Attachment 6

Minutes of PCAS WG, 2004
Meeting held August 29, 2004, 14:00 – 17:00
Kyoto, Japan

Participating members: Vladimir Majer (chair), Serguei Lvov (vice chair), Horacio Corti, Donald Palmer, Masaru Nakahara, Roberto Fernandez-Prini, Robert Wood, Andre Anderko, František Maršik, Josef Hruby, Josef Sedlbauer, Vladimir Valyashko

PRELIMINARIES

V. Majer called the meeting to order. Minutes of the previous meeting in Vejle, Denmark were accepted without comment. Andre Anderko was appointed as clerk of minutes.

Committee Leadership

V. Majer is stepping down as chairman as of January 2005. S. Lvov is ready to take over chairmanship. H. Corti is scheduled to become vice chairman, he expressed, however, some concern regarding his commitment to vice-chairmanship of the IAPWS Committee on educational outreach.

Priority Areas

pH of water at high temperatures. D. Palmer reported on the progress in this area. A questionnaire was sent out to experts in this field (Kunio Arai, Horacio Corti, Arthur Covington, Kang Ding, Glenn Hefter, Kevin Knauss, Serguei Lvov, Digby Macdonald, Eric Maughan, Donald Palmer, Peter Tremaine, Shinsuke Uchida, David Wesolowski, Thomas Wolery, Scott Wood, Andre Zeijseink). The topics are: definition of pH at high temperature and methods of measurement. So far, five people have responded. The goal is to prepare a publication with recommendations and submit it to a journal. PCAS WG approved this action unanimously.

Prediction of standard-state properties of nonelectrolytes. V. Majer, in collaboration with R. Fernandez-Prini and J. Sedlbauer, prepared a plan of the project and distributed it to the attendees. The objective is to prepare a technical report as an IAPWS guideline, an article to be published in Journal of Physical and Chemical Reference Data and a freely accessible database. Databases that are already in place at Arizona State and University of Liberec will be included in the project. Approximately 200 organic substances will be targeted to cover the largest number of structures rather than the largest number of individual species. Funding from IAPWS has been requested (12 k€ for 2.5 years) to facilitate the mobility of young researchers (under 40 years of age, not members of our group). The mobility support is intended mainly for visits to other labs rather than meeting participation. The possible young researchers include P. Vrbka (Institute of Chemical Technology, Prague), L. Mendez de Leo, H. Bianchi (Atomic Energy Commission, Buenos Aires), V. Diky (NIST – Boulder), K. Ballerat (Blaise Pascal University), N.V.

Plyasunova (Arizona State) and M. Slavik (U. of Liberec). V. Majer has sent the proposal to national delegates and the Executive Secretary; PCAS approved this action unanimously.

Ion pairing in 1-1 electrolytes. Donald Palmer reported no progress in this area. Robert Wood indicated the availability of results for 1-2 electrolytes from conductance measurements and predicted values from ab initio methods. Donald Palmer has results on complexation in $ZnCl_2$ and $NiCl_2$. However, these results are not directly relevant to this project. The PCAS WG does not want pursue activity in this area.

"Atlas" Monograph

D. Palmer reported that the monograph "Aqueous Systems at Elevated Temperatures and Pressure: Physical Chemistry in Water, Steam and Hydrothermal Solutions" was published by Elsevier in July 2004. IAPWS invested 10000 $ in technical preparation of the manuscript, royalties from sales will go to IAPWS. A copy will be sent to E.U. Franck in recognition of his early initiative to write this book. R. Fernandez-Prini indicated that the publishers expect to sell 1000-2000 copies. V. Majer thanked the Editors (D. Palmer, R. Fernandez-Prini and A. Harvey) for their work and dedication.

Book on thermodynamic data and measurement methods at high temperatures

V. Majer reported that an initiative to develop a compilation of high-temperature data (under coordination of V. Valyashko) was presented at Vejle 2003. Some criticism was raised in Vejle because of the lack of critical evaluation of the data and the arbitrary nature of the proposed lower temperature limit (200 °C), which would results in possible splitting of data sets. An Advisory board (Vladimir Valyashko, Vladimir Majer and Marc Assael) was nominated by EC to prepare a more detailed proposal of procedure so that the project can be considered for IAPWS sponsorship. A broad discussion on these aspects and timing of the project has taken place during winter and spring 2004.

In a later part of the meeting, Vladimir Valyashko gave a brief presentation on the proposed book. The objective is to give the user information on experimental methods, experimental data and their treatment. The originally proposed chapters were (1) phase equilibria (V. Valyashko, (2) PVT properties (H. Corti, V. Majer), (3) calorimetric data (V. Majer), (4) isopiestic data (Miroslaw Gruszkiewicz), (5) electrochemical data (D. Palmer, S. Lvov), (6) electrical conductivity (H.), (7) thermal conductivity (I. Abdulagatov, M. Assael) and (8) viscosity (I. Abdulagatov, M. Assael).

D. Palmer, M. Gruszkiewicz and S. Lvov expressed their difficulties to contribute to this project because of other heavy commitments. V. Majer attempted to enlist Christopher Wormald to collaborate, but it is unclear whether this will materialize. On the other hand, H. Corti has already written his chapter; also, most data are already in the computer.

Discussion on this topic continued during the week and a sound consensus was reached. Finally a proposal was formulated by the Advisory board for EC on September 2. The chapter on isopiestic data will be cancelled; V. Majer will take as a coauthor his research associate (K. Ballerat), S. Lvov will lead the chapter on electrochemical properties and will be helped by D. Palmer regarding the ORNL data.

Attachment 6

Reports regarding new Task groups and Committees

Metastability, Nucleation, Early Condensate, Droplet Sprays and Condensation. This group should provide a forum for researchers and practitioners to engage in debate on contemporary issues regarding the nonequilibrium thermodynamics of water and aqueous systems.

V. Marsik (Chair) listed persons (mainly out of IAPWS) working in this field and presented areas of interest to IAPWS: phase transitions and phase diagrams of aqueous systems, saturation line - bubble points and dew points, metastable water and metastable aqueous systems, nucleation – cavitation - boiling – condensation, bubble and droplet formation - two-phase flow, measuring techniques for transient quantities.

Recommendation to IAPWS: establish a task group within IAPWS.

Electrochemical Processes in High-Temperature Aqueous Systems

Serguei Lvov (Chair) gave a list of researchers involved in this task group (D. Macdonald, E. Maughan, M. Nakahara, T. Petrova, and S. Uchida) and listed main areas of interest to IAPWS: potentiometry, pH Measurements, electrochemical monitoring of solution chemistry, electrochemical kinetics measurements, corrosion metals and alloys, electrokinetic measurements, electrochemical production of substances (for example, hydrogen production), electrochemical production of electrical energy (for example, fuel cells), electrochemical conductance measurements..

Recommendations of PCAS WG: (*i*) continue the Task Group activities in 2004/2005, (*ii*) add D. Palmer to the members list, (*iii*) communicate with PCC WG to formulate details of the listed above areas of research.

Fuel Cell and H_2 Technologies

S. Lvov (Chair) reported on an initiative to establish a Committee with J. Pierre (invited consultant from Siemens Westinghouse, Pittsburg, PA). Several other PCAS WG members expressed interest.

The main areas that are important to IAPWS were suggested as follows: electrolysis of water, electrochemical oxidation of fuels, electrochemical reduction of oxygen, conductivity of water containing proton conducting membranes, electrochemical and chemical production of hydrogen using hydrothermal processes, development of fuel cell–turbine hybrid systems.

Recommendations of PCAS WG: create a task group on fuel cell and H_2 technologies: S. Lvov (chairman), H. Corti, M. Nakahara, and F. Marsik.

Properties and formulations for high temperature aqueous systems

V. Majer consulted on this topic A. Harvey, R. Fernandez-Prini, F. Marsik and J. Sedlbauer. The problem can be divided in two parts: (*i*) dilute solutions with interactions solute – solvent prevailing: these issues are addressed in a proposal of a project on hydration properties, (*ii*) concentrated solutions with interactions solute – solute playing also important role: this issue should be addressed in the next stage.

Recommendation to PCAS WG: support the hydration project, persons participating in this project will form the task group.

New members

V. Marsik proposed M. Sedlář of Sigma Research and Development Institute as WG member. Approved.

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Working group "Physical chemistry of aqueous solutions" (PCAS)

Chair: Vladimir Majer, vladimir.majer@univ-bpclermont.fr,
Blaise Pascal University / CNRS, Clermont-Ferrand, France
Vice-Chair: Serguei Lvov, lvov@psu.edu,
Pennsylvania State University, University Park, PA, USA

Establishing recommended data on thermodynamic properties of hydration for selected organic solutes

proposal for a project to be conducted under auspices of IAPWS and IUPAC (2005-2007)

Task group chairman: **Vladimir MAJER**

Task group members:

V. DOHNAL, P. Vrbka, Ustav fysikalni chemie, Vysoka skola chemicko-technologicka – Praha, 16628 Prague 6, CZECH REPUBLIC, *vladimir.dohnal@vscht.cz*

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A. H. HARVEY, Physical and Chemical Properties Division, NIST, Boulder CO 80305, USA, *aharvey@boulder.nist.gov*

V. MAJER, K. Ballerat, Laboratoire de Thermodynamique des Solutions et des Polymères, Université Blaise Pascal / CNRS, 63177 Aubière, France, *vladimir.majer@univ-bpclermont.fr*

Attachment 7

J. SEDLBAUER, M. Slavik, Katedra chemie, Universita Liberec, Liberec, CZECH REPUBLIC, josef.sedlbauer@vslib.cz

E.L. SHOCK, A.V. PLYASUNOV, N.V. Plyasunova, Department of Geological Sciences and Department of Chemistry and Biochemistry, Arizona State University, Tempe, AZ 85287, USA, Everett.Shock@asu.edu

Objective:

The objective of the project is to establish a database of thermodynamic properties of hydration for approximately 200 selected organic solutes at reference condition of 298.15 K and 0.1 MPa and as a function of temperature and pressure up to the near-critical region of water. The values of hydration properties for solutes covering different molecular structures will be calculated from the reliable experimental data for aqueous and pure solutes. The established database will be used as a standard for testing and establishment of new physico-chemical models and methods of molecular simulation as well as for developing semi-theoretical prediction schemes of interest for chemical engineering ,power cycle chemistry, environmental chemistry and geochemistry.

Description:

Thermodynamic properties of hydration (TPH) covered in the project are: the Gibbs energy of hydration $\Delta_{\mathrm{hyd}}G_2^\circ$, and its temperature and pressure derivatives (the enthalpy of hydration $\Delta_{\mathrm{hyd}}H_2^\circ$, the heat capacity of hydration $\Delta_{\mathrm{hyd}}C_{p,2}^\circ$ and the partial molar volume at infinite dilution V_2°), other TPH result from their combinations; for exact definitions and inter-relationship see Appendix 1. TPH express the difference between the property of a solute in the standard state of infinite dilution at a given temperature and pressure and that of an ideal gas at the same temperature and reference pressure of 0.1 MPa. Thus they characterise the transfer of a solute from a state where molecules are not interacting to the state where the solute molecules interact solely with the water solvent. Due to this definition they can be used conveniently in testing and conception of theoretical models and simulation approaches for dilute aqueous solutions developed by physical chemists. At the same time, TPH allow an easy calculation of partition coefficients (such as the Henry's law constant, air-water partition coefficient, relative volatility, etc.) and of the thermodynamic reaction constants for aqueous systems. Therefore they also have a practical value of interest for engineers and environmental chemists. In addition, the high temperature / high pressure TPH are particularly useful for characterization of phase and chemical equilibria in hydrothermal and power cycle systems.

TPH cannot be directly measured but are calculated from the experimental data characterising aqueous and pure solutes, which result from phase equilibrium, calorimetric and volumetric measurements. Appendix 1 summarises equations used to calculate TPH and lists types of experimental data that can be exploited.

The task group will select from the primary literature the best available experimental results for establishing a database of reliable values of TPH for 100 – 200 organic solutes and several common gases. In selecting the solutes, three main criteria will be observed: *i)* coverage of the widest range of molecular structures, indispensable for the development of theoretical models and group contribution prediction schemes *ii)* availability of reliable experimental data, particularly with regard to the HT/HP region, *iii)* technological and environmental importance of individual solutes. The database will comprise values at the reference condition T_r = 298.15 K and p_r = 0.1 MPa for about 200 solutes and at elevated temperatures ($T < 673$ K) and pressures ($p < 40$ MPa) for about 100 solutes. For several solutes the recommended TPH will be given up to the critical region of water where they undergo remarkable changes. A tentative list of the classes of solutes covered and their respective numbers are given in Appendix 2. Every effort will be made to supply a database that will not be biased by use of any particular correlation model for interpolating or extrapolating the data.

This project requires collaboration of researchers having complementary knowledge in data evaluation and in different experimental techniques used for obtaining data for aqueous and pure solutes. Participation of investigators from at least six institutions in four countries is expected. The Buenos Aires, NIST Boulder and Prague groups have particular expertise regarding experimental data on the Gibbs energy level for aqueous solutions while the Aubière (Clermont-Ferrand) group will focus mainly on derivative properties. They will all collaborate with the Tempe and Liberec groups where extensive databases for aqueous solutes are already available. TRC of NIST Boulder will supply all the recommended experimental data for pure organic compounds (under coordination of M. Frenkel). A particular feature of this project will be the participation of younger researchers, some of them in early stages of their careers, beside confirmed experts (listed in capitals) who collaborated already in the past and are members of international scientific bodies (IAPWS, IUPAC, IACT).

Outcome:

i) technical report to be presented as an IAPWS guideline*, ii)* a comprehensive article to be published in Journal of Physical and Chemical Reference Data, *iii)* a database (list of values, no software) freely accessible through the IAPWS and IUPAC web pages.

Time frame: Planned start date January 2005, duration of project 30 months

Milestones:

- October 2005 system selection closed, main experimental data sets selected
- March 2006 determination of recommended data for TPH at T_r = 298.15 K and p_r=0.1MPa completed
- August 2006 recommended TPH at HT/HP calculated for most systems, workshop organized during the International Conference on Chemical Thermodynamics in Boulder, CO
- January 2007 consistency verification and refinements completed
- June 2007 review paper submitted to JPCRD, the proposed IAPWS guide line circulated for evaluation, data base prepared to be available through the IAPWS web page after approval of the guideline at the IAPWS annual meeting

Anticipated impact:

The data on TPH are of interest for:
- *physical chemists* (model developers and simulators)
- *chemical engineers* (schemes for calculating phase and chemical equilibria in industrial aqueous systems including power cycles)
- *environmental chemists* (partitioning of solutes between air and water, cleanup of aqueous effluents)
- *theoretical geochemists* (development of prediction schemes for thermodynamic equilibrium constants of hydrothermal reactions)

Budget requested from IAPWS:

Total: **12k€** (5 k€ in 2005, 5 k€ in 2006, 2 k€ in 2007)
This budget will be used for *i)* facilitating mobility of young researchers (who are not members of IAPWS working groups) when working on project tasks (8 k€), *ii)* data compilation, evaluation and transfer, establishment of a database (4 k€).

Budget requested from other sources:

- IUPAC: 14 k€
- Participating laboratories: contribution to the project estimated to 48 k€

Note: This proposal was prepared by Vladimir Majer and consulted with Roberto Fernandez-Prini (PCAS WG) and Allan Harvey (TPWS WG) before its submission to IAPWS EC for discussion and vote during the 14th ICPWS in Kyoto (August 29 – September 3, 2004).

Appendix 1 to Attachment 7

Establishing recommended data on hydration properties for selected organic solutes

APPENDIX 1

Thermodynamic background and main classes of experimental data needed

Thermodynamic property (function) of hydration (TPH) – difference between a property in the standard state of infinite dilution (temperature and pressure of the system) and in the state of an ideal gas (temperature of the system and standard pressure of 0.1 MPa)

$$\Delta_{\mathrm{hyd}}X_2^\circ = X_2^\circ[T,p] - X_2^{\mathrm{ig}}[T,p_\circ] \qquad p_\circ = 0.1\ \mathrm{MPa}$$

Gibbs energy of hydration $\Delta_{\mathrm{hyd}}G_2^\circ$ **:**

Relationship with the Henry's law constant: $\Delta_{\mathrm{hyd}}G_2^\circ = G_2^\circ - G_2^{\mathrm{ig}} = RT\ln(k_{\mathrm{H},2}/p_\circ)$

Relationship with the Gibbs energy associated with dissolution of a liquid or solid solute

$$\Delta_{\mathrm{hyd}}G_2^\circ = \Delta_{\mathrm{sol}}G_2^\circ + RT\ln(f_2^\bullet/p_\circ) = \Delta_{\mathrm{sol}}G_2^\circ + RT\ln(\phi_2^\bullet p_2^{\mathrm{sat}}/p_\circ) + \int_{p_2^{\mathrm{sat}}}^{p} V_2^\bullet \mathrm{d}p$$

Relationship of $\Delta_{\mathrm{sol}}G_2^\circ$ to the symmetric limiting activity coefficient (liquid solutes)

$$\Delta_{\mathrm{sol}}G_2^\circ = G_2^\circ - G_2^{\bullet\mathrm{l}} = RT\ \ln\gamma_2^{\mathrm{R}\infty}$$

Relationship of $\Delta_{\mathrm{sol}}G_2^\circ$ to the solubility (sparingly soluble liquid or solid solutes)

$$\Delta_{\mathrm{sol}}G^\circ = G_2^\circ - G_2^\bullet = -RT\ln x_2^{\mathrm{sol}}\gamma_2^{\mathrm{H}} \cong -RT\ln x_2^{\mathrm{sol}}$$

Experimental data needed:
(aq) - Henry's law constants (gases), limiting activity coefficients (hydrophilic and moderately hydrophobic liquid solutes), solubilities (hydrophobic liquid and solid solutes)
(pure) - vapour pressures, gas nonideality corrections, densities of pure solutes

Enthalpy of hydration $\Delta_{\mathrm{hyd}}H_2^\circ$ **:**

Relationship with the enthalpy associated with dissolution

$$\Delta_{\mathrm{hyd}}H_2^\circ = \Delta_{\mathrm{sol}}H_2^\circ + \int_0^p (V_2^\bullet - T(\partial V_2^\bullet/\partial T)_p)\mathrm{d}p \quad T > T_{\mathrm{c}}$$

$$\Delta_{\mathrm{hyd}}H_2^{\circ} = \Delta_{\mathrm{sol}}H_2^{\circ} - \Delta_{\mathrm{vap}}H_2^{\bullet} + \int_0^{p_2^{\mathrm{sat}}} (V_2^{\bullet} - T(\partial V_2^{\bullet}/\partial T)_p)\mathrm{d}p \cong \Delta_{\mathrm{sol}}H_2^{\circ} - \Delta_{\mathrm{vap}}H_2^{\bullet} \quad T<T_{\mathrm{c}}$$

Relationship of $\Delta_{\mathrm{sol}}H_2^{\circ}$ to the data resulting from calorimetric experiments

$$\Delta_{\mathrm{sol}}H_2^{\circ} = (H_2^{\circ} - H_2^{\bullet}) = \lim_{n_2 \to 0} (\Delta_{\mathrm{sol}}H / n_2)$$

Experimental data needed:
(aq) - enthalpies of solution (dilute aqueous solutions)
(pure) - residual enthalpies (enthalpic departure function resulting from pVT data) for gases and supercritical fluids, enthalpies of vaporization (liquids) / sublimation (solids)

Heat capacity of hydration $\Delta_{\mathrm{hyd}}C_{p,2}^{\circ}$:

$$\Delta_{\mathrm{hyd}}C_{p,2}^{\circ} = C_{p,2}^{\circ} - C_{p,2}^{\mathrm{ig}}$$

Relationship of $\Delta_{\mathrm{hyd}}C_{p,2}^{\circ}$ to the data resulting from calorimetric experiments

$$C_{p,2}^{\circ} = c_{p,1} \cdot M_2 + \lim_{m_2 \to 0}\left(\frac{c_p - c_{p,1}}{m_2}\right)$$

Experimental data needed:
(aq)- specific heat capacities (heat capacity differences) of dilute aqueous solutions
(pure)- ideal gas heat capacities of solute

Partial molar volume at infinite dilution V_2° :

$$V_2^{\circ} = \frac{M_2}{\rho_1} - \frac{1}{\rho_1^2} \lim_{m_2 \to 0}\left(\frac{\rho - \rho_1}{m_2}\right)$$

Experimental data needed:
(aq)- densities (density differences) of dilute aqueous solutions

Appendix 1 to Attachment 7

Relationship between individual TPH:

$$\Delta_{\mathrm{hyd}}G_2^\circ = \Delta_{\mathrm{hyd}}G_2^\circ[T_\mathrm{r}, p_\mathrm{r}] - (T - T_\mathrm{r})\Delta_{\mathrm{hyd}}S_2^\circ[T_\mathrm{r}, p_\mathrm{r}] +$$

$$+\int_{T_\mathrm{r}}^{T}\left(\Delta_{\mathrm{hyd}}C_{\mathrm{p},2}^\circ\right)_{p_\mathrm{r}}\mathrm{d}T - T\int_{T_\mathrm{r}}^{T}\left(\Delta_{\mathrm{hyd}}C_{\mathrm{p},2}^\circ\right)_{p_\mathrm{r}}\mathrm{d}\ln T + \int_{p_\mathrm{r}}^{p}\left(V_2^\circ\right)_T\mathrm{d}p$$

where

$$\Delta_{\mathrm{hyd}}S_2^\circ[T_\mathrm{r}, p_\mathrm{r}] = (\Delta_{\mathrm{hyd}}H_2^\circ[T_\mathrm{r}, p_\mathrm{r}] - \Delta_{\mathrm{hyd}}G_2^\circ[T_\mathrm{r}, p_\mathrm{r}])/T_\mathrm{r}$$

T_r=298.15 K, p_r=p_o = 0.1 MPa

Symbols : 2 solute, 1 solvent ; superscript • - pure solute property, superscript °- standard state of infinite dilution, superscript ig – ideal gas
Note: thermodynamic properties of water are obtained from the equation of state for ordinary water substance (IAPWS-95 formulation)

Appendix 2 to Attachment 7

APPENDIX 2

Classes of compounds covered and tentative numbers of solutes included

Compounds of carbons and hydrogen (C-H)	55
Alkanes	
Cycloalkanes	
Unsaturated aliphatic hydrocarbons	
Aromatic and unsaturated monocyclic hydrocarbons	
Polycyclic hydrocarbons	
Compounds of carbon, hydrogen and halogen (C-Hal, C-H-Hal)	20
Fluoroderivatives	
Chloroderivatives	
Bromoderivatives	
Iododerivatives	
Mixed halogen derivatives	
Compounds of carbon, hydrogen and nitrogen (C-H-N)	30
Amines	
Nitriles	
Heterocyclic nitrogen compounds	
Miscellaneous nitrogen compounds	
Compounds of carbon, hydrogen and oxygen (C-H-O)	60
Ethers	
Alcohols and phenols	
Carbonyl compounds	
Acids	
Esters	
Heterocyclic oxygen compounds	
Miscellaneous oxygen compounds	
Compounds of carbon, hydrogen and sulphur (C-H-S)	15
Sulphides	
Thiols	
Heterocyclic sulphur compounds	

Other organic compounds	10
Compounds of carbon, hydrogen, halogen and oxygen (C-H-Hal-O)	
Compounds of carbon, hydrogen, nitrogen and oxygen (C-H-N-O)	
Compounds of carbon, hydrogen, oxygen and sulphur (C-H-O-S)	
Miscellaneous compounds	
Inorganic gases (H_2 O_2, N_2, CO_2, NH_3, H_2S, …)	10

THE INTERNATIONAL ASSOCIATION FOR THE PROPERTIES OF WATER AND STEAM

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Working group "Physical chemistry of aqueous solutions" (PCAS)

Chair: Vladimir Majer, vladimir.majer@univ-bpclermont.fr,
Blaise Pascal University / CNRS, Clermont-Ferrand, France
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Pennsylvania State University, University Park, PA, USA

Hydrothermal Experimental Data; Phase Equilibria and Solution Properties in Binary and Ternary Systems

Outline of the book to be published under auspices of IAPWS
and proposal of a procedure
(2004-2005)

Following the presentation of the proposal for a book on hydrothermal data at the IAPWS annual meeting in Vejle (2003), the Advisory Board (M. Assael, V. Majer and V. Valyashko), nominated by the EC, has undertaken a broad consultation with authors and a consensus was reached in Kyoto (August 2004). The following proposal was developed:

1. The main goal of the project is to prepare a monograph "Hydrothermal Experimental Data; Phase Equilibria and Solution Properties in Binary and Ternary Systems" dealing with

- high temperature measurement techniques,
- experimental data review and assessment,
- presentation of experimental values in tabular forms.

The database of experimental values on hydrothermal systems reaching to temperatures above 200°C was established by V.M.Valyashko and N.S.Ivanova (Kurnakov Institute RAS, Moscow, Russia) between 1998-2003. This database will provide a solid basis for the preparation of the book. A preliminary agreement was reached at the end of 2003 with the Publisher (John Wiley Ltd., London, UK).

2. The monograph will be organized into 7 chapters, each chapter dealing with a property of hydrothermal systems. The Editor of the book will be *V.M. Valyashko, Russia*. *J.M.H. Levelt Sengers* and *D.A. Palmer* have agreed to act as the English Editors after the chapters are available in the final form. The list of properties and responsible authors is as follows:

Chapter I (Phase Equilibrium data – V.M. Valyashko, Russia)
Chapter II (pVTX data – H. Corti, Argentina, V. Majer, France)
Chapter III (Calorimetric data – V. Majer, K. Ballerat, France)
Chapter IV (Electrochemical data – S.N. Lvov, D.A. Palmer, USA)
Chapter V (Electrical conductivity data – H. Corti, Argentina)
Chapter VI (Thermal conductivity data – I. Abdulagatov, Russia/USA, M.J. Assael Greece)
Chapter VII (Viscosity data - I. Abdulagatov, Russia/USA, M.J. Assael Greece)

The collective of authors is free to invite possibly other scientists to participate in the preparation of the book.

Each Chapter will consist of two parts: *text part* (thermodynamic background and the review of techniques, experimental data and treatment procedures) and *summary table* overviewing the data. This table will show for each property the following information: nonaqueous component(s) of system (chemical formula and name), range of parameters (concentration, temperature, pressure), type of data in the literature source, indication of data quality, code for the experimental technique used, literature reference, code for connection to the CD database and possibly other additional information. An Appendix on a CD will be produced presenting the direct experimental data (one table per system and reference). Brief specific information regarding the data presented, and information on the accuracy claimed by the author (if available), will precede each table.

3. Additionally to the aforementioned points, the members of the PCAS WG have come to the following agreement:

3.a. The collection will focus mainly on the data reaching above 200°C. This data limit will not be, however, considered as restrictive. For certain properties the chapter authors may consider the data below this limit if it makes sense and a better explanation of the nature of the data is so achieved.

3.b. The chapters will have no temperature limitation in a description of experimental techniques, property behavior or the methods of experimental data treatment. Moreover, the summary table will indicate the temperature ranges as reported by the original authors. The tables in the CD Appendix will contain mainly the data above 200°C; in some cases this temperature limit can be lowered provided the chapter authors add the data to the database.

3.c. Values of T, p, and x in the Summary Tables will be presented in uniform units (temperature - K. pressure - MPa, concentration range - molality or mole per cent as convenient). Experimental data in the CD Appendix will be presented as reported by authors. However, in a limited number of cases where a conversion is desirable (obsolete units etc.), all information necessary will be provided.

3.d. Copies of original papers presenting experimental data will be available to authors from V. Valyashko when necessary.

4. Timetable:

October 1, 2004 Final list of authors and chapter outlines submitted to the Editor. Every author should submit an official confirmation of his participation in the book preparation.
February 1, 2005 Authors decide on the final list of data sources to be included and if necessary complete the database accordingly. Papers published in the open literature, including theses, until the end of 2004 will be considered.
July 1, 2005 Drafts of chapters sent to the Editor.
December 15, 2005 Final manuscript ready for the submission to the Publisher.

5. The preliminary agreement with John Wiley Ltd. regarding the book is as follows. The book will contain about 500 printed pages. The Publisher will pay \$ 10 per printed page. The payment for the CD material will be the total sum of \$ 3500.

Since **no financial support from IAPWS is requested for this project** the payment from the Publisher will go to the authors and for compensating the expenses with the manuscript and data base preparation.

Submitted to EC by the Advisory board members. M. Assael, V. Majer, V. Valyashko
Kyoto, September 1, 2004

Appendix to Attachment 8

Appendix (book outline)

Hydrothermal Experimental Data; Phase Equilibria and Solution Properties in Binary and Ternary Systems

V.M. VALYASHKO, Editor
Kurnakov Institute RAS, Moscow, Russia

CHAPTER I **"Phase Equilibria in Binary and Ternary Hydrothermal Systems" (V.M. VALYASHKO, Kurnakov Institute RAS, Moscow, Russia)**
Introduction
Binary Systems *(Fluid and complete phase diagrams; Theoretical derivation and systematic classification of binary phase diagrams).*
Ternary Systems *(Graphical representation; Theoretical derivation and systematic classification of ternary phase diagrams)*
Estimation of Thermodynamic Functions and Equilibrium Constants from Experimental Data on Phase Equilibria.
Methods and Equipment for Studying Hydrothermal Phase Equilibria
Some Regularities of Hydrothermal Phase Behavior in Experimentally Studied Systems.

CHAPTER II **"PVTX Properties of Hydrothermal Solutions" (H.R. CORTI, Comision Nacional de Energia Atomica, Buenos Aires, Argentina; Vladimir MAJER, Blaise Pascal University, Clermont-Ferrand, France))**
Basic Principles and Definitions
Experimental Methods
Theoretical Treatment of PVTX-data for Ionic and Nonionic Solutes *(Standard partial molar volume; Partial molar volumes near critical conditions; Excess volume; Ion association effects on excess volumes)*
General Trends in Temperature, Pressure and Composition Dependencies of Standard Partial Molar Volume and Excess Volume for Ionic and Nonionic Solutes.
Recommendations for the Calculation of Standard and Excess Properties from Experimental Data.

CHAPTER III **"Calorimetric Properties of Dilute Hydrothermal solutions" (V. MAJER, K. BALLERAT, Blaise Pascal University / CNRS, Clermont-Ferrand, France)**
Thermodynamic Background: Heat Of Solutions, Heat Of Dilution, and Heat Capacity

Experimental methods
Theoretical Treatment of Calorimetric Data for Ionic and Molecular Solutes (*Standard and Excess Properties, Near Critical Behaviour, Ion Association Effects)*
General Trends in Temperature, Pressure and Composition; Depenencies of Standard and Excess Properties ror Ionic And Molecular Solutes
Recommendations for the Calculation of Standard and Excess Properties from Experimental Data.

Appendix to Attachment 8

CHAPTER IV **"High-Temperature Electrochemical Measurements of Aqueous Solutions" (S.N. LVOV, Pennsylvania State University, University Park, USA, D.A. PALMER, ORNL, Oak Ridge, USA)**

Introduction
Conventional High Temperature Electrochemical Cells
Hydrogen-Electrode Concentration Cell
Hydrothermal Electrochemical Measurements

CHAPTER V **"Electrical Conductivity in Hydrothermal Binary and Ternary solutions" (H.R. CORTI, Comision Nacional de Energia Atomica, Buenos Aires, Argentina)**

Basic Principles and Definitions
Experimental Methods
Data Treatment (*Dissociated and associated electrolytes; Getting information from electrical conductivity data)*
General Trends *(Specific conductivity as a function of temperature, concentration and density. The limiting molar conductivity; Molar conductivity as a function of concentration, temperature and density; Association constants)*
Conductivity in Ternary Systems

Chapter VI **"Thermal Conductivity of Hydrothermal Solutions" (I.M. ABDULAGATOV, NIST, Boulder, USA; M.J. ASSAEL, Aristotle University, Thessaloniki, Greece)**

Introduction
Experimental Methods *(Parallel Plate, Coaxial Cylinders and Transient Hot – Wire Apparatus, Theoretical Bases and Uncertainties of the Measurements)*
Experimental Thermal Conductivity Data for Hydrothermal Solutions *(Temperature, pressure and concentration dependencies of the thermal conductivity of aqueous solutions)*

Chapter VII **"Viscosity of Hydrothermal Solutions" (I.M. ABDULAGATOV, NIST, Boulder, USA; M.J. ASSAEL, Aristotle University, Thessaloniki, Greece)**

Introduction
Experimental Methods of the Viscosity Measurements at High Temperatures and High Pressures *(Capillary flow and oscillating disk apparatus; Theoretical bases and uncertainties of the measurements)*
Experimental Viscosity Data for Aqueous Solutions at High Temperatures and High Pressures *(Temperature, pressure and concentration dependencies of the viscosity of aqueous solutions)*