The IUPAC Stability Constants Database (SC-Database)

The definitive collection of all significant published metal-complex stability constants

Poster presented at the
IUPAC Congress/General Assembly
July 2001

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, 1898 - 2000.
- PC computer-based (32-bit) with very fast and friendly searching and display routines.
- Currently being updated to 2000 with extended features as project # 2000-004-2-500

Features:

- 19,000 references covering 8,000 ligands in 85,000 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 sample files from: **www.acadsoft.co.uk**

Output options

Output can be sent to:

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

Format can be:

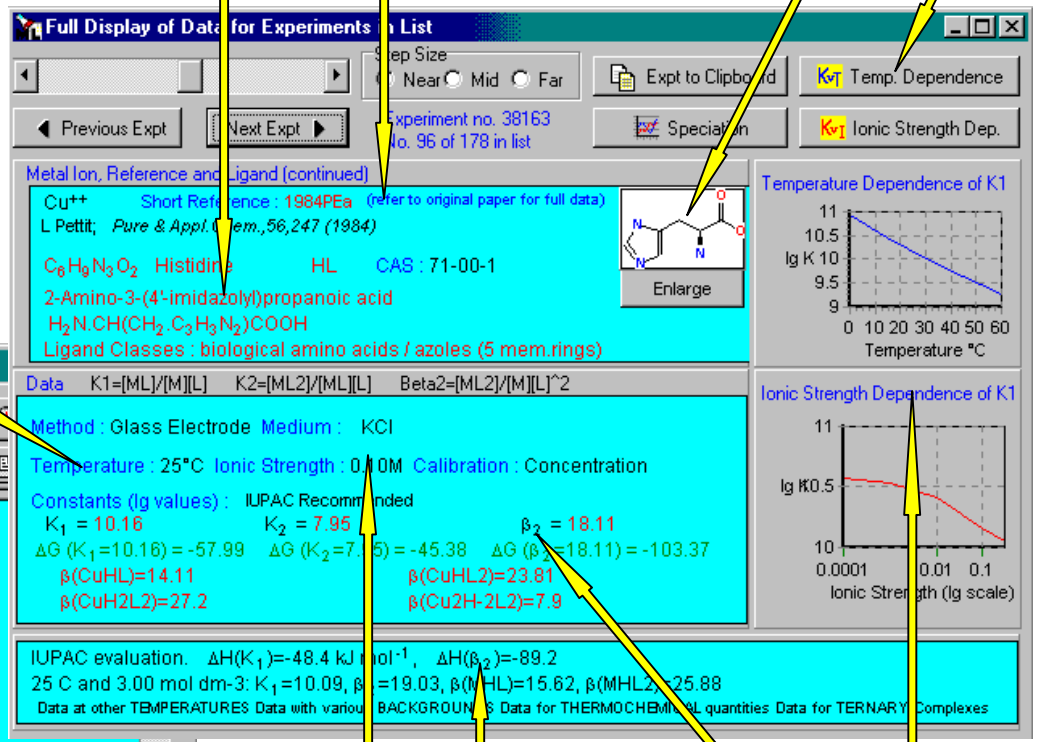
- **Single record**
- **Multiple records**

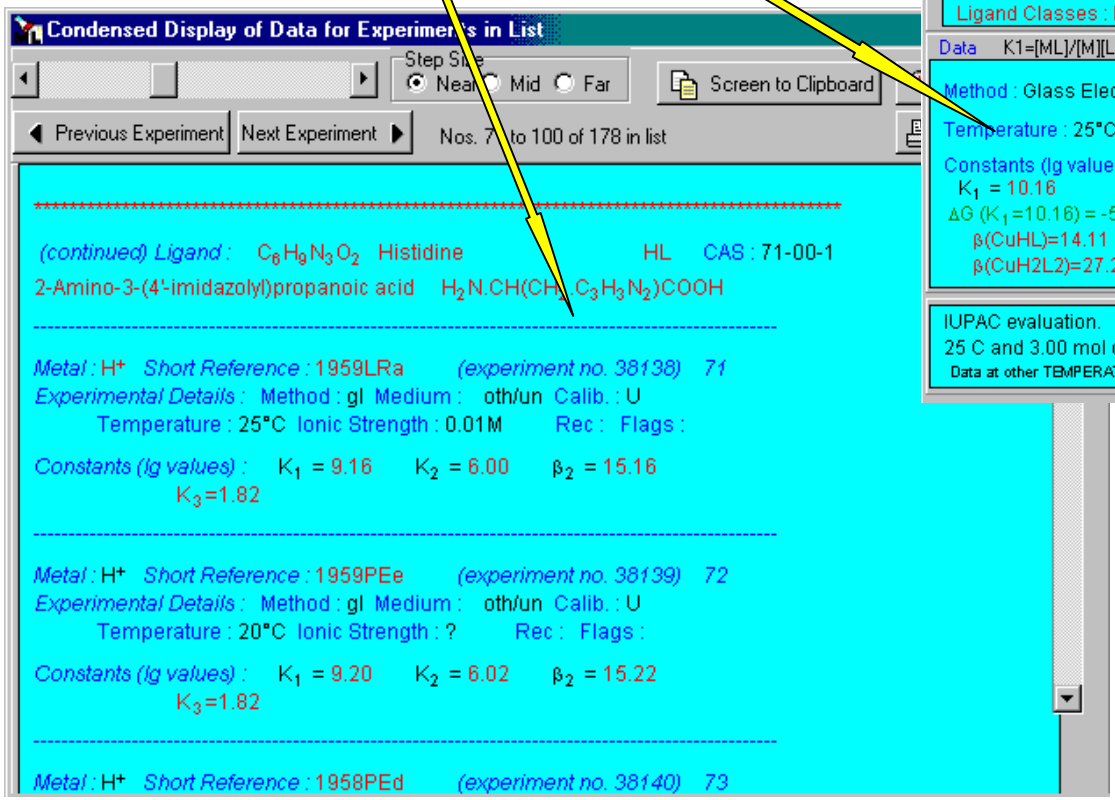
Instant access to other applications

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

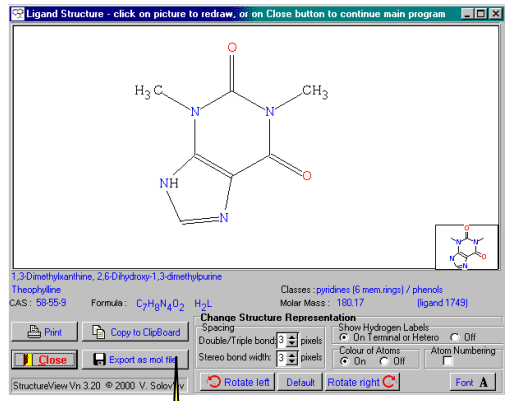
Ligands can be searched on any combination of :

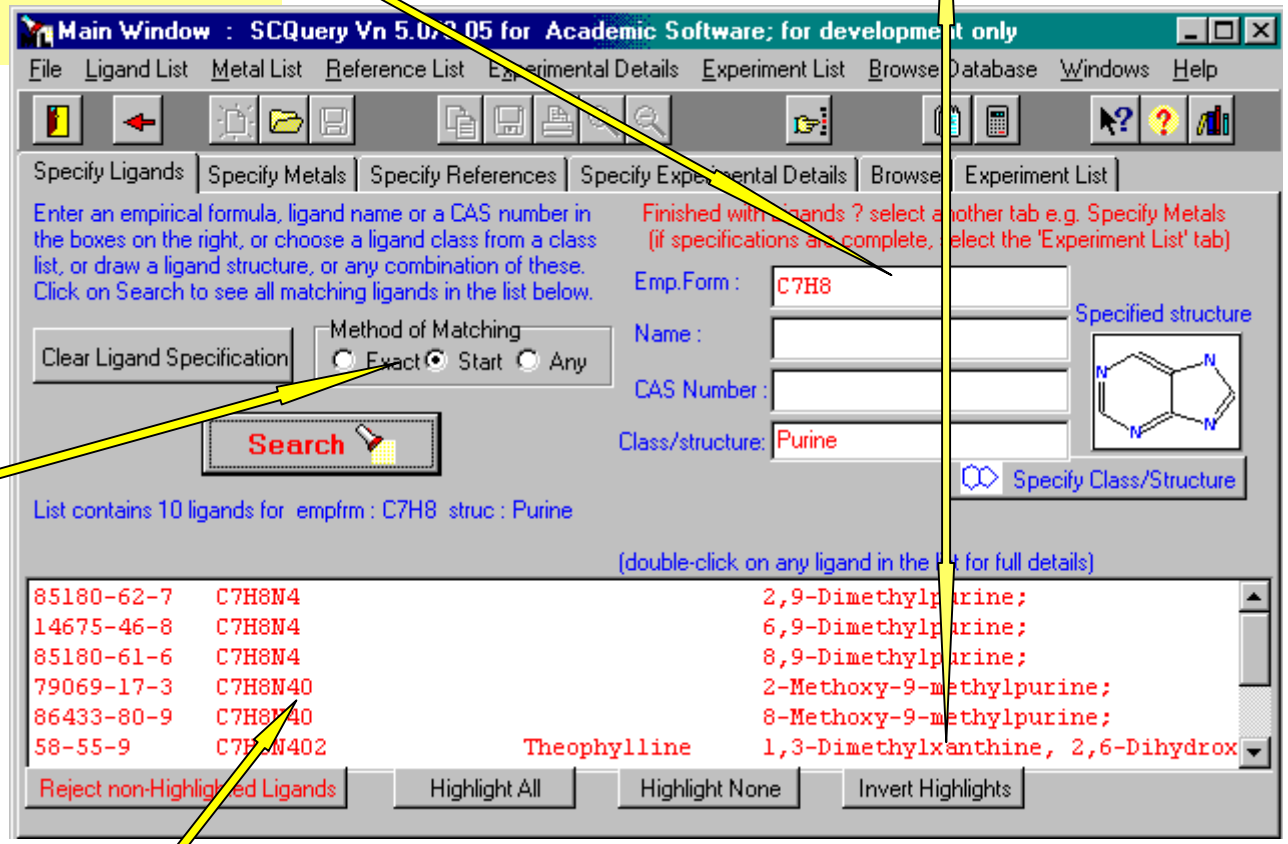
- empirical formula (or fragment)
- Name (or fragment) - full name or short name
- Any structure fragment
- Ligand class (from 34 classes)
- CAS-RN

Searching can be:

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

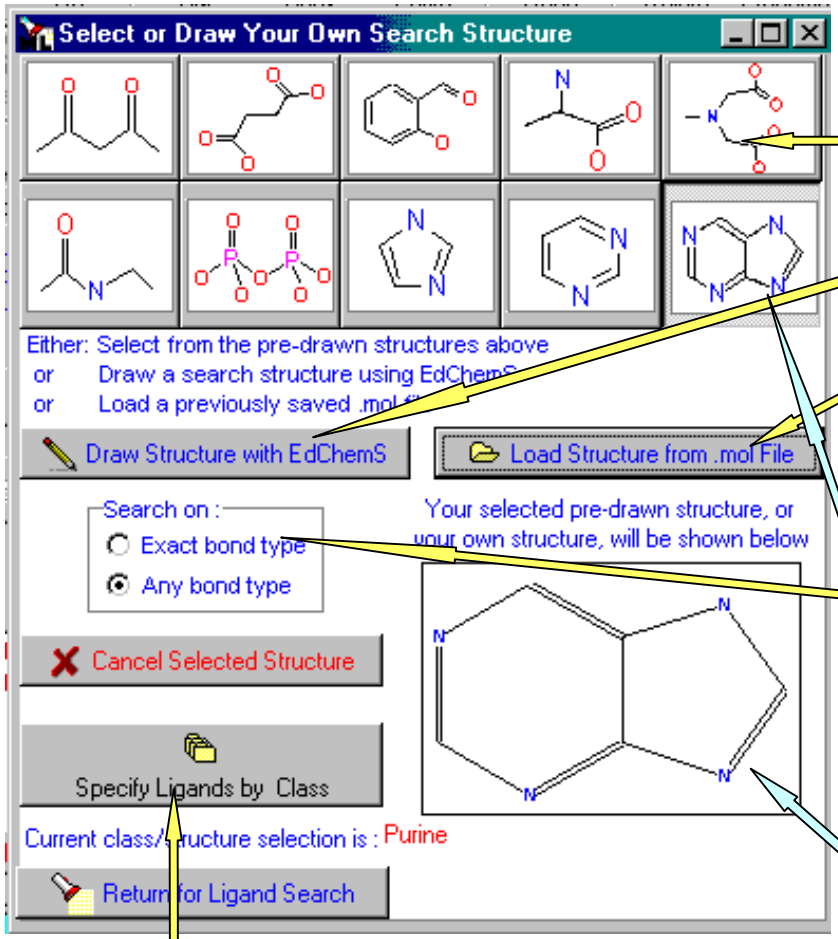
Double-clicking on an entry in the ligand list displays the structure and other details





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

Searching by ligand (sub-structure searching)

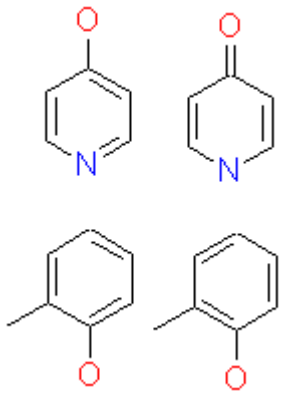


Choose from:

- 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:

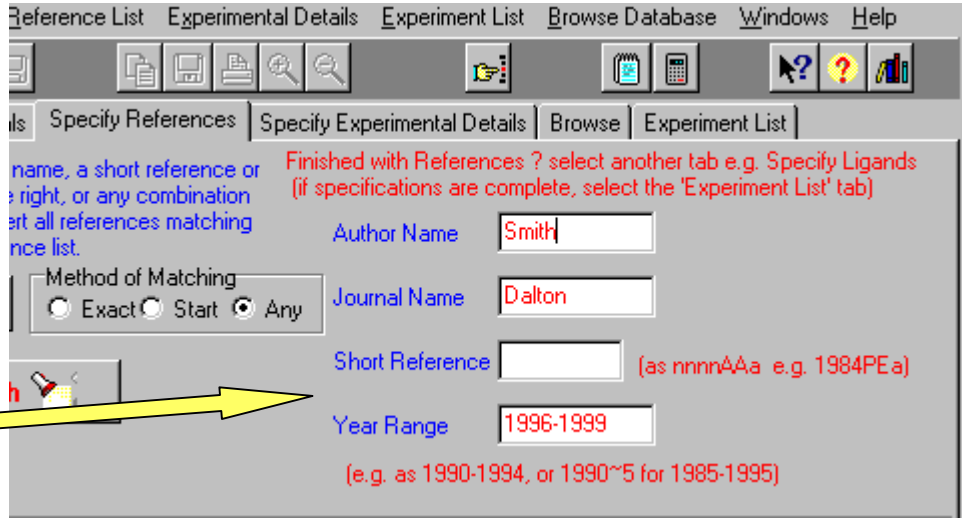
- saved as a *mol* file *or*
- printed *or*
- copied to the clipboard for use in other applications.

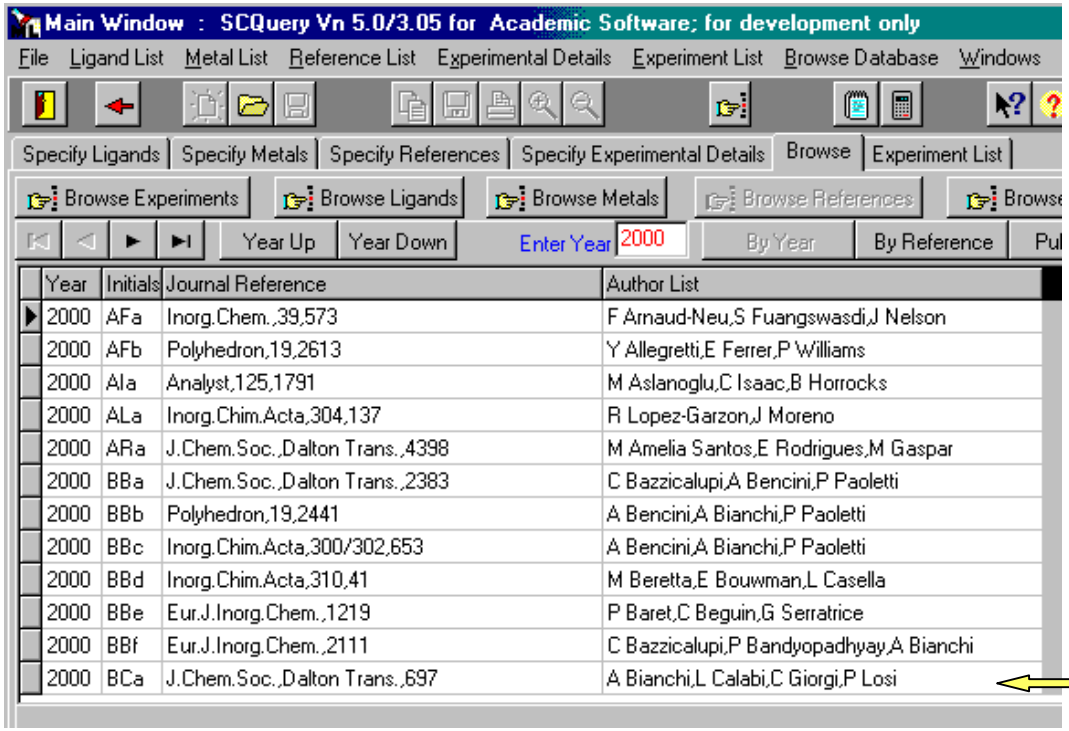
Searching by reference or author

About 13,000 authors are cited in 18,500 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)





Year	Initials	Journal Reference	Author List
2000	AFa	Inorg.Chem.,39,573	F Arnaud-Neu,S Fuangswasdi,J Nelson
2000	AFb	Polyhedron,19,2613	Y Allegretti,E Ferrer,P Williams
2000	AIa	Analyst,125,1791	M Aslanoglu,C Isaac,B Horrocks
2000	ALa	Inorg.Chim.Acta,304,137	R Lopez-Garzon,J Moreno
2000	ARa	J.Chem.Soc.,Dalton Trans.,4398	M Amelia Santos,E Rodrigues,M Gaspar
2000	BBa	J.Chem.Soc.,Dalton Trans.,2383	C Bazzicalupi,A Bencini,P Paoletti
2000	BBb	Polyhedron,19,2441	A Bencini,A Bianchi,P Paoletti
2000	BBc	Inorg.Chim.Acta,300/302,653	A Bencini,A Bianchi,P Paoletti
2000	BBd	Inorg.Chim.Acta,310,41	M Beretta,E Bouwman,L Casella
2000	BBe	Eur.J.Inorg.Chem.,1219	P Baret,C Beguin,G Serratrice
2000	BBf	Eur.J.Inorg.Chem.,2111	C Bazzicalupi,P Bandyopadhyay,A Bianchi
2000	BCa	J.Chem.Soc.,Dalton Trans.,697	A Bianchi,L Calabi,C Giorgi,P Losi

Author Name	Count	Latest/Earliest
Marshall	24	1995KMb1954BBb
Marsicano	12	1995CMa1976HMb
Marteau	1	1974MCa
Martel	1	1955MKb
Martelet	2	1972CMd1972CMe
Martell	188	2000SMc1952MPa
Martelli	1	1966EMa
Marthen	1	1952LMa
Marti	1	1969BMb
Martin	86	1996AKa1937MTa
Martin-Faber	1	1981SMb
Martin-Frere	3	1965MAb1957MAc

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

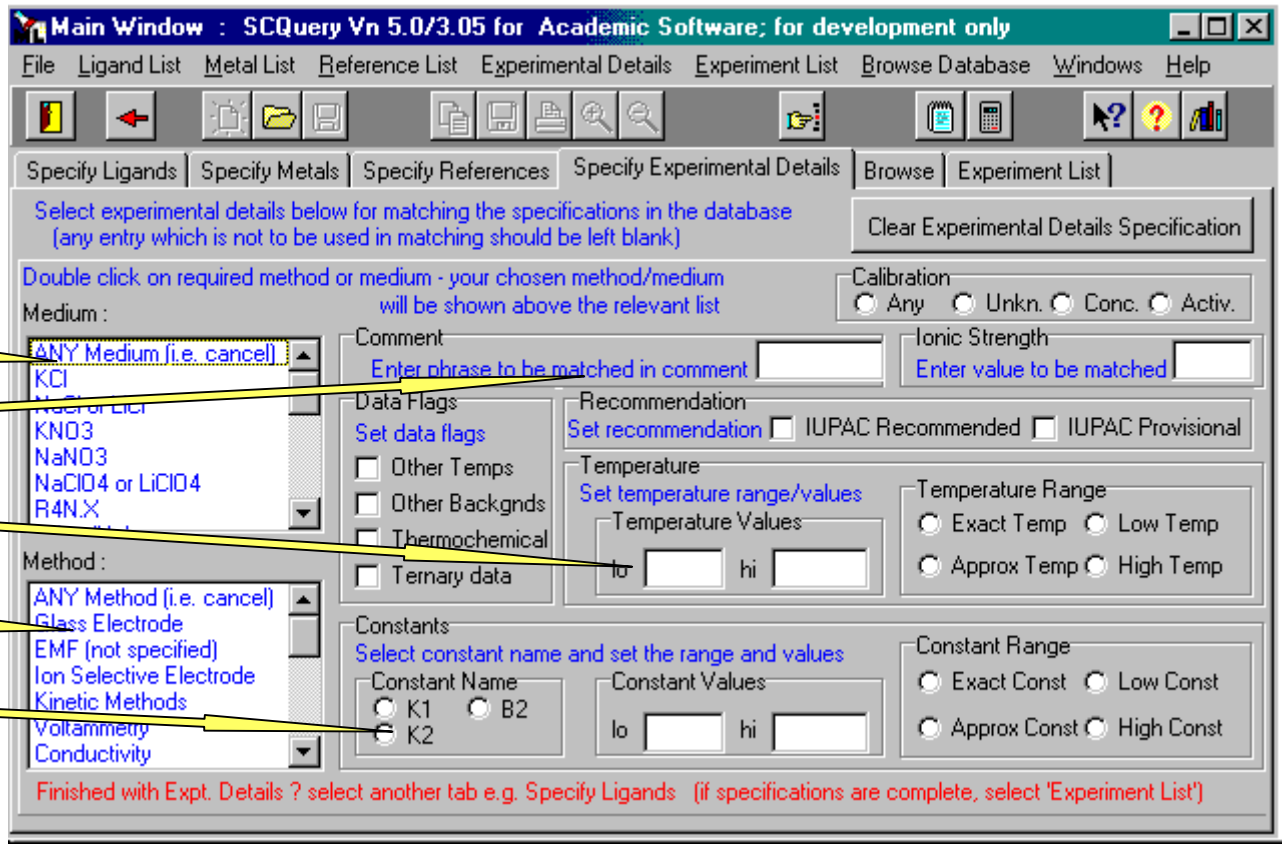
alkaline earth metal ions

lanthanide ions

Searching by experimental details

Experimental details may be searched by:

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



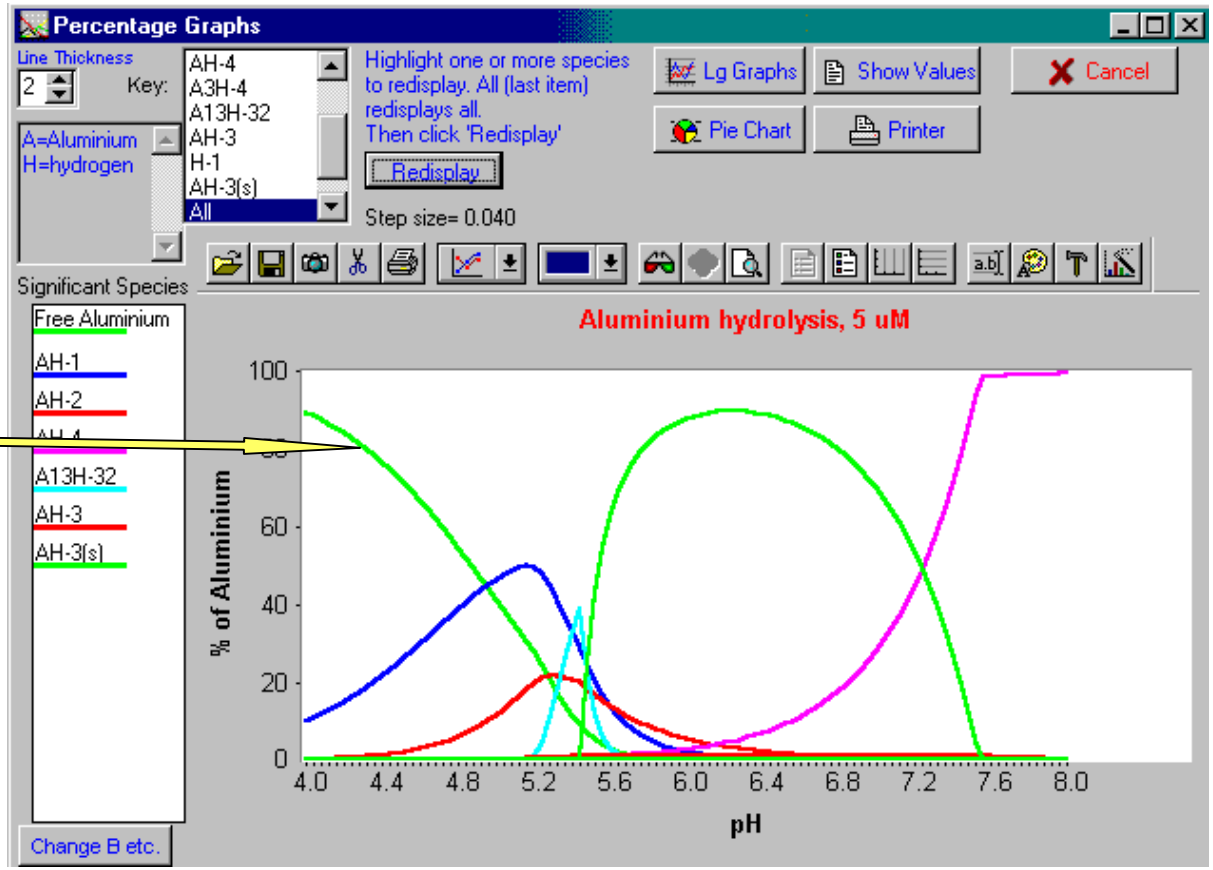
Speciation

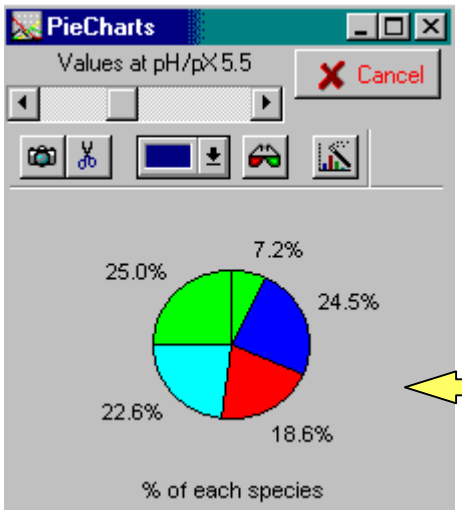
Can handle up to:

- 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)



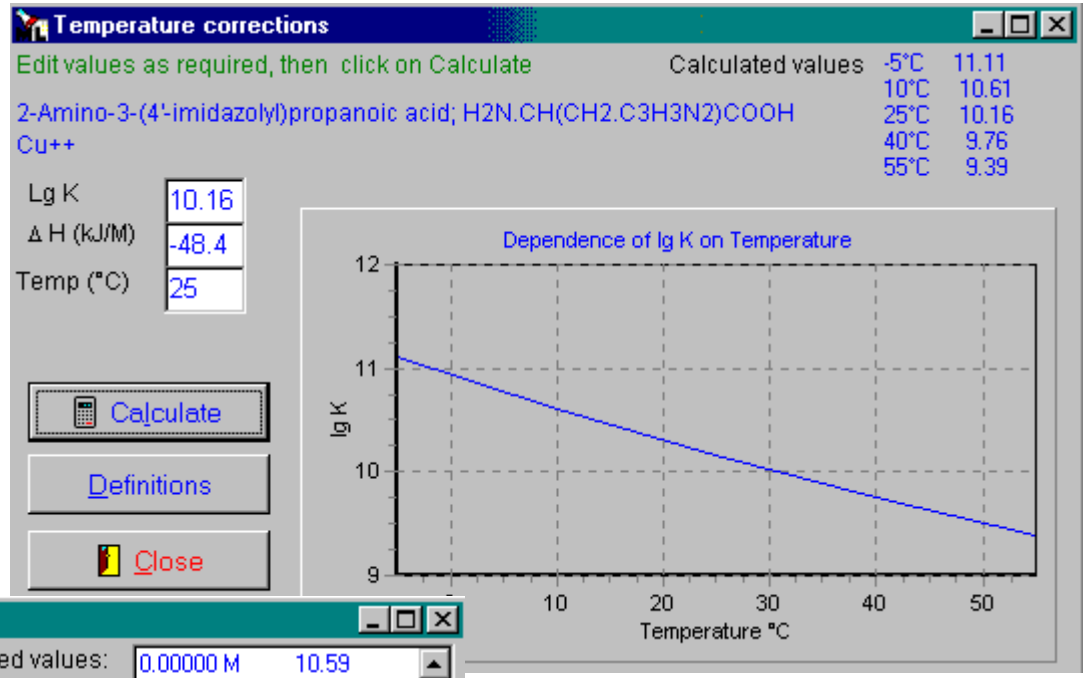


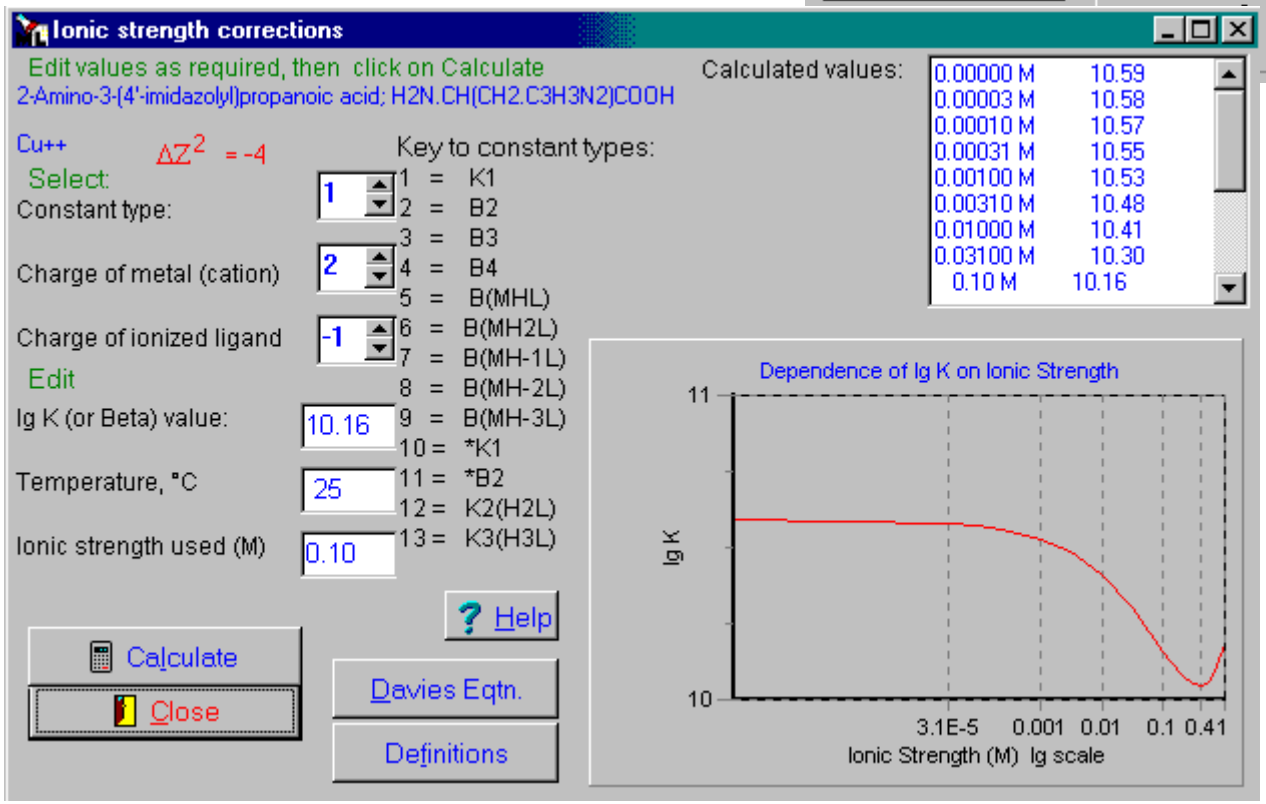
Curves may be plotted as:

- 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 under development.

Current Developments

SC-Database is currently being updated, and new features added, in partnership with project: # 2000-004-2-500

- All significant journals publishing stability constants are being checked up to 2000
- Structures, in mol file format, for all ligands are being added
- Sub-structure searching is being included, together with a dedicated structure drawing package (*EdChemS*)
- An edited sub-set of *SC-Database* has been prepared and is included with *SC-Database* and with *SolEq*.(*Solution Equilibria; principles and applications*). This will be made freely available through www.acadsoft.co.uk

Contact Details

Data collection coordinated by **K.J.Powell** k.powell@chem.canterbury.ac.nz

Database conflation and management by **L.D.Pettit** lesp@acadsoft.co.uk

Structure searching software by **V. Solov'ev** solvit@ipac.ac.ru

Database software and distribution by **Academic Software** www.acadsoft.co.uk