

IUPAC Project Progress Report

Project number: 2000-003-1-500

Project Title: Ionic Strength Corrections for Stability Constants

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Report:

1. Current status of project:

The project, as initially designed, was completed two years ago but the project has been enlarged significantly to extend its usefulness. It now consists of a suite of inter-linked programs as follows:

The controlling program: 'The Adjustment, Estimation and Uses of Equilibrium Constants in Aqueous Solution'.

- 1) The SIT program as described in the last report.
- 2) Electrolytes: to calculate activity coefficients and water activity using Pitzer and Lin-Tseng-Lee equations.
- 3) Acid-base: to calculate acid-base equilibria in electrolytes and seawater for over 260 acids.
- 4) Temperature Effects: to calculate temperature dependence of log K values using 8 thermodynamic equations of increasing complexity.
- 5) Oxygen solubility: To calculate oxygen solubility in 22 electrolytes, natural fluids and seawater as a function of temperature, salinity etc.
- 6) Speciation. The powerful speciation package which is also part of the IUPAC Stability Constants Database.
- 7) Titration and speciation simulations: a dynamic and real-time simulation program.

In addition, other programs are planned if resources are available. The initial versions of these programs are now available for inspection and evaluation. They could be provided as a CD or as a compressed zip file of about 6.5 GB provided a mechanism for distribution can be established.

2. Progress relative to 'milestones':

Original project now completed and the work has been extended within the project as agreed by IUPAC in summer 2003.

3. Difficulties encountered (or concerns): none

4. Projected completion date (documents ready for external review):

The current version is available for review, with initial details of possible future extensions.

5. Intended outputs and the dissemination plan for this project:

Programs and data files can be made available on the IUPAC web-site, and on any other interested sites or as a CD if distribution costs are met.

6. Work on this project has identified issues and/or opportunities for related projects:

The CD referred to above offers many exciting possibilities but availability and distribution would have to be considered. Distribution via the internet is one possibility.