The IUPAC Stability Constants Database—Completion of Data Collection up to 2006

The IUPAC Stability Constants Database (SC Database) is the most comprehensive compilation of stability constants available, now covering the years 1877 to 2002. It is a major research tool for those involved in equilibrium modeling of environmental, biological, and industrial systems, and it is the primary source of data for the Critical Evaluations of Stability Constants that are published regularly by the IUPAC Analytical Chemistry Division (Division V).

The SC Database records solution equilibrium data ($\lg K, \Delta H, \Delta S$) abstracted from 55 mainstream journals. It includes all of the data from the previous volumes published before 1972 by IUPAC and RSC. Publications from 1972 to 2002 were evaluated and abstracted through a series of projects by Commission V.6, then Division V. The database now contains some 105,500 records (pages of data) from 22,000 references for 9,000 ligands, forming a unique compilation of significant published solution equilibrium constants.

The SC Database can be searched by ligand (formula, name, fraction of name, structure fragment, ligand class), metal ion, author, reference, method, medium, or any combination thereof. Data resulting from an SC Database search can be exported to a powerful speciation program or to programs for temperature and ionic strength corrections. Coupled with its ancillary programs, it has no equivalent competitor.

There is no indication that the publication of articles on solution equilibria has declined in the past 10 years, although there have been changes in the popularity of specific journals for this work (e.g., an increasing use of biological journals and study of biologically relevant ligands). Furthermore, the average number of records derived from each article has remained essentially constant. This trend indicates a continuing interest in the field and also an ongoing need for literature evaluation and abstracting of data.

The continuing flow of publications and the shifting focus of experimental work (and published data) onto new classes of ligands (e.g., biological buffers, ligands used in medicinal and pharmaceutical applications, and macrocyclic ligands) ensures an ongoing demand for IUPAC’s SC Database. It also ensures an ongoing need for IUPAC projects that will contribute to the Critical Evaluation of Stability Constants.

The current database can be ordered at <www.iupac.org/divisions/V> or <www.acadsoft.co.uk>. Each of these sites offers a downloadable demo version of the database.

The aim of the present project is to:
• bring the literature coverage in the SC Database up to date to 2006, to be accomplished by 2008 (Coverage is currently complete to the end of 2002 for 26 mainstream journals, to 2001 for 11 journals, and to 2000 for nine journals of the 55 that are currently abstracted.)
• expand the team of experts who supervise data entry and oversee quality control
• establish a succession of experts to continue this work beyond the current project

Members of the project team who are responsible for literature abstracting, data evaluation, and data entry are Kip Powell (New Zealand), Tamás Gajda (Hungary), Igor Sukhno (Russia), and Erich and LanChi Königsberger (Australia). Expressions of interest from additional experts are welcome.

For more information, contact Task Group Chairman Kip Powell <kip.powell@canterbury.ac.nz>.


---

**Searching by ligand**

Ligands can be searched on any combination of:
- empirical formula (or fragment)
- Name (or fragment) - full name or short name
- Any structure fragment
- Ligand class (from 34 classes)
- CAS-RN

Searching can be:
- exactly as specified
- matching from start only
- from anywhere within the entry

Double-clicking on an entry in the ligand list displays the structure and other details.

Search results are presented as a list of ligands matching the search criteria. Ligands required by the user are selected from this list.