

IUPAC Project Progress Report

Date: July 2007

Task Group Leader: Kip Powell

Project number: 2005-014-1-500

Project Title: IUPAC Stability Constants Database. Completion of data collection to 2006.

Report:

1. Current status of project:

The project involves on-going literature evaluation and entry of data into files that are then conflated into the master database by Academic Software.

In this reporting period data have been entered from J. Chemical Engineering Data 2006; Talanta 2005 and 2006; Thermochemica Acta 2005 and 2006; J. Coordination Chemistry 2005; Inorganica Chimica Acta 2005; J. Inclusion Phenomena 2005 and 2006; Transition Metal Chemistry 2005 and 2006; J. Solution Chemistry 2005; New Journal of Chemistry 2005; J. Inorganic Biochemistry 2004-2006; Coll. Czech Chem Commun. 2005 and 2006; Monatsh. 2005; Koord. Khim. 2005; some 400 pages of data from missed articles in older journals.

2. Progress relative to 'milestones':

The above completions of data entry should be gauged alongside the following: (a) a total of 56 main stream journals will be abstracted to the end of 2006; (b) including the above there are now some 15 journals complete to 2004, 8 complete to 2005, and 9 complete to 2006; (c) the work is concentrating on those journals with a high frequency of relevant articles – several journals not up to date beyond 2000-2003 have few relevant articles (e.g. J. Amer. Chem. Soc. and Anal. Chem.), while others are difficult to access on a regular basis.

Journals that continue to be difficult to access include Acta Chimica Sinica; Ann. Chim (Rome); Bull. Soc. Chim. Fr.; Chem. Speciation Bioavail.; Gazz. Chim. Ital.; J. Indian Chem. Soc.; Polish J. Chem.; Radiochim. Acta.; Z. Naturforsch. The cost of obtaining articles from these on interloan is prohibitive. However, recent informal arrangements have been made for supply of articles from Radiochimica Acta (Paul Brown) and Bull. Soc. Chim. Fr. (Montserrat Fillela).

3. Difficulties encountered (or concerns):

In addition to data entry this project aims to establish an ongoing team of (at least three) data management experts, each member of which will undertake a 3 year commitment. With these commitments starting in successive years this would establish a continuum of expertise. This aspect of the project has not been successful to date. One team member, although making a personal contribution, has not been able to hire a graduate student to assist with data entry and is therefore not able to generate the level of input anticipated. The second team member, after delays to commencement on this project, finally withdrew entirely (in April 2007). To date there has been no success in finding a replacement for him or finding a third team member.

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

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:

An article on SC-Database was published in CI in the October 2006 issue, the first in the series on Tools of the Trade.

6. If your project is within 6 months of completion, how do you plan to utilise any remaining budget for this project?

N/A

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:

The ongoing maintenance of *SC-Database* after the completion of this project is a major concern. This is compounded by the fact that the involvement of Academic Software as database managers is not likely to extend much beyond the completion date of this project.

The current understanding with the IUPAC Executive is that the Division (viz. the SSED) will undertake the ongoing abstracting, entering and quality control of the data, while an approved new manager will have responsibility for database management and distribution. There has been an inadequate outcome on each of these facets. Firstly, the TG member who brought SSED links to the project is the one who has now withdrawn. Secondly, the agreed new manager, FIZ-Chemie, who indicates an intention to establish a web-based version for IUPAC, has been unresponsive to communication since visiting them in November 2006.