# *International Association of Chemical Thermodynamics*
# IACT

**Minutes of the Meeting of the Board of Directors**
**Salon Leo (4F), Tsukuba International Congress Center**
**(Epochal Tsukuba)**
**Sunday August 1st 2010 from 10.30 to 11.50**

Present at the meeting:

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| Chairman | Dr. A.R.H. Goodwin |
| Past Chair | Prof. J.-P. E. Grolier |
| Secretary | Dr. J.H. Dymond |
| Treasurer | Prof. T.W. De Loos |
| Members | Prof. T. Atake |
| | Prof. M. Frenkel |
| Counsellors | Prof. Watson Loh |
| | Prof. Li-Xian Sun |
| | Prof. Mary Anne White |
| Observers | Dr. R. Chirico |
| | Prof. J. Fernández |

**1. Preliminary Matters, and any Announcements**

The Chairman opened the meeting by welcoming everyone. The agenda was approved without change.

**2. Apologies**

Apologies were received from Prof. J. Boerio-Goates, Prof. E Vogel, Prof. T.M. Letcher, Prof. S. Randzio, Prof. J.P.M. Trusler, Prof A. Victorov, and Prof. W.A. Wakeham.

**3. Minutes of the Santiago de Compostela Meeting, 2009**

The Minutes of the Meetings held in Santiago de Compostela, Spain on July 2nd 2009 were approved and signed.

**4. Secretary's Business**

**4.1 *IACT Publicity at 21st ICCT***

It was agreed to display the IACT banner on the front of the table on stage at the IACT Business Meeting on Thursday.

**4.2 *IACT Awards 2010***

Rossini Lectureship Award Winner:

The 2010 Rossini Award winner is Prof. Dr. Gerd Maurer from the Department of Mechanical and Process Engineering, University of Kaiserslautern, Germany who will present the Rossini Lecture on *Phase Equilibria in Chemical Reactive Fluid Mixtures*. The certificate will be presented by Dr. Goodwin immediately before his lecture. Prof. Maurer will be introduced by Prof. R. Weir.

2010 Junior Award Winners:

There were 12 applications for the Junior Awards this year. A committee was set up under Prof. J-.E. Grolier to review these applications – other members were Prof. T. Atake and Prof. S.L. Randzio. The Committee reviewed and ranked the applicants independently and arrived at practically the same ranking. Besides the scientific "weight", the age, sex and country were also taken into consideration. The Committee considered that the first five candidates deserve receiving the Award. They further considered the total number of candidates and that the Award is not only a financial help to participate to the ICCT 2010 but also an honorific distinction to encourage young researchers, and suggested that the number of Awardees could be increased by one or two. As a result of discussion with the ICCT Conference Organisers, it was decided that 7 awards would be made in 2010. It is to be noted that they represent 5 different countries; there are four male and three female winners.

Thanks were expressed to Prof. Grolier and his committee.

The award winners are:

Dr. Yoshimitsu KOHAMA (male, age 29, Japan), PhD Tokyo Institute of Technology, Post Doc Los Alamos National Laboratory. *AC Specific Heat and Magnetocaloric Effect Measurements for Short Pulsed Magnetic Fields.*

Dr. Takeshi YAMADA (male, age 29, Japan), PhD Tokyo Metropolitan University and University Blaise Pascal Clermont-Ferrand, Post Doc Institute for Solid State Physics Tokyo, Japan. *Phase Transitions and Dynamics of Water in Nano-Porous Copper Rubeanate.*

Dr. Ala BAZYLEVA (female, age 28, Belarus), PhD Belarusian State University Minsk, Post Doc University of Alberta Edmonton, Canada. *Phase behavior of Athabasca bitumen*.

Dr. Gennady GOR (male, age 28, Russia), PhD (in Physics) St Petersburg State University, Post Doc Rutgers State University of New Jersey, U.S.A.. *Thermodynamics of Adsorption-Induced Deformation of Mesoporous Solids.*

M.S. SANTOSH (male, age 25, India), PhD expected date 2011 National Institute of Technology Mangalore, India. *Volumetric, Refractometric and Excess Properties of Glycylglycine in Aqueous FeCl2 solution at temperatures T = (288.15 to 318.15) K.*

Maria TOIKKA (female, age 25, Russia), PhD (in Chemistry) expected date 2010 St Petersburg State University, Russia. *Experimental Study of Thermodynamic Peculiarities of the Reacting Systems: Critical States, Phase and Chemical Equilibrium in the Quaternary System with Ester Synthesis Reaction*.

Hongli LIU (female, age 29, China), PhD in progress within a "sandwich program" between Hunan Central University (China) and Osaka Kinki University, Japan. *Thermodynamic Properties of o-, m- and p-Structure Isomers.*

Framed Certificates will be presented to these award winners by Dr. Goodwin just before the IACT Business Meeting.

IUPAC Poster Prizes: IUPAC has offered 3 Poster Awards to this Conference. The winners will each receive a certificate and a personal copy of the Green Book.

There will be six judges as there are 304 posters. Three judges are from IACT (Dr. J. Dymond, Dr. M. Frenkel and Prof. T.M. Letcher) and three appointed by the ICCT Organising Committee.

Presentation of the Poster Prizes will be made by Dr. Dymond during the Closing Ceremony on August 6$^{th}$ in the Main Hall of the Tsukuba International Congress Centre.

**4.3** ***Arrangements for the IACT Business Meeting***

a) The meeting will be preceded by the following Presentations, chaired by Dr. Chirico, each of which will be 10-minutes followed by a short (5 min.) question session:

Extension of ThermoML - the IUPAC standard for thermodynamic data communications: M. Frenkel and R. Chirico

Applied Thermodynamics of Fluids – A.R.H. Goodwin

Guidelines for temperature modulated DSC - J.-P. E. Grolier

Thermodynamic study on hydrogen storage materials of metal organic frameworks and metal hydrides - Li-Xian Sun

b) The presentations of Junior awards will then be made.

c) As per last time, slides have been prepared in PowerPoint for the Business meeting, with the following information posted on the IACT website:

- Agenda
- Minutes of the Warsaw meeting
- Financial statement

**4.4** ***Arrangements for the 2010 Election to the Board of Directors***

The composition of the present Board is:

*Elected Members:*

Prof. J.-P. Grolier, Clermont-Ferrand, France (past Chairman) (2008-2012)

Prof. Julie Boerio-Goates, Provo, Utah, U.S.A . (2008-2012) [first term]

Dr. J.H. Dymond, Glasgow, UK (Secretary) (retires 2010)

Prof. Tooru Atake, Yokohama, Japan (2008-2012) [second term]

Prof. Th. W. De Loos, Delft, The Netherlands (Treasurer) (retires 2010)

Dr. Michael Frenkel, Boulder, Colorado, U.S.A. (retires 2010)

Dr. Anthony R.H. Goodwin, Sugarland, Texas U.S.A.(Chairman) (2008-2012)

Prof. T.M. Letcher, Durban, South Africa (retires 2010)

Prof. Alexey Victorov, St. Petersburg, Russia (2008-2012) [first term]

Prof. Eckhard Vogel, Rostock, Germany (retires 2010)

Prof. W.A. Wakeham, Southampton, UK (2008-2012) [first term]

*Counsellors:*

Prof. Watson Loh, Campinas, SP, Brazil (2008-2012) [first term]

Prof. Stanislaw Randzio, Warsaw, Poland (first term ends 2010)

Prof. Li-Xian Sun, Dalian, China (first term ends 2010)

Prof. J.P. Martin Trusler, Imperial College, London, UK (2008-2012) [first term]

Prof. Mary Anne White, Halifax, Canada (Counsellor, retires 2010)

Five Board Members, plus one Counsellor, will be retiring in 2010. Dr. Goodwin expressed thanks to all those retiring at this time.

As per the Constitution, a Nominating Committee of three Board members was set up: Profs. Ron Weir (chairman), Trevor Letcher and Jean-Pierre Grolier. A list of five candidates was proposed. All five have agreed to allow their names to stand for election.

Dr. Robert (Rob) Chirico (U.S.A.)

Professor Josefa Fernandez (Spain)

Professor Luis Galicia-Luna (Mexico).

Professor Manual Minas de Piedade (Portugal)

Professor Derish Ramjugernath (South Africa).

This slate of nominees was posted on the IACT website, with an invitation to submit additional names, but none were forthcoming. Board members recommended approval of these nominations, for confirmation at the Business Meeting.

**4.5** ***Arrangements for the Election of the Chair-Elect, Secretary and Treasurer***

Dr. Chirico was appointed as Secretary. This leaves the position of Chair-Elect and Treasurer still to be filled.

**4.6** ***Arrangements for the Appointment of Counsellor***

It was noted that there is a vacancy for one Counsellor.

**5. Treasurer's Report**

The Santander bank balance at April 27th 2009 was GBP 5639.93. There was no cash on hand.

In this financial year, IACT has received USD 1000 (£672.63) donation from Elsevier for the Junior Awards, and £40.39 in bank interest. The only payment was for "life membership" as an Associated Organisation for USD 1000 (£633.19, with bank transfer fee of £25). The bank balance at April 26th 2010 was GBP 5694.76.

Adoption of the accounts was moved by Prof. Frenkel and seconded by Prof. White, and unanimously approved.

It was noted that as Prof. de Loos retires as Treasurer at this Business Meeting, arrangements should be made by the new Board to have the accounts independently examined.

**6. 21st ICCT-2010, Tsukuba, Japan**

Prof. Atake reported that, earlier this year, the Japanese Government had contacted the organisers to say that their Majesties, the Emperor and Empress of Japan, would be attending the Opening Ceremony and Welcome Reception. This was a great honour, but the information had to be kept confidential until close to the time of the Conference.

He said that financially the Conference was sound. Information on the numbers of participants would be given at the Closing Ceremony.

**7. Update on Projects : Project Leader's name in parentheses**

**7.1** ***Project on Thermochemistry of Chemical Reactions*** **[M.A.V. Ribeiro da Silva]**

This is a long-running project. Prof. Manuel A. V. Ribeiro da Silva had divided his original manuscript into two sections: *Thermochemistry of Chemical Reactions: 1 Terminology and Symbols* (Recommendations) and *Thermochemistry of Chemical Reactions: II. Experimental Methods for the Determination of Bond Energies* (Technical Report).

Members of the IUPAC Division 1 Physical and Bio-Physical Chemistry Division Committee commented that with the passing of time, Part II should be updated to include important new methods. There had also been critical comments from one or two members of ICTNS about Part I. Prof. Weir (new ICTNS President) was keen to see a conclusion to this project and had suggested that the two documents be reunited as a Technical report (which does not require unanimous approval of reviewers, as is the case for an IUPAC Recommendation). In view of Professor Ribeira da Silva's understandable reluctance to embark on yet another revision, the Division I Committee at its recent meeting suggested that this project should now be written off. However, Prof. Weir was still trying to encourage Prof. Manuel da Silva to revise his manuscripts.

**7.2** ***Project on Guidelines for Modulated-Temperature Differential Scanning Calorimetry*** **[J.-P.E. Grolier]**

Prof. Grolier will meet co-editors in Tsukuba to discuss the contributions. The final document will be prepared as soon as possible.

**7.3** ***Vapour-Liquid Critical Properties*** **[K.N. Marsh]**

Prof. Ken Marsh will work with Profs. Costa Tsonopoulos and Eugene Nikitin on part 12 that will update the early parts (2, 3, 5, and 6; published in 1995 and 1996) on hydrocarbons.

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

The project was satisfactorily concluded with the publication of this paper in *J. Phys. Chem. Ref. Data.* Vol. 39, No. 1 (2010) (404 pages).

**7.5** ***Establishing Recommended Data on Thermodynamic Properties of Hydration for Selected Organic Solutes*** **[J. Sedbauer]**

Data retrieval from literature sources has been completed, the hydration properties (in most cases recalculated from their original format) entered into the databases, and data processing finished. Submission of the manuscript and accompanying databases is expected shortly, followed by submission of drafts of the IUPAC Technical Report and the IAPWS Guideline.

The project will be presented at two conferences this year, each of them attended by one person from the Task Group:

The 20th International Conference on Physical Organic Chemistry, Busan, Korea, 22-28 August 2010.

14th International Symposium on Solubility Phenomena and Related Equilibrium Processes, Leoben, Austria, July 25-30 2010.

Board members recommended that :

i. Publication should be in J. Phys. Chem. Ref. Data.

ii. Dr. Sedbauer should contact Dr. Frenkel regarding the database.

iii. Dr. Sedbauer should contact IUPAC regarding the financing of publicity after the end of a project. It may be necessary to make a new project proposal.

**7.6** ***Guidelines for Reporting of Phase Equilibria Measurements*** **[T.W. de Loos]**

There was a delay due to the illness a key contributor, Dr Gupta.

**7.7** ***Experimental Thermodynamics: Applied Thermodynamics of Fluids*** **[A.R.H. Goodwin]**

The book was reviewed by Ron Weir and Jack Lorimer (ICTNS) and a revised version prepared and sent to the publisher. This volume (14 chapters and 500 pp.) will be available in November 2010.

**7.8** ***Heat Capacities of Liquids, Solutions and Vapours*** **[T.M. Letcher]**

Prof. Lorimer (ICTNS) and Dr Dymond sent a list of corrections and comments to Prof. Letcher at the beginning of April 2010. Publication of this volume by the Royal Society of Chemistry is expected in August 2010.

**7.9** ***Extension of ThermoML – the IUPAC Standard for Thermodynamic Data Communications*** **[M. Frenkel]**

Part 4 on Biomaterials has been published:

ThermoML-An XML-Based Approach for Storage and Exchange of Experimental and Critically Evaluated Thermophysical and Thermochemical Property Data. 4. Biomaterials. R.D. Chirico, M.Frenkel, V. Diky, R.N. Goldberg, H. Heerklotz, J.E. Ladbury, D.P.Remeta, J.H. Dymond, A.R.H. Goodwin, K.N. Marsh, W.A. Wakeham, *J. Chem. Eng. Data*, 2010, 55 (4), pp 1564–1572.

A draft of Part 5 has been prepared for discussion at a Task Group meeting in Tsukuba, with planned submission to *J. Chem. Eng. Data* in October 2010.

ThermoML* – an XML-based Approach for Storage and Exchange of Experimental and Critically Evaluated Thermophysical and Thermochemical Property Data. 5. Speciation and Complex Equilibria. Michael Frenkel, Vladimir Diky, Robert D. Chirico, Robert N.

Goldberg, Heiko Heerklotz, John E. Ladbury, David P. Remeta, John H. Dymond, Anthony R. H. Goodwin, Kenneth N. Marsh, William A. Wakeham, Stephen E. Stein, Paul L. Brown, Erich Königsberger, Peter A. Williams.

A no-cost extension to the project to end-2010 to complete this project on speciation issues was granted by IUPAC.

Parts 4 and 5 will be combined with other minor, but necessary, extensions to ThermoML and will be submitted to *Pure & Appl. Chem.* to complete the project.

**7.10** ***Thermodynamic Study on Hydrogen Storage Materials: Metal Organic Framework s and Metal or Complex Hydrides*** **[Li-Xian Sun]**

This is going well, with a number of research publications providing additional data. A task group meeting will be held in Tsukuba.

**7.11** ***A critical evaluation of the viscosity and density of molten copper and tin*** **[M.J. Assael]**

All references for the viscosity and density of molten copper and tin have been collected, data were transferred into a database, and critically evaluated. Based on these evaluations correlations were developed and these correlations were presented and discussed at the International Association for Transport Properties (IATP) Meeting in Santiago de Compostela, Spain on July 2-3, 2010.

Following this presentation the correlations will be submitted to *Pure and Applied Chemistry*, *High Temperatures – High Pressures* and to a journal consulted by practitioners in the metal casting industry (still to be decided).

The results will be presented at the next 19th European Thermophysical Properties Conference.

## 8. IACT Membership 2010-2012

It was noted that membership is only relevant for attendance at Business meetings, which all attendees at the ICCT are welcome to attend.

For people who wished to propose nominees for election to the Board of Directors of IACT, a web link was established from the ICCT website to the IACT website inviting such nominations. It was agreed that this method should be followed in future.

## 9. IACT Website

This will be up-dated when the draft Minutes of these various meetings have been prepared, at which time the completed projects and the publication list will also be brought up to date.

## 10. Publications 2008-2010

A publication list is appended to these Minutes.

## 11. Possible new projects

**11.1** ***Mechanical and Isentropic Coefficients of Liquid Systems, Pure and Mixed.*** **[T.M. Letcher]**

This proposal was unanimously approved in Santiago de Compostela. Prof. Letcher will submit a project proposal to IUPAC.

**11.2** ***Guidelines on Isothermal Titration Calorimetry*** **[J.-P. E. Grolier]**

Prof. Grolier said that there were no standardisation procedures and insufficient metadata for this procedure and that a project with instrument manufacturers was required. He was encouraged to consider a project proposal.

**11.3** ***Experimental Thermodynamics. Volume IX. Experimental Transport Properties***

Dr. Goodwin said that the IAPT (International Association of Transport Properties) were keen to update this volume. He would see if this could be the subject of a project proposal submitted to IUPAC via IACT.

## 12 Any Other Business

### 12.1 *Tribute to Dr. Henry Kehiaian and Awards in his Name*

Prof. Grolier asked if he could give a tribute to Dr. Henry Kehiaian, who had given so much to Thermodynamics, right up the time before his death earlier this year. Members readily agreed to this, with a short tribute to be given during the IACT Business Meeting on Thursday and an expanded Tribute written for the IACT website.

It was agreed that a fitting memorial to Dr. Kehiaian would be the establishment of travel awards for young scientists. Prof. Grolier agreed to discuss this possibility with the family and make recommendations.

### 12.2 *Publishing*

Some concern was expressed about the advent of open access journals. However, there appears to be little interest in these and publishers are not worried. It was agreed that it would be useful to have a panel discussion on publishing at the next meeting.

## 13. Date of next meeting

The meeting of the New Board will be held on Friday August 6$^{th}$ 2010 in Tsukuba International Congress Centre.

**Signed…….. Date……**

**Chairman**

**Item 10. Publications 2008-2010**

*Heat capacities*

Heat Capacity of Liquids: Critical Review and Recommended Values. Supplement II, by Milan Zábranský, Zdenka Kolská, Vlastimil Růžička Jr., Eugene S. Domalski, *J.Phys.Chem.Ref.Data* Vol. 39, No. 1, 2010 (404 pages).

*Electrolyte Data Collection* - Volume XII DECHEMA, Frankfurt.

Part.5a: Specific Conductivities of Concentrated Solutions of Lithium Salts in Binary Organic Solvent Mixtures of Carbonates. J. Barthel et al. (2010).

*Critical Properties*

Vapour-Liquid Critical Properties of Elements and Compounds. 11. Organic Compounds Containing B + O; Halogens + N, + O, + O + S, + S, + Si; N + O; O + S, + Si. D. Ambrose, C. Tsonopoulos , and E. Nitikin, *J. Chem. Eng. Data*, 54, 669-689 (2009).

*XML-based IUPAC Standard*

ThermoML-An XML-Based Approach for Storage and Exchange of Experimental and Critically Evaluated Thermophysical and Thermochemical Property Data. 4. Biomaterials. R.D. Chirico, M.Frenkel, V. Diky, R.N. Goldberg, H. Heerklotz, J.E. Ladbury, D.P.Remeta, J.H. Dymond, A.R.H. Goodwin, K.N. Marsh, W.A. Wakeham, *J. Chem. Eng. Data*, 2010, 55 (4), pp 1564–1572.

*Thermodynamics of Hydration*

Thermodynamics of Non-Reactive gases Dissolved in Water at Ambient Temperature (T ≥333 K): an update. J.L. Alvarez and R. Fernández Prini, *Journal Solution Chemistry*, **37**(10), 1379-1392 (2008).

*Ionic Liquids*

Thermodynamic and Thermophysical Properties of the Reference Ionic Liquid: 1-Hexyl-3-methylimidazolium Bis[(trifluoromethyl)sulfonyl]amide (including Mixtures). Part 1.Experiment Methods and Results. (IUPAC Technical Report) Kenneth N. Marsh, Joan J. Brennecke, Robert D. Chirico, Michael Frenkel, Andreas Heintz, Joseph W. Magee, Cor J. Peters, Luis Paulo N. Rebelo, and Kenneth R. Seddon , *Pure Appl. Chem.*, Vol. 81, No. 5, pp. 781–790 (2009).

Thermodynamic and thermophysical properties of the reference ionic liquid: 1-Hexyl-3-methylimidazolium bis[(trifluoromethyl)sulfonyl]amide (including mixtures). Part 2. Critical evaluation and recommended property values (IUPAC Technical Report). Robert D. Chirico, Vladimir Diky, Joseph W. Magee, Michael Frenkel and Kenneth N. Marsh, *Pure Appl. Chem.*, Vol. 81, No. 5, pp. 791–828 (2009).

*Book:*

Future Energy – Improved, Sustainable, and Clean Options for Our Planet, Ed. T.M. Letcher, [ISBN 978-0-08-054808-1] Elsevier, 2008.

**Articles in Chemistry International**

*The Project Place*

Future Energy: Improved, Sustainable, and Clean Options for our Planet, T. Lectcher, *Chem. Int.*, Vol. 30, No. 2, 20-21 (2008).

Expension of ThermoML – The IUPAC Standard for Thermodynamic Data Communications. *Chem. Int.*, Vol. 30, No. 3, 18 (2008).

Applied Thermodynamics of Fluids. *Chem. Int*., Vol. 30, No. 5, 19-20 (2008).

A Critical Evaluation of the Viscosity and Density of Molten Copper and Tin. *Chem. Int*., Vol. 31, No. 5, 17 (2009).

*Making an imPACt*

Thermodynamic and Thermophysical Properties of the Reference Ionic Liquid: 1-Hexyl-3-methylimidazolium Bis[(trifluoromethyl)sulfonyl]amide (including Mixtures). Part 1.Experiment Methods and Results. (IUPAC Technical Report) Kenneth N. Marsh, Joan J. Brennecke, Robert D. Chirico, Michael Frenkel, Andreas Heintz, Joseph W. Magee, Cor J. Peters, Luis Paulo N. Rebelo, and Kenneth R. Seddon , *Chem. Int*., Vol. 31, No. 4, 28 (2009).

Thermodynamic and thermophysical properties of the reference ionic liquid: 1-Hexyl-3-methylimidazolium bis[(trifluoromethyl)sulfonyl]amide (including mixtures). Part 2. Critical evaluation and recommended property values (IUPAC Technical Report). Robert D. Chirico, Vladimir Diky, Joseph W. Magee, Michael Frenkel and Kenneth N. Marsh, *Chem. Int*., Vol. 31, No. 4, 28 (2009).

*Provisional Recommendations*

Thermochemistry of Chemical Reactions: 1. Terminology and Symbols. *Chem. Int*., Vol. 30, No. 5, 22 (2008).

*Bookworm*

Future Energy – Improved, Sustainable, and Clean Options for Our Planet, Ed. T.M. Letcher, Elsevier, 2008. *Chem. Int*., Vol. 31, No. 1, 22 (2009).

*Where 2B & Y*

Challenges in Thermodynamics Applied to Materials World. *Chem. Int*., Vol. 31, No. 5, 32 (2009).