

IUPAC Project Progress Report

Project number: 2000-004-2-500

Project Title: IUPAC Stability Constants Database

Task Group Leader: L. D. Pettit

Report:

1. Current status of project: Progressing to plan

Data collection, co-ordinated by Prof. K. Powell, is proceeding well, collecting both data published since 2000, and filling in gaps with data omitted from previous years. The database now holds data from 27 references for 2003, 199 references for 2002 and 265 references for 2001.

Currently the database holds stability constant data on 8858 ligands; 313 new ligands since April 2004 (all with .mol file structures) from 22045 references and holds 104260 records (ligand-metal-reference combinations).

The interrogation software has been modified to allow inspection of constants directly from the various 'Browse' menus..

2. Progress relative to 'milestones': On schedule

3. Difficulties encountered (or concerns): Nothing particular

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

The current database is always available for external review

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

The database is currently distributed on CD, with a printed manual

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

The database is now used in Strasbourg for 'data mining' based on sub-structure fragments. We are now actively discussing with IUPAC the formal transfer of the database to IUPAC over the coming years and, this month, have had a meeting with Prof. K. Powell to discuss the possibilities. We have jointly submitted some proposals to IUPAC.