

## IUPAC Project Progress Report

**Date:** July 2007

**Task Group Leader:** Igor V. Sukhno

**Project number:** 2006-010-1-500

**Project Title:** The Adjustment, Estimation and Uses of Equilibrium Reaction Constants in Aqueous Solution

### Report:

1. Current status of project: The project was started in June 2006
2. Progress relative to 'milestones':
  - a) Collected during June 2006 – June 2007 period published SIT and Pitzer-related parameters are currently being analyzed.
  - b) A version of the SIT program to correct stability constants for changes in seawater salinity and in electrolyte mixtures now is ready and tested.
  - c) A program to calculate the solubilities of N<sub>2</sub> and rare gases now is ready and tested.
  - d) The second task group meeting in full project staff (Dr. Igor Sukhno, Dr. Vladimir Buzko, Dr. Leslie D. Pettit) is in preparation. This meeting will take place in 18.08.2007–23.08.2007 in UK (Academic Software, Otley, Yorks LS21 2PW). The project progress for June 2006 – June 2007 period will be discussed. After this meeting the new version of project software will be placed on IUPAC (<http://www.iupac.org/projects/2006/2006-010-1-500.html>), Academic Software (<http://www.acadsoft.co.uk>) and Aqua Solution Software (<http://public.kubsu.ru/aquasolsoft/>) web sites.
3. Difficulties encountered (or concerns): nothing significant
4. Projected completion date (documents ready for external review): 1 July 2008
5. Please list all of the intended outputs and the dissemination plan for this project (viz. articles, CD, conference presentations; etc.). These may have been expanded since project approval:

### Outputs

- Public Domain software and free CD software
- IUPAC Technical Report
- Manuscript to be published in Journal of Solution Chemistry

### Dissemination Plan

To be made freely and easily available to the scientific community via the internet and on CD. Presentation of the Software at IUPAC sponsored conferences.

To advertise the final Software product and to disseminate it, via the Internet, among the research groups working in the field.

6. If your project is within 6 months of completion, how do you plan to utilise any remaining budget for this project? –
7. Work on this project may have identified new problems, issues, challenges, emerging topics, opportunities for related projects, etc. Please indicate these here so that the Division can follow up on them: –