

Working Group PCAS  
Physical Chemistry of Aqueous Systems

Present: Chialvo, Corti, Fernández-Prini, , Levelt-Sengers, Majer (Chair), Nakahara, Palmer, Peters, Plyasunov; Regazzoni; Ueno, Tremaine

MINUTES

Monday, July 22 2002

Minutes of 2001 and Action Arising

Vladimir Majer opening the meeting, the clerk of minutes (P. Tremaine) appointed. The agenda was adopted with the addition of ICRNs. Minutes from Gaithersburg (2001) and Prague (2000) were approved.

Progress in Priority Areas:

- ***pH of Water:***

Don Palmer distributed Sergei Lvov's report which refers to the outstanding ICRN on pH sensors.

ACTION (PCAS members) Provide feedback to Sergei in (i) the accuracy and technical content of the report and (ii) a short statement of proposed future actions.

- ***Prediction Standard Properties of Aqueous Non-Electrolytes***

No report has been received from the project co-ordinator (R.H. Wood). There was discussion about how to achieve closure or a well-defined product from the project. It was agreed that the objective should be to develop a prioritised list of useful equations of state, the shortcomings and advantages of each, and a clear list of needs.

ACTION (Majer, Plyasunov) To prepare a draft statement and to contact Bob Wood regarding the continuation.

- ***Ion-pairing of Strong Electrolytes***

Don Palmer made a short report of work at ORNL.

ICRN's

- ***ICRN 10: pH Measurements***

After discussion, it was agreed that the ICRB should be extended by 1 year so that the pH report can be finalized by Lvov.

ACTION (Majer): To move extension at the EC.

- ***ICRN 11: Priorities of Salts in Steam***

ACTION (Palmer, Fernández Prini): To complete draft closing statement by September.

- ***ICRN 12: Kinetics of Oxygen and Hydrogen Electrode reactions***

ACTION (Lvov, Majer): Vladimir will e-mail Sergei to obtain draft closing statement by September.

### *IUPAC Report*

- Roberto Fernández Prini reported on the recent off year IUPAC meeting in Switzerland and changes in IUPAC priorities and procedures for project selection. He stressed the importance of developing IUPAC connections, and the desirability of developing a joint project. Anneke Sengers noted that TPWS has a joint project on transport properties of steam.

ACTION (PCAS Members): To identify possible projects to Roberto.

### *Round Table Preparation*

- There was a general discussion of the need for industrial dialogue to identify projects with long-term impact and potential funders. Don Palmer noted new DOE programs for targeted special projects. V. Majer noted new E.U. funding programs for partnerships with industry. Don noted EPRI support from targeted areas, usually identified by EPRI who then approach the researcher. Marasu Nakahara will identify new Japanese programs for international collaboration.

### *International Collaborative Grant*

- The US and Czech National Committees propose a 5-month collaborative grant for a PhD student, Tomas Nemec from the Institute of Thermomechanics in Prague to work at ORNL to prepare a database of thermodynamic data of interest for nucleation in superheated steam. Discussion on Thursday noted the need to operate a car at ORNL which justifies relatively high budget (\$9,000 stipend being proposed), travel to be paid by the Czech partner. ACTION: Approved.

- The desirability of young scientists returning to their home country after an collaborative grant was discussed. ACTION (Fernandez Prini) to formulate a statement of intent to be signed by the candidate and host country.

**Thursday, July 25 2002**

### **Discussion of the 2003 Meeting (August 29 – September 3)**

- Next years conference will be held in Denmark Possible conflicts with two meetings were noted:  
ISHR conference 2<sup>nd</sup> week of September in China  
IUPAC General Meeting Ottawa  
A desire was expressed to have aqueous chemistry people from the Technical University in Lyngby present during a part of meeting

### **ICPWS Conference in 2004**

- The committee supports the inclusion of the names “high temperature”, “aqueous systems” in connection with the suggested names “power generation” and “environment” in the title of the Conference.
- We support the continued focus on high temperature water and steam and expansion into new areas of application. We do not support expanding into areas of application that are unrelated to high pressure and/or high pressure water or aqueous solutions where other expert organizations are present.

### Membership

- A proposal to move Dr Marsik from PCC to PCAS was approved.

### ICRNs

- **Formulation for NaCl(aq):**  
Experimentalists now use a self consistent package of (i) Hill eqn of state + (ii) Archer & Wang Debye Huckel constant + (iii) Archer formulation for properties of NaCl(aq). The use of the new IAPWS formulations requires a self-consistent formulation for NaCl(aq) as an urgent priority. It would be desirable to incorporate new data to extend the range of validity once the compatibility issue is solved (two separate and successive actions envisaged).

### Guidelines

- **Equilibrium Constants for the Solubility of Gases (Harvey et al.)** The Guideline was approved if amended to note this definition of Henry's Law (function of T only) is specific to this guideline.

### Atlas

Don Palmer made a report to the combined working groups on progress and deadlines. The issue of appendices and supplementary material was discussed. The following actions and decisions were noted.

- The NIST version of the steam tables should be included on a read-only CD ROM
- Chapter deadline November 30, 2002
- Submission deadline April 30, 2003
- The inclusion of collecting hard-copy tables in an appendix is an editorial decision

### Priority Areas

- **Standard State Thermodynamic Properties of Aqueous Organic Solutes.**  
There was extensive discussion of the equations of state summarized in Vladimir Majer's lecture at the Symposium. A decision was made to form a Task Group to prepare guidelines on the application and database development of these and other similar treatments. Members were nominated: Majer (chair), Plyasunov, Fernandez Prini, Sedlbauer, Wood, Harvey, Tremaine, one Japanese member.

ACTION (Majer) To draft a statement for the Task Force and to contact members to make a progress before the next IAPWS meeting in Denmark.

- **Measurements and Standards of pH**  
Don Palmer tabled a proposal to form a Task Force (i) for developing an assessment of measurement techniques for pH in water & steam, and (ii) revised pH scale for high T & p Palmer (chair), Lvov, Nakahara, Ding, Jensen, Johnston, Tremaine  
ACTION (Palmer) To draft a statement and to contact members to arrange a first meeting at or before the next IAPWS meeting in Denmark

**Future of IAPWS and Restructuring Discussion**

- **Most Important Project :**”  
“Atlas”
- **New Directions**  
The following trends were noted:  
Deregulation and demise of national and corporate labs  
Initiate education program or initiative  
Focus on ultra-supercritical cycles possible in future
- **Alternative Structures**  
Maintain “3 seminar structure” (one separate and two joint sessions) of the annual meeting  
Implement one or more Task Forces in PCAS to address specific issues  
Hold a simplified ICPWS every 3 years; replace proceedings with synopses or journal issues.