# The IUPAC Stability Constants Database (*SC-Database*)

## The definitive collection of all significant published Metal-complex stability constants

## Summary

**Background**:

- Designed to contain all significant published metal-complex stability constants.
- Contains all data from the book volumes published by Royal Society of Chemistry and IUPAC, 1957-1974.
- Data from all significant journals, 1877 - 2002.
- PC computer-based (32-bit) with very fast, user-friendly searching and display routines.
- Currently being updated from 2002.

**Features**:

- 22,000 references covering 9,000 ligands in 105,500 records.
- Searchable on any combination of ligand, reference or experimental details.
- Data displayed, printed or saved in many ways.
- Interactive software for speciation, ionic strength and temperature corrections included.
- A tool for industry, research and teaching.
- Download **DEMO** database from: www.acadsoft.co.uk

## Output options

*Output can be sent to:*

- **Screen** or to:
- **Printer**; **Clipboard** or **Disk file**

*Format can be:*

- **Single record**
- **Multiple records**

Instant access to other applications

Metal and reference details

Ligand details

Ligand structure

Experimental details

Constants

Other data

*Thumbnail graphs of:*
Temperature dependence
Ionic Strength dependence

Output of multiple records to printer, clipboard or disk includes full references

## 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

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

*Searching can be:*

- exactly as specified *or*
- matching from start only *or*
- from anywhere within the entry

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

## Searching by ligand (sub-structure searching)

*Choose from:*

- 10 pre-defined sub-structures
- use the built-in structure editor, ***EdChemS***
- load a mol file (*e.g.* from ***Chem Draw*** or ***Isis Draw***) from disk

*Match by:*

- exact bond type
- any bond type (to allow for resonance)

Here the sub-structure **purine** has been selected

*Ligand class:*
Ligands are assigned within 34 classes

*Once displayed, structures may be:*

- saved as a *mol* file *or*
- printed *or*
- copied to the clipboard for use in other applications.

## Searching by reference or author

About 13,000 authors are cited in 22,000 references from 750 journals and sources.

*SC-Database may be searched on:*

- year range or
- journal, (any fragment of name, volume or page number) or
- author (any surname or name fragment)

*SC-Database may also be browsed by:*

- author or
- journal

## Searching by metal ion

Metal ions may be searched on:
any of over 130 metal ions (*e.g.* Cu+, Cu++, Cu+++)
alkali metal ions
alkaline earth metal ions
lanthanide ions

## Searching by experimental details

Experimental details may be searched by:

- medium
- words in comments
- temperature
- method
- K values

## Speciation

Can handle up to:

- 12 components
- 28 species
- 3 solid phases

Species distribution curves may be plotted as:

- percentage plots
- lg conc. plots
- lg S plots (when insolubles present)

Curves may be plotted as:

- a function of pH
- a function of any reactant (pL)
- as a pie-chart, recalculated interactively for any pH/pL

## Temperature and Ionic Strength Dependence

Temperature dependence may be calculated from the van't Hoff equation, provided the ΔH value is known.

Ionic strength dependence may be calculated from the Davies equation.

Ionic strength correction using SIT is freely available from www.acadsoft.co.uk

## Current Status

*SC-Database* is currently being updated through IUPAC project: #2005-014-1

- All significant journals publishing stability constants are being abstracted
- Structures, in mol file format, are included for all ligands
- Sub-structure searching is a feature, together with a dedicated structure drawing package (*EdChemS*)
- *Mini-SCDatabase*, the edited sub-set of *SC-Database* is ideal for teaching. It is included with *SC-Database* and with *SolEq*.(*Solution Equilibria; principles and applications*).
- A **DEMO** database is available from:
  www.acadsoft.co.uk or www.iupac.org/divisions/V/index.html

## Contact Details


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