



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

Full Display of Data for Experiments in List

Step Size: Near Mid Far

Expt to Clipboard

Temp. Dependence

Previous Expt Next Expt

Experiment no. 38163
No. 96 of 178 in list

Special In

Ionic Strength Dep.

Metal Ion, Reference and Ligand (continued)

Cu⁺⁺ Short Reference : 1984PEa (refer to original paper for full data)
L Pettit, Pure & Appl. Chem., 56,247 (1984)

C₆H₉N₃O₂ Histidine HL CAS : 71-00-1

2-Amino-3-(4-imidazolyl)propanoic acid
H₂N.CH(CH₂.C₃H₃N₂)COOH

Ligand Classes : biological amino acids / azoles (5 mem.rings)

Enlarge

Temperature Dependence of K1

lg K 10
9.5
9

0 10 20 30 40 50 60
Temperature °C

Ionic Strength Dependence of K1

lg K 0.5
10

0.0001 0.01 0.1
Ionic Strength (lg scale)

Data K1=[ML]/[M][L] K2=[ML2]/[ML][L] Beta2=[ML2]/[M][L]^2

Method : Glass Electrode Medium : KCl

Temperature : 25°C Ionic Strength : 0.01M Calibration : Concentration

Constants (lg values) : IUPAC Recommended

K₁ = 10.16 K₂ = 7.95 β₂ = 18.11

ΔG (K₁=10.16) = -57.99 ΔG (K₂=7.95) = -45.38 ΔG (β₂=18.11) = -103.37

β(CuHL)=14.11 β(CuHL₂)=23.81

β(CuH₂L₂)=27.2 β(Cu₂H₂L₂)=7.9

IUPAC evaluation. ΔH(K₁)=-48.4 kJ mol⁻¹, ΔH(β₂)=-89.2

25 C and 3.00 mol dm⁻³: K₁=10.09, β₁=19.03, β(MHL₂)=15.62, β(MHL₂)=25.88

Data at other TEMPERATURES Data with various BACKGROUNDS Data for THERMOCHEMICAL quantities Data for TERNARY Complexes

Experimental details

Constants

Other data

Thumbnail graphs of:
Temperature dependence
Ionic Strength dependence

Condensed Display of Data for Experiments in List

Step Size: Near Mid Far

Screen to Clipboard

Previous Experiment Next Experiment

Nos. 71 to 100 of 178 in list

(continued) Ligand : C₆H₉N₃O₂ Histidine HL CAS : 71-00-1
2-Amino-3-(4-imidazolyl)propanoic acid H₂N.CH(CH₂.C₃H₃N₂)COOH

Metal : H⁺ Short Reference : 1959LRa (experiment no. 38138) 71

Experimental Details : Method : gl Medium : oth/lun Calib. : U

Temperature : 25°C Ionic Strength : 0.01M Rec : Flags :

Constants (lg values) : K₁ = 9.16 K₂ = 6.00 β₂ = 15.16
K₃=1.82

Metal : H⁺ Short Reference : 1959PEe (experiment no. 38139) 72

Experimental Details : Method : gl Medium : oth/lun Calib. : U

Temperature : 20°C Ionic Strength : ? Rec : Flags :

Constants (lg values) : K₁ = 9.20 K₂ = 6.02 β₂ = 15.22
K₃=1.82

Metal : H⁺ Short Reference : 1958PEd (experiment no. 38140) 73

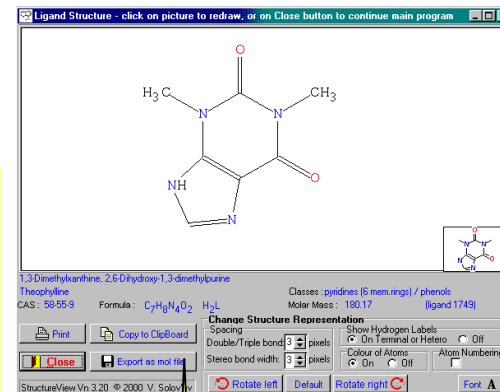
Output of multiple records to printer,
clipboard or disk includes full references

Searching by ligand

Ligands can be searched on any combination of :

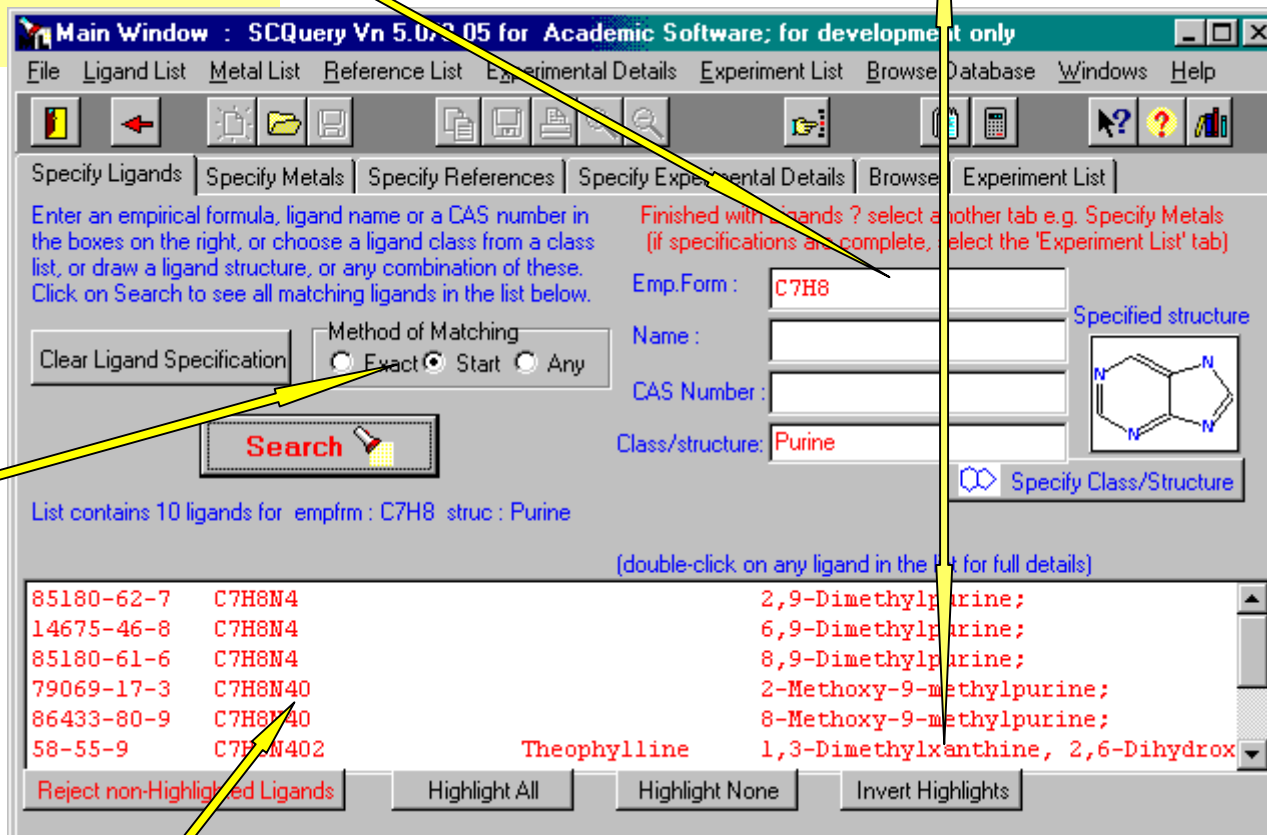
- empirical formula (or fragment)
- Name (or fragment) - full name or short name
- Any structure fragment
- Ligand class (from 34 classes)
- CAS-RN

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



Finished with ligands ? select another tab e.g. Specify Metals (if specifications are complete, select the 'Experiment List' tab)

Emp. Form : C7H8

Name :

CAS Number :

Class/structure: Purine

List contains 10 ligands for empfrm : C7H8 struc : Purine

(double-click on any ligand in the list for full details)

85180-62-7	C7H8N4	2,9-Dimethylpurine;
14675-46-8	C7H8N4	6,9-Dimethylpurine;
85180-61-6	C7H8N4	8,9-Dimethylpurine;
79069-17-3	C7H8N4O	2-Methoxy-9-methylpurine;
86433-80-9	C7H8N4O	8-Methoxy-9-methylpurine;
58-55-9	C7H8N4O2	Theophylline 1,3-Dimethylxanthine, 2,6-Dihydroxy

Reject non-Highlighted Ligands Highlight All Highlight None Invert Highlights

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)

Select or Draw Your Own Search Structure

Either: Select from the pre-drawn structures above
or Draw a search structure using EdChemS
or Load a previously saved .mol file

Draw Structure with EdChemS Load Structure from .mol File

Search on:
 Exact bond type
 Any bond type

Cancel Selected Structure

Specify Ligands by Class

Current class/structure selection is : Purine

Return for Ligand Search

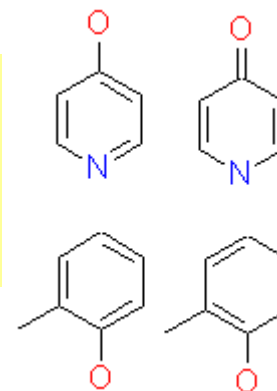
Here the sub-structure **purine** has been selected

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)



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)

Reference List Experimental Details Experiment List Browse Database Windows Help

Specify References Specify Experimental Details Browse Experiment List

name, a short reference or right, or any combination of all references matching the reference list.

Finished with References ? select another tab e.g. Specify Ligands (if specifications are complete, select the 'Experiment List' tab)

Author Name

Journal Name

Short Reference (as nnnnAAa e.g. 1984PEa)

Year Range (e.g. as 1990-1994, or 1990*5 for 1985-1995)

Method of Matching
 Exact Start Any

Main Window : SCQuery Vn 5.0/3.05 for Academic Software: for development only

File Ligand List Metal List Reference List Experimental Details Experiment List Browse Database Windows

Specify Ligands Specify Metals Specify References Specify Experimental Details Browse Experiment List

Browse Experiments Browse Ligands Browse Metals Browse References Browse

Year Up Year Down Enter Year 2000 By Year By Reference Pul

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	Ala	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

Groups of Metals

Hydrogen / Deuterium Lanthanides

Any Metal Ion Alkali Metals

Own Metal Group Alkaline Earths

Metal Ions: Cu, Ni, Zn

Searching by experimental details

Experimental details may be searched by:

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

Main Window : SCQuery Vn 5.0/3.05 for Academic Software; for development only

File Ligand List Metal List Reference List Experimental Details Experiment List Browse Database Windows Help

Specify Ligands Specify Metals Specify References Specify Experimental Details Browse Experiment List

Select experimental details below for matching the specifications in the database
(any entry which is not to be used in matching should be left blank)

Double click on required method or medium - your chosen method/medium will be shown above the relevant list

Medium : ANY Medium (i.e. cancel) KCl NaCl KNO3 NaNO3 NaClO4 or LiClO4 R4N.X

Method : ANY Method (i.e. cancel) Glass Electrode EMF (not specified) Ion Selective Electrode Kinetic Methods Voltammetry Conductivity

Comment: Enter phrase to be matched in comment

Data Flags: Set data flags. Other Temps Other Backgnds Thermochemical Ternary data

Constants: Select constant name and set the range and values. Constant Name: K1 B2 K2. Constant Values: lo [] hi []

Temperature: Set temperature range/values. Temperature Range: Exact Temp Low Temp Approx Temp High Temp

Calibration: Any Unkn. Conc. Activ.

Ionic Strength: Enter value to be matched

Clear Experimental Details Specification

Finished with Expt. Details ? select another tab e.g. Specify Ligands (if specifications are complete, select 'Experiment List')

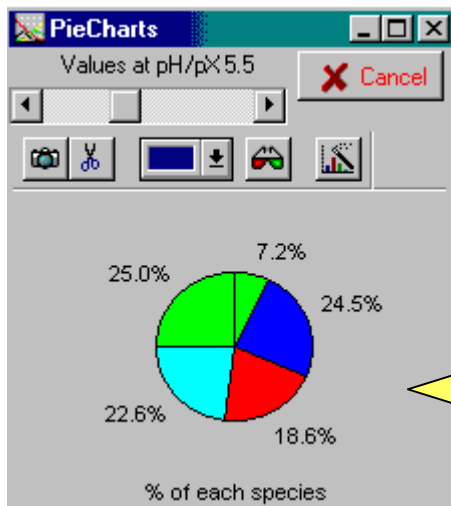
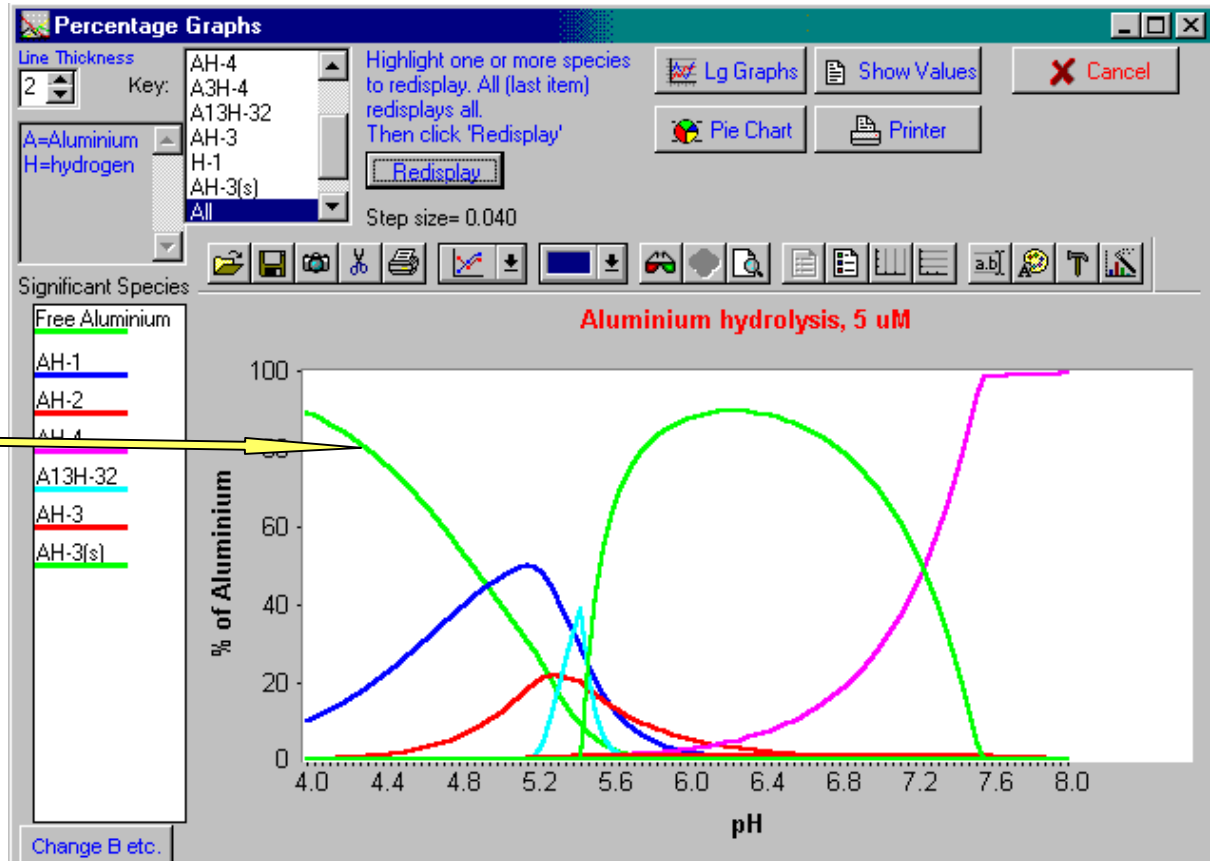
Speciation

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)

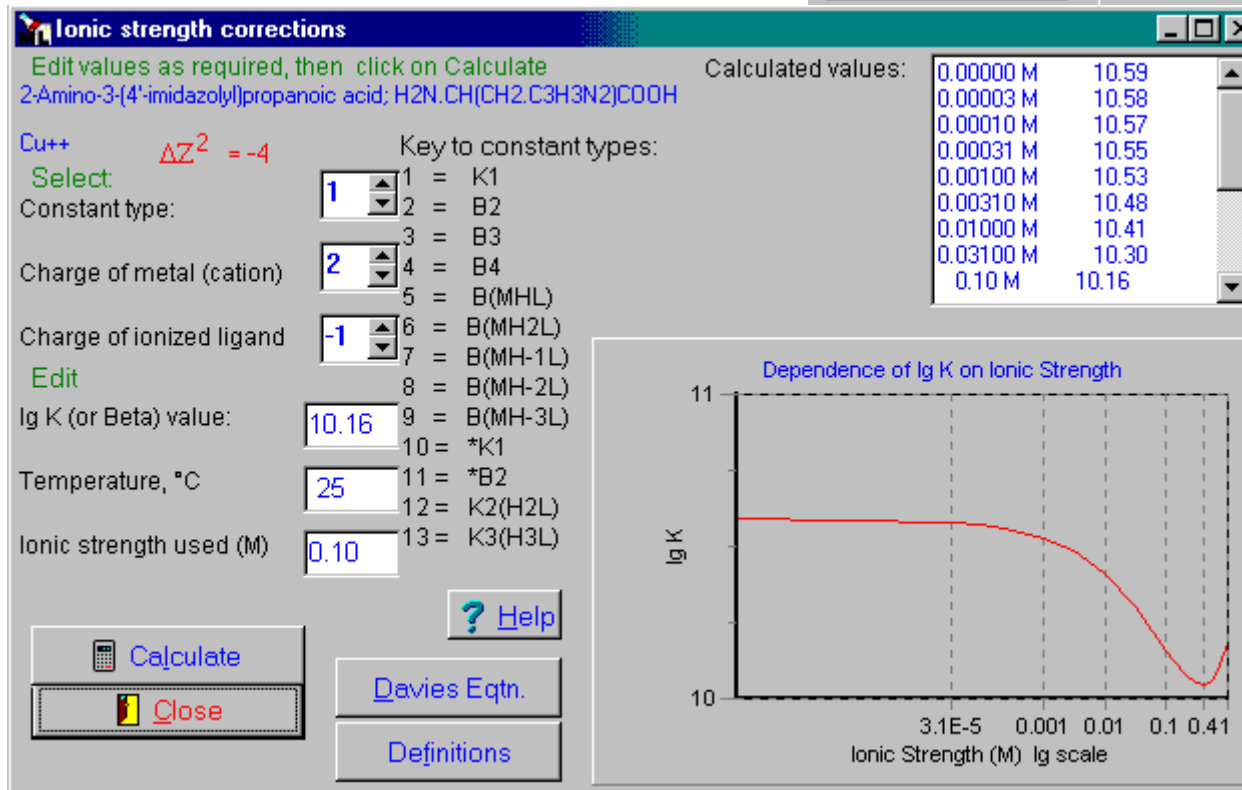
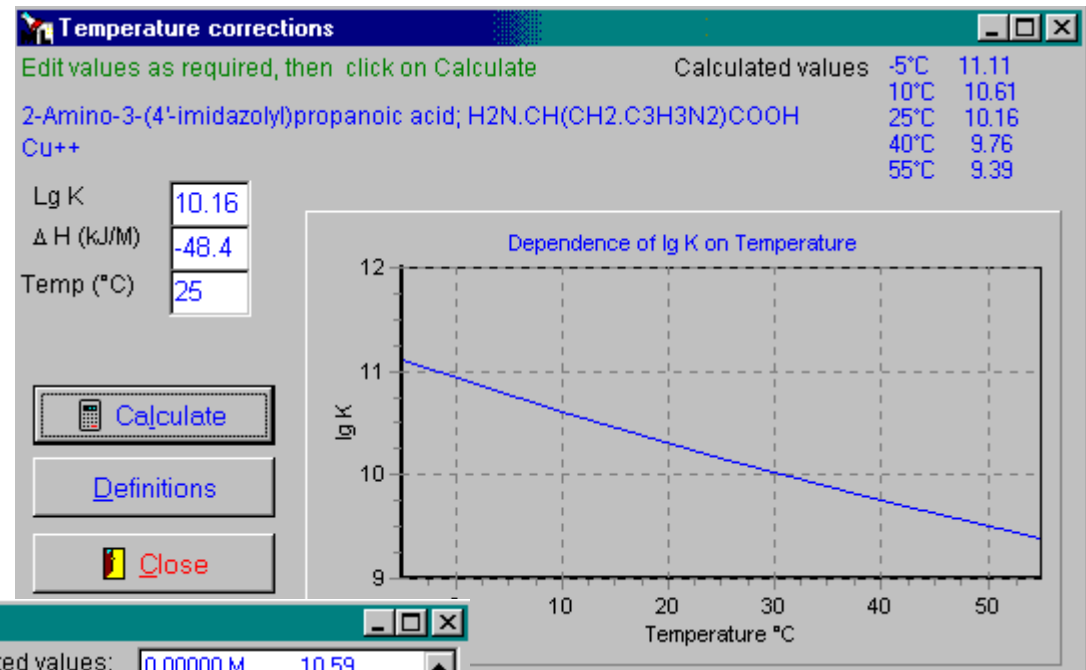


Curves may be plotted as:

- 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

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Database software and distribution by **Academic Software**

www.acadsoft.co.uk