Minutes of Meetings of IUPAC Commission I.2 on Thermodynamics

Berlin, Germany, 8-10 August 1999

0900-1300h, 0900-1700h and 0900-1230h

Present at the meetings at the Freie Universität, Berlin:

Chair	R.D. Weir
Secretary	J.H. Dymond
Titular Members	U.K. Deiters T.W. De Loos J.P.-E. Grolier T.M. Letcher
Associate Members	V.A. Durov M.A.V. Ribeiro da Silva A. Schiraldi M. Sorai E. Vogel M.A. White
National Representatives	T. Boublik G. Kaptay I. Wadsö
Observers	J.M.G. Barthel D.G. Friend
Present during part of the meeting	T. Cvitas (Sunday, item 2.14) G. Della Gata (Monday, Tuesday) A. Heintz (Sunday) G. Somsen (Tuesday, item 2.14) J.M.P. Trusler (Monday) W.A. Wakeham (Monday) G. Wilson (Sunday, item 2.14)

1. Preliminary Matters and Announcements

Opening of Meeting at 0900h, Sunday 8 August 1999.

The Chair welcomed and introduced those present. He noted that the following were unable to attend: J.C. Ahluwalia, C. Airoldi, R.A. Alberty, J.A.R. Cheda, A.R.H. Goodwin, J.L. Laynez, K. Murphy, H. Pak, F. Rouquerol, S. Stølen, Hai-Ke Yan.

1.05 The Agenda was accepted as written.

1.1 The Porto (1998) 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 according to plan. Publications circulated were the book volumes *Viscosities of Aqueous Solutions* Part 3c, $AgClO_4$ - $Cl_4O_{16}Th$ and Part 3d, CoO_4S-O_6SU, J. Barthel, R. Neueder and R. Meier 1998, Dechema Chemistry Data Series Vol. XII. The volume on

Conductivities, Transference Numbers and Limiting Ionic Conductivities, Part 1d. Carbonates, Dechema Chemistry Data Series Vol X is in press, and a further volume on Amides is expected in 2001.

Commission I.2 congratulated Professor Barthel and his group for their impressive output. It was noted that new Project Submission Forms should be completed after the Halifax meeting for future books.

2.2 Participation of Commission I.2 in IUPAC's "Horizontal Projects".

2.2.1 Chemistry of Advanced Materials. Reporter: Weir

Weir reported that this project was now complete

2.3 Recommendations regarding Legendre Transforms in Chemical Thermodynamics Reporter: Weir

Weir reported that Professor Alberty had written to Prof. Plieth, Commission I.3, to try to resolve the difficulties with Section 3.2 of the report. Alberty had suggested that Plieth might write an addendum to be published with the report. It was agreed to take this forward to the Joint Meeting with I.3 [see under 5.05]

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

Blackwell Scientific declined to publish the book when the draft copy greatly exceeded the agreed length, and the volume will now be published by Elsevier. As a result of the delay in finding a new publisher, authors had been requested to up-date their chapters by September 1st 1999 with an expected publication date of March 2000. Some authors had asked for a longer period to revise their chapters but this should not delay publication by more than a month or two.

2.5 Nomenclature for Phase Diagrams with Particular Reference to Vapour-Liquid and Liquid-Liquid Equilbria. Reporter: De Loos/Deiters

This project was completed with publication of the paper in *Pure and Applied Chemistry* 70 (1998) 2233-2257. Copies are to be submitted to the *Journal of Chemical Thermodynamics* and *Fluid Phase Equilibria* and a synopsis prepared for the *Journal of Chemical Education*.

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

Ribeiro da Silva presented a final draft of this paper. Publication is planned in the *Journal of Chemical Thermodynamics* and *Pure & Applied Chemistry*. [See also 5.04].

Commission members were invited to send comments to Ribeiro da Silva

2.7 Subcommittee on Thermodynamic Data. Reporter: Deiters

The current state of the projects as follows:

a. Critical Compilation of Vapour Liquid Critical Properties.

The coordinator Dr. Young has now retired from the project. His preliminary draft on halogenated compounds has passed to K. Marsh who, with Dymond, will complete this major contribution following a computer search to cover recent years. A paper on oxygenated compounds other than alkanols is in an advanced state of preparation. Work is still outstanding on nitrogen-containing compounds and poly-functional compounds; these may be the subject of new projects following the Halifax meeting.

b. Critical Compilation of Activity Coefficients at Infinite Dilution.

A very large database has been developed with more values to be derived from other experimental measurements. Unfortunately, a lack of sufficient time for the coordinator to work on this project, together with the practical difficulty of finding suitable international collaboration, has led to the reluctant decision to terminate this worthwhile project. It is hoped that this might become a new project at a later time if circumstances change.

c. International Thermodynamic Tables of the Fluid State. Benzene.

This project had come to a halt, following the development of a Helmholtz equation of state for the whole fluid surface, as a result of termination of funding for this work. As a result of a successful application to IUPAC for financial support, the volume could be now be completed with assistance to prepare tables and help with the graphics work. Publication is planned for 2000.

d. International Tables of the Fluid State. Carbon Dioxide.

Work on this IUPAC volume had come to a halt due to pressing engagements by Wagner and Span at Bochum. Span was now able to resume collaboration. Publication is planned for 2000.

e. Vapour-Liquid Equilibria and Related Properties in Binary and Ternary Mixtures of Ethers, Alkanes, and Alkanols.

The final workshop of this project was held as part of the 15th ICCT (IUPAC) in Porto, Portugal, 30-31 July 1998. The workshop proceedings were published as a special issue of *Fluid Phase Equilibria* 156 (1999) 1-236. The project is now completed.

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

The first workshop of this new project is being organised by Professor Matteoli in Pisa December 15-18, 1999. The scope of this meeting will be quite general, with attention to be focussed on a few key systems for later workshops. The response to the first circular was good, with 65 intending participants and some 60 presentations (oral plus poster) offered. A successful application has been made to IUPAC for financial support for scientists from the former eastern-bloc countries.

Publication of the proceedings is planned for *Fluid Phase Equilibria*, with Matteoli and Deiters as Guest Editors.

g. Heintz reported their intention to start a new project on low temperature molten salts (organic), which are useful as solvents because of low vapour pressure in chemical reactions and catalytic systems, with a workshop in 2001.

Heintz and Deiters will complete a New Project Submission Form.

Membership:

Dr. R. Span (Bochum) was proposed as a new member of the subcommittee; the Commission approved.

Members of Commission I.2 thanked U. Deiters and the members of the Subcommittee and the other volunteers for all their work.

2.8 Subcommittee on Transport Properties. Reporter: Wakeham

Wakeham reported on the current state of the projects:

122/1/83 Definitive correlation of transport properties of fluids
Work has been completed on the viscosity of toluene at atmospheric pressure/saturation line and on the thermal conductivity of propane.
New projects are on the viscosity of toluene as a function of pressure; viscosity of iso-butane; study of the intermolecular potential of water and viscosity of alkali halides.
The round-robin on the transport properties of R134a is completed. The report will be written by 2001.
Publications will appear shortly on the following: viscosity of toluene at atmospheric pressure/saturation line; viscosity of butane; and thermal conductivity of propane. Already published is Reference correlation on the viscosity of propane, E. Vogel, C. Kuchenmeister, E. Bich and A. Laesecke, J. Phys. Chem. Ref. Data 27 (1998) 947-970.

122/2/85 Internationally available data bank.
This project is now terminated, though the Stuttgart data bank was still being maintained for use of subcommittee members and others.

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

Work is proceeding to obtain international agreement on the viscosity of liquid water, and to propose a suitable fluid with a viscosity some 100 to 1000 times that of water as an additional viscosity standard.

122/4/91 Transport properties of fluids - theory and representation
Work is this area is in progress.

It is planned to start a new project on transport properties of molten metals where differences in viscosity of a factor of 10 occur in measurements from different groups. The results of a feasibility study will be presented at the Commission meeting in Halifax. Because of the large discrepancies in the literature viscosity data for toluene at elevated pressures, a new experimental project will probably be set up in 2001.

The next meeting of the subcommittee will be September 3 and 4, 1999 in Erlangen, Germany, prior to the 15th. European Thermophysical Properties Conference.

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

2.9 New Edition of Experimental Thermodynamics Vol II. Reporter: Weir

Volume VI. *Measurement of the Thermodynamic Properties of Single Phases* : Editors: Goodwin, Marsh and Wakeham. The ten Chapters comprise 31 sections. Contributions had been requested by end-May, but authors of 18 sections had still to submit manuscripts. These would probably all be received by end-December. There were problems with two sections, where authors had withdrawn. The one on Silicon Spheres as Mass Standards would be omitted and a new author was required for the section on Molten Salts. Kaptay has possible contacts for this.

Volume VII. *Measurement of the Properties of Multiple Phases*: Editors: de Loos and Weir. The timescale is similar to that for volume VI. A new author is required for Chapter 7.

As a result of IUPAC taking over the publication of *Pure and Applied Chemistry*, Blackwell Scientific will no longer publish IUPAC monographs. It is necessary to find a new publisher for these volumes - a number of possibilities were suggested. Publication is expected by 2001.

2.10 16th ICCT, 7-11 Aug 2000, Halifax, Canada. Reporter: White

Hotel rooms and dormitory accommodation have been booked, as have the meeting rooms, which will be on campus at Dalhousie University. Professor White pointed out the substantial savings to be made from use of a campus site ($50 000 in this case).
It was planned to raise at least $40 000, the minimum for a good conference; so far 28% had been secured. Sponsors prefer to give money for specific purposes such as funding a plenary lecturer, or taking advertising space in conference booklets.

White outlined the symposia: Connections between theory and experiment; Thermodynamics of materials [battery materials, molecular materials, session in honour of P.A.G. O'Hare, pharmaceutical materials, superconductors, others]; Thermodynamics of nuclear materials; Biological thermodynamics; Symposium on standards (in honour of NIST's 100th. anniversary); fluids and fluid mixtures; Other aspects of chemical thermodynamics; new approaches to thermodynamics education. It was hoped that NIST would contribute funds as the Symposium in their honour was being held at their request.

Details were also given in a handout on Sponsors and Exhibitors, Internationary Advisory Committee, Conference Organizing Committee and Scientific Program Committee.

The email list of potential participants is being compiled and the first "flyer" will be sent out in September to be followed shortly thereafter by a "call for papers". All correspondence is to be done through email and the website [http://is.dal.ca/~icct].

It was suggested to hold workshops on Global phase diagrams (Deiters) and applications of thermodynamics to food science (Schiraldi).

Weir thanked White for her report and wished her well with the future organization.

2.11 17th. ICCT,` 28th. July to 2nd. August, 2002, Rostock, Germany Reporters: Heintz, Vogel

Heintz and Vogel gave preliminary details. The registration fee will be about $250 (depending on the level of sponsorship). Low cost accommodation is available. Meetings will take place in the City Hall, with the possibility of several parallel sessions.

It is planned to have 7 sections: Molecular modelling and statistical thermodynamics, Nonelectrolytes, Complex reacting mixtures, Fluid phase equilibria (including Global phase diagrams), Surface Chemistry, New and advanced materials (including polymers), and Biothermodynamics (including pharmaceuticals). Workshops will be held on Thermochemical, thermodynamic and transport properties of halogenated compounds and mixtures, calorimetry and membranes (including solubility and transport).

A copy of the IUPAC Sponsorship form as completed for the Halifax meeting will be sent to Heintz and Vogel to aid completion of the form for Sponsorship of the 17th. ICCT.

2.12 Venue for the 18th. ICCT meeting in 2004.

The offer for Greece (2.12.3) having been withdrawn, there were two offers remaining, China (2.12.1) and Spain (2.12.2). It was agreed that Weir would define what we require and ask Yan and Cheda to provide the necessary detailed information so that a decision could be made at the Commission meeting in Halifax in 2000.

Weir will send full details to members from those offering to host the 2004 ICCT one month in advance of the Halifax meeting .

2.12.1 Beijing, P.R. China Reporter: Weir

Professor Hai-Ke Yan was unfortunately unable to be present, but Professor J.-S. He from Commission IV.2 presented a series of slides showing the International Convention Centre in north-east Beijing (the proposed site for the Conference) with its 2500-seater theatre and many smaller air-conditioned rooms suitable for parallel sessions; the 4-star International Hotel with Banqueting Hall for 1000 within 3 minutes walk of the Conference site; and lower-cost accommodation at a further distance from the Convention Centre.

The proposed registration fee was $350, to include a reception, a conference dinner and daily refreshments. Students would pay $175. Professor He thought that a half-day tour might be included in this fee. He quoted hotel prices ranging from $70 to 80 per person in the 4-star hotel down to $15 per person in cheaper hotels.

Wadsö indicated that this was a conscientious group who would organise a good conference. Members pointed out the increased number of publications from Chinese thermodynamicists, the need to encourage them and the fact that only one previous ICCT had been held in Asia. Questions were asked about the distance of the cheaper accommodation from the Convention Centre. It was agreed that transport by bus would be a great advantage. White recommended that ICTAC and ICCT be held in the same venue at the same time in 2004.

It was agreed that Weir would write to Yan to check the dates with a note of further questions, including the possibility of an excursion covered by the registration fee. He will also contact ICTAC.

2.12.2 Near Madrid, Spain Reporter: Weir

Weir reported (Tuesday) that a package had been received from Cheda the previous evening, with a formal letter of invitation from Professor Nunez Dalgado, Head of the Physical Chemistry Department, Universidad Complutense de Madrid, to host the 18th ICCT in July 2004. Meetings would be held in the Faculty of Medicine at the University, with additional lecture rooms available in a nearby faculty if it was necessary to have more than 4 parallel sessions. Accommodation in hotels would cost from US$ 70 to US$ 190 (20 to 30 mins walk to the Conference; metro alternative) with dormitory accommodation available at the Conference site from US$ 30 to US$ 60. Registration fees would be US$ 370, or US$ 140 for students, paid 3 months early, otherwise US$ 450 and US$ 200. Proposed Conference topics were Statistical Thermodynamics, Thermodynamics of Materials, Biological Thermodynamics, Colloids and Surfaces, Thermodynamic Standards, Experimental Thermodynamics, Theoretical Thermo-dynamics and Modelling, Thermodynamics Education and Other Topics.

Members queried the stated intention to hold the meeting concurrently with the "Mediterranean Conference on Calorimetry and Thermal Analysis", which would have to be rescheduled to take place in 2004.

It was agreed that Weir would write to Cheda with a note of further questions to establish, for example, what was covered by the registration fee.

2.12.3 Greece Reporter: Weir

It was reported that Professor Panayiotou had withdrawn his offer to host the 18th. ICCT in 2004 because of the higher costs associated with the holding of the Olympics in Greece that year
He indicated that 2006 would be more suitable for hosting the Conference in Greece.

2.13 Guidebook for Organizers of IUPAC ICCTs. Reporter: Wier

The value of this information to prospective organizers would be greatly enhanced by having the information on diskette. Professor Grolier undertook to arrange this. It is important also to have available the mailing list from the most recent conference.

2.14 Forthcoming change in IUPAC operation Reporter: Wier

Weir reported that the present Commission structure of IUPAC would cease at the end of 2001. All current projects would have to be completed by that date or else would have to be submitted as new projects under the new project-based system which had been in position since January. Funding would in future be available for approved projects. Professors Cvitas (president) and Wilson (vice-president) of the Physical Chemistry Division Committee joined us to answer questions about the effect of these changes. Approval of new projects will be given by the Division Committee which, for the period 1999-2001 will consist of the officers plus Commission chairmen. The composition post-2001 has not been decided.

Our ICCTs would continue to receive IUPAC sponsorship following satisfactory completion of the Advance Information Questionnaire, but no funding is associated with this. For funding, it would be necessary to submit a proposal to hold an ICCT as a new project.

There was further discussion by members on Tuesday, when Professor Somsen (past-president of the Physical Chemistry Division Committee) was present. The Commission felt that its activities would translate smoothly to the new scheme, with continuation of the biennial ICCT affording an opportunity for a meeting of all those involved in projects, plus other interested thermodynamicists.

Weir thanked the officers of the Physical Chemistry Division Committee for coming to talk to the Commission.

2.15 Guidelines for Publication of Equations of State Reporter: Deiters

The Guidelines appeared in *Chemical Engineering Science*, 69 (1998) 69-81 and it is planned to publish the article also in *Fluid Phase Equilibria*. Deiters has copies for distribution to members.
This project is now complete.

2.16 Guidelines for Publication of Equations of State II. Mixtures Reporter: Deiters

Deiters reported that he was getting together a team to work on this project, and would give a further report at the Commission meeting in Halifax.

2.17 Chemical Thermodynamics in the 21st. Century in Industry, Chemical Technology, Biochemistry and Medicine Reporter: Letcher

This project is now complete following publication by Blackwells Scientific. A description of the book appeared in *Chemistry International* 21 (1999) 84-85, and it is to be reviewed in the *Journal of Chemical Thermodynamics.*

2.18 Global Phase Diagrams of Fluid Mixtures Reporters: Deiters, Boublik

A workshop held near Cologne towards the end of March 1999 attracted about 50 participants. The proceedings will appear in PCCP in the final edition this year/ first edition next year.

Deiters and Boublik will report on the feasibility of a new project at the Commission meeting in Halifax in 2000.

2.19 Biological Buffers: Data Required and the Feasibility Study Reporter: Weir

There was no report as Murphy was absent. Wadsö stressed the importance of this topic and suggested we discuss it with Commission I.7.

[Joint meeting with Commission I.7: see under 5.06]

2.20 The Journal of Chemical Thermodynamics. Reporters: Wakeham/Weir

Weir reported that the recent changes to include papers in fluid phase equilibria, biochemical thermodynamics, polymers and invited review articles had been very successful. Statistics for the past three years were as follows:

	Papers submitted	Papers accepted	Printed pages	Time from receipt to acceptance
1996	161	127	1460	104 days
1997	170	137	1554	109 days
1998	149	127	1631	107 days

Some adverse comments were expressed about the cost of the journal and the length of the reviewing process. Little can be done about the former, and the latter was generally considered very reasonable for a reputable journal with a serious refereeing process. Delays often arose from authors taking time to revise their manuscripts

The special memorial issue for Professor McGlashan will contain 14 papers and should be published in October.

2.21 Standards, Calibration and Guidelines in MicroCalorimetry Reporter: Wadsö

Wadsö presented a draft paper entitled “Standards in Isothermal Microcalorimetery”, from the working group A.E. Beezer, G. Olofsson, K. Murphy, F. Rouquerol, J. Sipowska and I. Wadsö and invited comments from Commission members.

Della Gatta invited comments on the draft “Standards for Differential Scanning Calorimetry”, prodced by the working group G. Della Gatta, M.J. Richardson, S.M. Sarge and S. Stølen. He commented on the good collaboration from members of the group.

It was planned to produce these in final form for the Commission meeting in Halifax, 2000, for subsequent publication in the *Journal of Chemical Thermodynamics*, *Thermochimica Acta* and *Calorimetry and Thermal Analysis*.

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. Secondary publications should also be considered.

2.22 IUPAC Project on Thermochemical, Thermodynamic and Transport Properties of Halo-compounds and Mixtures Reporter : Deiters

This was taken as part of item 2.7

2.23 New Calorimetric Techniques Reporter: Wadsö

Wadsö reported that there was a real need for a guide for new users. He had decided to write a non-IUPAC book with his son, so this would not be a new IUPAC project.

2.24 Thermodynamics in Education Reporter: Letcher

Letcher said that he planned to explore with others with a special interest in education whether it was worthwhile to initiate a new project in this area, and would report at the Commission meeting in Halifax.

3.0 Finances of the I.2 Commission. Reporter: Weir

Weir reported that the Physical Chemistry Division would have $52 000 for 2000, of which some $12 000 was earmarked for a Division Committee meeting. This averaged out to about $6 000 per Commission for projects. In addition, the Treasurer had reserves of $270 000. For large projects or inter-Divisional projects, application should be made to the Project Committee.

[After the meeting, Weir and Dymond estimated the funding requirements for approved projects for 2000 and 2001 to be $ 11 500 and $7 500 respectively. These were placed before the Division Committee.]

4.0 Membership Reporter: Weir

Under the regulations, the number of Titular Members in the Commission should be 8; current membership is 6. At a meeting of the Titular Members, it was agreed to propose Professor E. Vogel and Prof. M.A.V. Ribeiro de Silva as Titular Members.

[These were approved at the Bureau meeting].

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. Members are asked to communicate any changes to the secretary.

5.0 Other business

5.01 Weir noted that the next meeting of Commission I.2 would take place in Halifax, Nova Scotia on August 5 and 6, 2000.

5.02 Web site. Dr. Fabienne Meyers, IUPAC secretariat, joined us for a short meeting on Tuesday when she spoke about the IUPAC web site map (*Chemistry International* 21 (1999) 113) and described the contents of the Home page, News and notices, Organizations and people, Standing Committees, Divisions, Projects, Reports and recommendations, Publications and Conferences and Symposia. Project descriptions should be checked by coordinators; additions/ corrections should be sent to fabienne@iupac.org. Additional information can be placed in separate folders.

It was considered by members that we should have our own web site so that we could highlight our activities and achievements and draw attention to future events. Della Gatta offered help in setting this up. Members are asked to send ideas for the web page to the Secretary or Chairman.

<u>It was agreed that Dymond and Weir would agree the format of the web page with the aim of opening it for January 1st. 2000.</u>

<u>Weir will write to Della Gatta's University regarding the possibility of their setting up the web site.</u>

5.03 Joint IUPAC-CODATA Project on Standardization of Physico-Chemical Property Electronic Data Files
Reporter: Kehiaian

Dymond opened the 30 minute meeting by welcoming the many members of IUCOSPED, and described the various data activities of the Commission and its subcommittees. He stated the need for a universally-agreed format for data storage and exchange through the Internet, with programmes to convert to and from the format used in various publications and by participants in each project.

Kehiaian (IUCOSPED Project Coordinator) introduced the project which is specifically to design computer-readable Standardized Electronic File Formats (SELF Formats) for presenting numerical data, as well as metadata, on physico-chemical properties as they appear in primary sources. This project will involve not only data users, but also data publishers, data centres and data bank managers. Authors will

be encouraged to submit to the journal editors their data in the SELF Format, in parallel with their article. Each publisher of data, whether printed or electronic, can continue with their own usual format for each particular property, but the objective is to have the data available for each property from all sources in uniformly documented SELF format. This will greatly improve data extraction and dissemination.

Kehiaian pointed out that the project had been awarded $ 100 000 under the ICSU Grants Programme 2000 for new innovative projects. The membership of IUCOSPED includes 17 property experts, 7 database or software developers, 6 members of important organizations plus 3 members associated with CODATA.

IUCOSPED meetings in Berlin would consider existing data file formats and proposals for SELF formats, definitions and standardization of electronic data files and examples of property data and their presentation.

Weir wished IUCOSPED well in their endeavours which would greatly improve our work of data collection from journals and data sharing.

5.04 Joint meeting with Commission I.1 on Physicochemical Symbols, Terminology and Units

Reporter: Weir

Definitions for the Green Book

Weir welcomed members of Commission I.1 and reported that the changes noted in the Geneva minutes would appear in the next edition of the Green Book. There was some discussion about the term "thermal power". It was agreed that this should appear in the section on Chemical Thermodynamics.

Wadsö raised the question of notation for "apparent molar volume". It was agreed that a superscript "app" should appear in the section on Chemical thermodynamics.

Strauss (chairman I.1) reported that it was the intention to complete the draft of the Green Book by September 1999 with publication about mid-2000. They were looking into the possibility of a web site for greater availability.

Thermochemistry of Chemical Reactions [Item 2.6]

There was some discussion over choice of some symbols. Mills (I.1) agreed to send written comments to Ribeiro da Silva. Other commission members were invited to comment.

Standards in Isothermal Microcalorimetry [part of Item 2.21]

The use of "isothermal" when conditions were not strictly isothermal was discussed. It was suggested that quotation marks might be used with a clear definition given in the text.

Weir thanked members of I.1 for their helpful cooperation.

5.05 Joint meeting with Commission I.3 on Electrochemistry. Reporter: Weir

Recommendations regarding Legendre Transforms in Chemical Thermodynamics

At the Joint Meeting, attended by W. Plieth, C. Brett, G. Wilson, D. Schiffrin and J. Rusling, of the Commission on Electrochemistry, Weir summarised the history of this project, through the 6 draft reports, and suggested that I.3 might write an addendum to point out that there was an alternative method of approach to electrochemical potential. After discussion, the feeling was that this would not be appropriate for an IUPAC publication but rather that Alberty should be asked to revise the section to fit in with the definition in the Green Book. Schiffrin agreed to draft a revised version of the relevant section by the end of October. Once agreement has been reached, the publication will be submitted to *Pure and Applied Chemistry* and the *Journal of Chemical Thermodynamics*. It was suggested that an abridged version would be useful for workers in biochemistry.

Weir thanked members of I.3 for their constructive comments and assistance for the completion of this project.

5.06 Joint meeting with Commission I.7 on Biophysical Chemistry. Reporter: Weir

a) Biological Buffers

Weir welcomed members of Commission I.7 [Hauser (chair), Goldberg (Secretary), Wüthrich, Eisenberg, Kitigawa, Thévenot] and referred to the Geneva minutes where it was stated that Goldberg would contact Murphy to build a group and promote a horizontal project between I.2 and I.7. Goldberg stated that there was a need for pK's, and ΔH and ΔC_p for ionization for some 20 to 40 buffers. This would involve a fair amount of data collection from different experiment-al studies, but would be a very useful project, especially with a computer programme for calculation of the composition of solutions at given temperature and ionic strength. This would probably take 1 year full-time.

Weir agreed to contact Murphy to find out his position concerning this project.

b) Recommendations for the measurement and analysis of results obtained on biological solutions with DSC

Hauser presented this draft manuscript, authored by H.-J. Hinz and F.P. Schwartz, and invited comments from members of I.2. Input was also to be sought at the Calorimetry Conference. The intention was to publish it in *Pure and Applied Chemistry* and then in biological journals.

Members of I.2 are asked to send comments to Hauser.

c) Standards in Isothermal Microcalorimetry [part of Item 2.21]

The use of "isothermal" was discussed. It was suggested that quotation marks might be used with a clear definition given in the text. Wadsö requested comments on this document to be sent as soon as possible.

Kaptay mentioned that there was no reference to high-temperature calorimeters. Wadsö agreed to look into this, but noted that there was a lack of reference data.

d) Standards for Differential Scanning Calorimetry [part of Item 2.21]

Della Gatta gave copies of this manuscript to members of I.7 and invited their comments.

Weir thanked members of Commission I.7 for their helpful discussions.

Membership I.2 Commission
as approved at the 69th Bureau meeting 14 Aug 99

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	Prof. 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. Boublík	Czech Republic
1998-2001	Prof. G. Kaptay	Hungary
1994-2001	Dr. J.L. Laynez	Spain
1996-2001	Professor Hyungsuk Pak	Republic of Korea
1994-2001	Dr. I. Wadsö	Sweden
1996-2001	Professor Hai-Ke Yan	P.R. China

ANNEX A

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