

IAPWS Annual Meeting 2007, Lucerne PCAS Minutes

Monday Morning

Present: Serguei Lvov (Chair), Masaru Nakahara; Peter Tremaine (Clerk of Minutes); Masakatsu Uneo; Notiyuki Yoshi; Frantisek Marsik; Milan Sedlar; Pavel Safarik; Tomas Nemec; Jana Ehlerova.

1. **Opening Remarks** were made by Serguei Lvov (Chair). Members introduced themselves with a short description of their research interests. Peter Tremaine was appointed Clerk of Minutes.

2. **Minutes from 2006 meeting (Witney)** were unanimously approved as written.

Actions Arising: One outstanding action from 2006. Horacio Corti has expressed concern about the difficulties he is having in attending meetings as co-chair. He was not able to come to Lucerne. The question will be discussed on Thursday.

3. **IAPWS International Collaboration:** Peter Tremaine presented the proposal by Canada (Tremaine) and the Czech Republic (Sedlbauer). Both national committees support the proposal. Questions related to two aspects of the proposal were discussed by Tremaine. (i) Budget: the budget of \$16,000 is based on the stipend of a Canadian graduate student after tuition is deducted. (ii) The draft proposal was incorrectly sent to the Executive Director rather than to the Chair of PCAS for distribution. The project is for measurements on copper (II) complexation vs T as part of research to support the hydrogen co-generation as part of the Gen IV Initiative. Two students have been identified as candidates. The request for \$16,000 is higher than past proposals. It will be reduced to \$14,000 for a 10 month stay. The proposal identifies Ms. Jitka Felcmanova for the exchange, with Ms. Jana Eherlova as 2nd choice. Both are Dr. Sedlbauer's PhD students. Dr. Tremaine and Dr. Trevani will supervise the experimental portion of the project; Dr. Sedlbauer will supervise fitting the SOW group additivity model to the new data. The project is not related to the recently completed collaborative project by Jana Eherlova, Tremaine and Sedlbauer, which was to develop group additivity models for aromatic organic solutes in high temperature water.

MOVED (Lvov): To approve the project. Unanimous approval (Tremaine: abstained).

4. **ICRNs and Releases:** Lvov invited the committee to discuss reasons for so few ICRNs to arise from PCAS. It was agreed to identify possible new ICRNs and further discuss the issue on Thursday.

ICRN Number 10 (pH Measurements) and ICRN Number 13 (Surface tension of Aqueous Solution): Members agreed in 2006 to transfer ICRN 13 to PCAS. Both were extended by 3 years at that time last year.

New Release: Ionization Constant of Water. The draft release prepared by Lvov was approved by the Evaluation Committee (A. Harvey, P. Tremaine, M. Nakahara). The question of whether releases should have an acknowledgement to indicate the members of the evaluation committee and other contributors. It was agreed that acknowledgements can be included where appropriate.

5. **New Members:** No new members were suggested.

6. **Task Groups and Committees:**

6.1. **Joint Electrochemical Society/IAPWS Symposium (Washington, 2007):** Dr. Lvov presented a status report on the Symposium. The call for papers attracted 25 submissions and will result in a 2-day symposium. The WG compliments Lvov on this very successful initiative.

6.2. **Data Book Project:** Dr. Lvov presented a status report on the Data Book Initiative, Prof. Valashkov (editor). The chapter 2 by Dr. Majer has been withdrawn and will be omitted. Three chapters

are complete, three are completed as drafts. The project is on schedule. The draft manuscript is expected to be submitted to the publisher by Prof. Valashkov by December 2007.

6.3: Joint IUPAC/IAPWS Project on Standard Partial Molar Properties of Solutes Dr. Lvov presented a letter from Dr. Fernandez Prini expressing concern about the status of the project, and a letter from Professor Majer to IUPAC explaining that he has left his position as Director of the Thermodynamics Lab at Blaise Pascale, and that the project cannot be continued. The committee expressed deep concern that IAPWS was not contacted by Dr. Majer to explore solutions.

ACTION (Lvov): To write Dr. Majer requesting a wrap-up status report, and recommendations by which the project might be saved.

Tuesday Morning

Present: Serguei Lvov (Chair), Masaru Nakahara; Peter Tremaine (Clerk of Minutes); Masakatsu Uneo; Notiyuki Yoshi; Frantisek Marsik; Milan Sedlar; Pavel Safarik; Tomas Nemec; Jana Ehlerova.

7. Actions from Witney:

(7.1) Membership: Horacio Corti has expressed concern about the difficulties he is having in attending meetings as co-chair. The question of attendance from several counties was under review during this meeting by a special committee.

ACTION (Lvov): To communicate the results of the Executive Committee decision on this point to Horacio after Friday's meeting. If Horacio cannot continue, an e-mail election for co-chair will be held.

8. IAPWS International Collaboration: Jana Ehlerova presented results from her recently completed collaborative project with Dr. Tremaine (University of Guelph) and Dr. Sedlbauer (University of Liberec), which was to measure values for the ionization constant of o-, m-, and p-nitrophenol under hydrothermal conditions as part of her PhD thesis project which is to develop group additivity models for aromatic organic solutes in high temperature water. A manuscript entitled "Spectrophotometric Determination of the Ionization Constants of Aqueous Nitrophenols at Temperatures up to 225 EC" by Ehlerova, Trevani, Sedlbauer and Tremaine has been written and will be submitted to J. Phys. Chem.

The Working Group congratulated Ms. Ehlerova on her very successful project and report presentation.

MOVED (Lvov): To accept the PowerPoint report, as successful completion of the project. **APPROVED (Unanimous)**

ACTION (Tremaine, Sedlbauer): To provide the manuscript by Christmas 2007, for information.

Tuesday Afternoon (Joint with TPWS)

Present (PCAS): Serguei Lvov (Chair), Masaru Nakahara; Peter Tremaine (Clerk of Minutes); Masakatsu Uneo; Notiyuki Yoshi; Frantisek Marsik; Milan Sedlar; Pavel Safarik; Tomas Nemec; Jana Ehlerova..

Present (TPWS): Hans Joachim Kretzschmar (Chair); Alan Harvet; Jan Sengers; Rainer Feistal; Dan Friend; Koichi Watanabe; Jeff Cooper; Alexandrov; Ines Stoecker, Petra Spitzer.

9. Seawater Symposium and Decisions

Rainer Feistal and Petra Spitzer presented the talks on seawater as listed in the agenda. Rainer noted that the release is based on the new seawater formulation outlined in his presentation, and submitted for publication.

IT WAS AGREED: that TPWS and PCAS should proceed on the understanding that approval will be contingent of acceptance of the new formulation by IAPSO.

MOVED (R. Feisal) that the working groups accept the draft release, subject to review by the editorial committee. **APPROVED (Unanimous)**

Thursday Morning (Joint with TPWS)

Present (PCAS): Serguei Lvov (Chair), Masaru Nakahara; Peter Tremaine (Clerk of Minutes); Masakatsu Uneo; Notiyuki Yoshi; Frantisek Marsik; Milan Sedlar; Pavel Safarik; Tomas Nemec; Jana Ehlerova..

Present (TPWS): Hans Joachim Kretzschmar(Chair); Alan Harvey; Jan Sengers; Rainer Feistal; Dan Friend; Koichi Watanabe; Jeff Cooper; Alexandrov; Ines Stoecker.

10. Release on the Ionization Constant of Water

A. Harvey presented the Editorial Committee report on the proposed release by S. Lvov. The Committee consisted of Alan Harvey (Chair); M. Nakahara, P. Tremaine, and D. Palmer (withdrew),

S. Lvov presented two additional changes:

(i) Q is now defined to be dimensionless

(ii) The limit at zero density of K_w (hyp 1-m std state) is not equal to K_w^G (ideal gas std state) because the standard-state transfer term is non-zero.

The Working Groups discussed minor changes to the list of symbols to improve clarity.

MOVED: (A. Harvey; second S. Lvov): that the working groups accept the formulation subject to minor correction by the Editorial Committee: **APPROVED (Unanimous).**

ACTION (Hans-Joachim Kretzschmar): To raise the issue of whether the release must be based on a published paper and whether the release can deviate from the material in the paper on which it is based.

ACTION (Working Party Members): Minor corrections must be submitted to A. Harvey by lunch time today.

11. Symposium on Molecular Simulation:

After the presentations, the working groups discussed two questions at PCAS request: (i) whether the IAPWS mandate should include Hydrogen Co-generation; (ii) whether TPWS would be prepared to initiate work on developing releases on the density and dielectric constant of D_2O and $NaCl(aq)$.

IT WAS AGREED: that a strong effort should be made to support the symposium on cogeneration at the ICPWS.

IT WAS AGREED that, if the need is clarified, TPWS would consider a request to produce an ICRN could be written to highlight the need for measurements and/or formulations for the density and dielectric constant of D_2O and $NaCl(aq)$.

ACTION: (Peter Tremaine, Jeff Cooper) to draft a short statement of each problem with key references.

12. PCAS Meeting: Final Actions

Collaborative Project: Frantisek Marsik presented the report for the project of Andre Mican's project (S. Lvov and F. Marsik, supervisors).

MOVED (Lvov): that the report be accepted. **APPROVED (Unanimous)**

New name of the WG: Serguei Lvov proposed to rename the WG to Physical Chemistry of Aqueous Systems. **APPROVED (Unanimous).**

Future of PCAS: Possible candidates for PCAS WG chair in the future were discussed. It was decided to continue the discussion at IAPWS 2008 meeting in Berlin.

13. The meeting adjourned at 4:00 pm.