

IUPAC Project Progress Report

Date: September 2008

Project number: 2005-014-1-500

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

Task Group Leader: Kip Powell

Starting date: September 2005

Report:

The project involves on-going literature evaluation and entry of data into files that are conflated by Academic Software. In this reporting period data have been entered from: Ann. Chim. 2000, 01, 03, 05 and 06; Dalton 06; Inorg Chem. 03, 04, 05, 06; J. Inclusion Phenomena 06; Chemical. Geol. 01 to 06; Eur. J. Chem. 03; Chem. Eur. J. 03, 04; some 300 pages of data from older journals.

1. Projected completion date: November 2009
2. Have the project objectives been modified during the last 6 months?
Yes. See item 8 below.
3. Please list the task group members involved in the work during the last 6 months.
Bela Gyurcsik, Kip Powell.
The assistance of Paolo de Zorzi in providing access to the Italian literature is much appreciated.
4. Difficulties encountered (or concerns):
Since commencement of the Project the Hungarian workers (Tamas Gajda and Bela Gyurcsik) have lost access to SciFinder, which is an essential tool for data entry on new ligands. This has considerably increased the workload for the TGC.
5. Please list the to-date results (outputs) of the project
6. Please list the dissemination events (viz. articles, CD, conference presentations; etc.)
 - (i) already accomplished; Academic Software (Leslie Pettit) presented a paper at the Solubility Phenomena Conference in Dublin in August.
 - (ii) planned N/A
7. If your project is within 6 months of completion, how do you plan to utilise any remaining budget for this project? N/A
8. 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.
 1. Following discussions with the Secretary General in March 2009 and meetings with Academic Software in April 2009, the TGC prepared a proposal regarding the future of the Stability Constants Database, to take effect at the end of the currently-funded project. The Division V President was briefed on this proposal. The proposal was sent to the Bureau's Executive Committee and approved in August 2009.

As will be outlined in a separate document, this proposal reflected
(a) the difficulties experienced in enlisting a team of suitably qualified and motivated persons to take over the on-going task of literature evaluation, data entry and verification, and

(b) the difficulties encountered in working with a web provider who initially undertook to prepare a web-based version of the database, prepare a web interface for data entry, and manage the master files, apparent commitments that have now all been withdrawn.

The agreement reached with the Bureau is that data collection will terminate at the end of the current project (which will complete data compilation from the literature to the end of 2006) and that the database will be made available through IUPAC as a frozen compilation, until such time as interested parties within IUPAC identify a need to continue the work in what is then seen as a timely fashion and format for identified end-users.

2. Thinking of the Division's future commitment to critical evaluations of equilibrium data in homogeneous solution, it is clear that the SSED is under-resourced with members who have an interest and expertise in equilibria in homogeneous solution.