
Grolier presented a progress report on the IUCOSPED Project, which had been received from Henry Kehiaian. Copies are available from the Secretary.
- 5.03 New Projects
Grolier suggested the following two projects:
Thermophysical properties of polymers: to include $\Delta_f H$, T_f , glass transition temperatures and thermo-mechanical coefficients over extended temperature and pressure ranges.

Guideline for temperature modulated DSC.

5.04 ICCT 2006

A verbal proposal had been received from Michael Frenkel (NIST, Boulder, U.S.A.) to host the 19th. ICCT jointly with the 16th. Symposium on Thermophysical properties at the University of Colorado at end-June 2006.

[Note added: On receipt of the written proposal from Mickey Haynes and Michael Frenkel, Dymond forwarded copies to Commission members for comment. He has also written to Cheda (Madrid, Spain) and Panayiotou (Thessaloniki, Greece) who had previously indicated an interest in submitting a proposal for the ICCT in 2006.]

5.05 Joint Meetings

(a) Commission I.1.

A new edition of the Green Book "Quantities, Units and Symbols in Physical Chemistry" would be published shortly. Suggestions on new sections for inclusion in the fourth edition should be communicated to Jeremy Frey. Commission I.1 welcomed the setting up of the International Committee on Chemical Thermodynamics, as the means of providing a link to the new Commission on Units.

(b) Commission I.3

Electrochemistry was served by the International Society of Electrochemists, which was research based and I.3 would not be seeking to continue in any other form. Professor Ahlberg, University of Göteborg was suggested as a link to the electrochemical community.

(c) Commission I.7

Commission I.7 on Biophysical Chemistry reported on their recent publication: Measurement and analysis of results obtained on biological substances with differential scanning calorimetry, H.-J. Hinz and F.P. Schwarz, *Pure Appl. Chem.*, **73**, 745-759 (2001). Possible new projects were on Isothermal titration studies and Redox potentials of proteins.

Membership I.2 Commission
as approved at the 69th Bureau meeting 14 Aug 00

Members (8)

1989-2001	Prof. R.D. Weir	Chair
1994-2001	Dr. J.H. Dymond	Secretary
1994-2001	Dr. T.W. De Loos	
1996-2001	Prof. U.K. Deiters	
1996-2001	Prof. J.-P.E. Grolier	
1991-2001	Prof. T. Letcher	
1994-2001	Prof. M.A.V. Ribeiro de Silva	
1994-2001	Prof. E. Vogel	

Associate Members (8)

1998-2001	Prof. J.A.R. Cheda
1996-2001	Professor V.A. Durov
1996-2001	Dr. A.R.H. Goodwin
1996-2001	Dr. K. Murphy
1998-2001	Prof. A. Schiraldi
1998-2001	Prof. M. Sorai
1998-2001	Prof. S. Stølen
1998-2001	Prof. M.A. White

National Representatives (7)

1991-2001	Dr. Claudio Airoldi	Brazil
1996-2001	Professor T. Boublik	Czech Republic
1998-2001	Prof. G. Kaptay	Hungary
1994-2001	Dr. J.L. Laynez	Spain
1996-2001	Professor Hyungsuk Pak	Republic of Korea
2000-2001	Professor B. Toshev	Bulgaria
1994-2001	Dr. I. Wadsö	Sweden
1996-2001	Professor Haike Yan	P.R. China

ANNEX A

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