NIST Critically Selected Stability Constants of Metal Complexes Database
Version 8.0 For Windows

Users' Guide

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The National Institute of Standards and Technology (NIST) uses its best efforts to deliver a high quality copy of the database and to verify that the data contained therein have been selected on the basis of sound scientific judgment. However, NIST makes no warranties to that effect, and NIST shall not be liable for any damage that may result from errors or omissions in the database.

ACKNOWLEDGMENTS

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INTRODUCTION

The NIST Critically Selected Stability Constants of Metal Complexes Database is a reference work covering a tremendous number of interactions for aqueous systems of organic and inorganic ligands with protons and various metal ions. Over 18,000 papers have been examined, representing over 99,000 metal-ligand systems, and only data which meet the criterion of well-documented, careful work were considered for inclusion. Furthermore, the data were scrutinized for consistency by comparison both with the same systems by different authors and with similar systems. All data included herein have met these selection guidelines. Bibliographic citations are linked to each ligand-proton or ligand-metal combination retrieved.

The informational scope of the NIST Critically Selected Stability Constants of Metal Complexes Database is very similar to that of the six-volume set by Martell and Smith (*Critical Stability Constants*, Plenum Press, New York, London 1974, 1975, 1977, 1976, 1982 and 1989) except that most of the data have been rescrutinized, errors corrected, and some 50% new material has been added, effectively superseding the values found in the published hardbound volumes.

22,898 protonation constants under specified conditions of temperature and ionic strength for over 4,700 ligands, are given. In addition, 3429 heats of protonation and 3016 entropies of protonation are also given from data provided in the original literature.

Most of these ligands have been investigated with all sorts of metal ions, and hence the stability constants and thermodynamic constants reported herein constitute the largest part of the over 99,000 pieces of data. The interactions of metal ions with ligands usually result in a large number of chemically distinct species. Thus, in addition to the ordinary stability constants, all other constants have been extracted from the literature to give the complete thermodynamic equilibrium descriptions of the systems in question. There are 49,447 equilibrium constants as well as 7,577 heats of reactions and 6,519 entropies for metal ions other than hydrogen.

Additionally, there are 1357 ligands included which did not meet the criteria of selection. For these, the metal ions studied and the bibliographic citations are included, but not the data. These constitute 970 protonation studies and 10,560 metal ion studies for which constants were not abstracted but complete literature references are given.

The NIST Critically Selected Stability Constants of Metal Complexes Database is an important tool for quickly locating a needed equilibrium constant or associated heat of reaction with complete references. Every

abstracted ligand possesses a structural formula for quick identification. Therefore the program is very easy to use. The data are critically selected, so that the values chosen are the most reliable.

The Version 8.0 of the database is now a Windows application. It should be easier to use for most Users. Yet, an effort was made to maintain the efficient "look and feel" and color schemes of the original Versions 1.0 - 5.0, so the previous users would not be distracted by having to learn a new interface.

SYSTEM REQUIREMENTS

a. 80486 PC or greater with Windows® 98, NT, 2000, ME or XP
b. Hard disk with at least 37 MB free space
c. Color monitor, VGA or greater
d. Optional printer: any 80 column printer supported by the operating system
e. CD-ROM drive for installation

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INFORMATION IN THE DATABASE

The term "ligand" is used below to refer to any specific organic or inorganic complexor, chelator, molecule, ion, anion, base, zwitterion, charge-transfer complexor, precipitant, etc. The term "metal" is used synonymously with H^+, M^{n+}, $R_nH_{(4-n)}N^+$, $B(OH)_3$, and others.

The heart of this database is the stability constants, enthalpies and the entropies of proton and metal ion equilibria with ligands in aqueous solution under defined conditions of ionic strength and temperature. The data is critically scrutinized for accuracy and consistency, but all authors are identified for a given ligand-metal study without association of a particular author with a particular constant.

Therefore, the search for equilibrium constants in this Database is achieved by looking for a desired Ligand with a desired metal. This search can be done by 1) Ligand name or name parts; 2) by formula; 3) by combination of these; and 3) by browsing the database sequentially. A further searching refinement is possible by "locking on" to the desired metal or metal oxidation state in all of the above searches. Most people restrict their searches by Ligand Name parts.

The yellow opening window menu bar has four active commands:
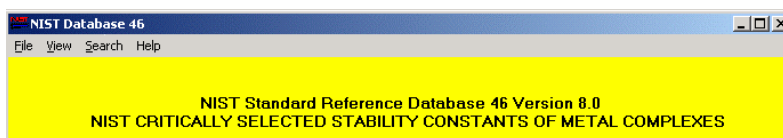
The bottom of this window has seven initially inactive command buttons:

These activate as necessary after a ligand or data are shown.

To locate a ligand, use the Search command on the menu bar followed by Ligand, Formula or Browse. These three open an appropriate dialog box where search parameters are entered. These search actions show one ligand at a time meeting the search criteria.

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The black window shows a serial number, a formula, the type of ligand, its name, and a structural formula. For those ligands that do not meet the critical selection criteria, this window shows only the serial number, name and a box indicating that "Published data do not meet the criteria for critical selection"

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File View Search Help

520   C10H16N2O8   H4L
Ethylenedinitrilotetraacetic acid (EDTA)

HO_2CCH_2 CH_2CO_2H
            $N-CH_2CH_2-N$
HO_2CCH_2 CH_2CO_2H
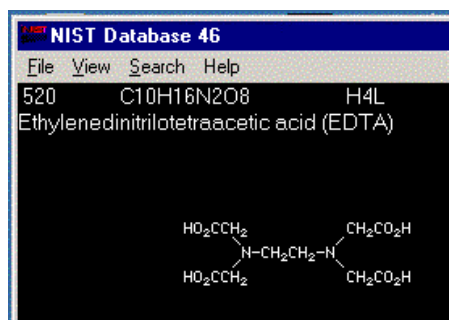
The bottom left most three-command buttons are now active for navigating the Next or Previous ligand. When the desired ligand is displayed, its data may be shown by clicking on the Data command button.

The metal-ligand data and optional bibliographic information for each ligand metal system are shown on one of two standard <u>data displays</u>: a BLUE equilibrium-constant-values display or a RED thermodynamic-constant-values ($\Delta H°$ and $\Delta S°$) display. The standard <u>data display</u> turns GREEN for those ligands and metal ions for which critical constants are not given. However, the metals studied are shown, and their bibliography is accessible.

NIST Database 46

File View Search Help

14496   14615   15116

$C_{10}H_{16}N_2O_8$ H4L   Ethylenedinitrilotetraacetic acid (EDTA)

HO_2CCH_2 CH_2CO_2H
            $N-CH_2CH_2-N$
HO_2CCH_2 CH_2CO_2H

| Mg^{2+} | [MHL]/[ML][H] | log K 4.0^{118} | 25 °C | μ 0.1 |
| Mg^{2+} | [MHL]/[ML][H] | log K 3.85 | 20 °C | μ 0.1 |

Next   Previous   Data   More   Metal   Bibliography   Footnotes
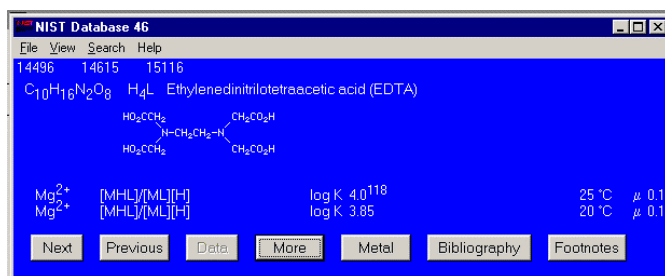
Each BLUE stability constant <u>data display</u> shows the following information:
   a. empirical chemical formula
   b. type of ligand, e.g. H_4L
   c. full chemical name(s) with structural formula
   d. metal ion
   e. equilibrium quotient

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f. logarithm of the equilibrium constant (range of agreement among different papers)
g. temperature
h. ionic strength
i. footnotes (if any)
j. The top line: internal record number, the record number being displayed, and final record number with this ligand. These are useful for reporting problems.

Each RED thermodynamics constant <u>data display</u> has the following information:
a. empirical chemical formula
b. type of ligand, e.g. H_4L
c. full chemical name(s) with structural formula
d. metal ion
e. equilibrium quotient
f. ΔH or ΔS [Joules and calories listed] (range of agreement among different papers)
g. temperature
h. ionic strength
i. footnotes (if any)
The top line: internal record number, the record number being displayed, and final record number with this ligand. These are useful for reporting problems.
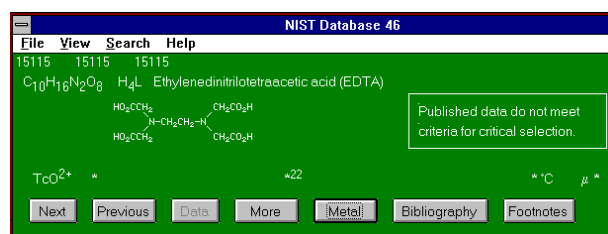
Each GREEN non-critical display has the following information:
a. full chemical name
b. box with text, "Published data do not meet the criteria for critical selection"
c metal ion
d. footnote, "The non-critical data may be found in the reference."
e. temperature headers and ionic strength headers (empty)
f. The top line: internal record number, the record number being displayed, and final record number with this ligand. These are useful for reporting problems.

Whenever there is more than one page of data with a given ligand, the next page can be accessed by clicking on the More command button.

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The Print Data command is available under File command of the menu bar. It offers to print all of the data with this ligand. To print only data with a particular metal, use the Metal command button to choose that metal first.

The Metal command button is available whenever data is displayed. It opens a dialog box to limit data display to only that metal.

The Bibliography command button displays complete bibliography for the currently displayed metal-ligand combination.

The Print Bibliography command is available under File command of the menu bar.

The Footnotes command button displays any footnotes that may be present in the data.

It is possible to find ligands which contain data with a certain metal or oxidation state. Click on the Metal command in the Search found on the menu bar. A dialog will open to first specify the metal element, which leads to a dialog to choose the particular oxidation state. Subsequent ligand searches then retrieve only ligands that contain this metal among its data listing.

> The database bibliography can be searched directly from the Author command found on the menu bar under Search. It is an added feature and is unrelated to the search for data. The dialog box provides for searching the literature citations by Author with a combination of any other part of anticipated references such as publication year, journal abbreviation and page numbers.

> For each hit, the yellow display has a complete reference followed by each ligand studied and a list of metals studied with each ligand.

INSTALLATION

Place the CD-ROM in the CD drive. In Windows 98, 2000, NT, Me or XP

Start the installation by either double-clicking on the install file SETUP.EXE on the CD via the Windows Explorer or My Computer, or by clicking on the Start button, selecting Run and entering the appropriate location for the installation file e.g. D:\SETUP.EXE (if the CD-ROM drive is assigned the letter D:).

Follow the remainder of the Installation instructions.

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If you have downloaded the version with source code from web, it will be installed by default. Otherwise the code will not be installed, but can be copied off of the accompanying CD-ROM.

To start the program, go to the start button, Programs, NIST, and click on critical.

A NIST Metal Complexes Database Program Group will be created at the end of the installation.

After installation, the following 34 files should be present for the program to function properly. In addition, there should be 7 files with DLL extension and 6 OCX files and a User Guide.DOC. The program does not create or use any other files:

BIB.DAT	CODE4.DAT	LMBIB.DAT
BINV3.DAT	CODE5.DAT	MASTER.STR
BPOINTER.DAT	CODE6.DAT	OVERFLOW.WDS
CODE1.DAT	CRITICAL.EXE	POINTER.DAT
CODE2.DAT	INV3.DAT	REFNUMB.DAT
CODE3.DAT	LIGNUMB.DAT	VALUES.DAT
USER GUIDE.DOC		

USE OF THE DATABASE

A. STARTING AND STOPPING

To run the database from Windows environment double click on the program icon.
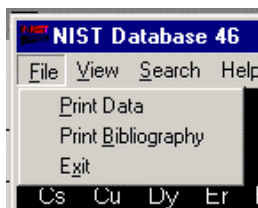
You may exit the program any time by clicking Exit (File menu).

B. HELP MENUS
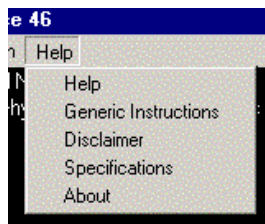
The Help menu has 5 submenus:
Help:
   details of all commands with examples
General Instructions:
   highly abbreviated highlights to help searching
Disclaimer:
   legal statement
Specifications:
   database contents
About:
   Authors and e-mail contacts

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C. LIGAND SEARCHING BY NAME
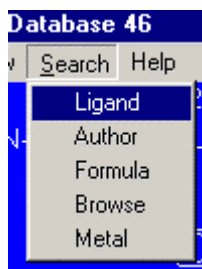
Note: All ligand names in the database start with a capitalized first letter and continue with lower-case letters.

The Ligand search command (Search menu) provides a dialog box asking for "LIGAND SEARCH WORDS?"

One can search either for a specific ligand name or for all ligands or indexes that contain a specific string of characters. <u>The search keys typed here are intrinsically upper-case and lower-case sensitive.</u> All ligand names in the database start with a capitalized first letter and continue with lower-case letters. Thus "Glycine" and "glycine" will find different sets of ligands. To do a case-insensitive search uses all capital letters only. Thus "GLYCINE" will pick up all Glycines and glycines.

Keeping the above in mind, here are the rules:
1. A single search word must have at least 3 consecutive alphabetical letters.
2. Two or more search words are separated by a space.
3. Commas cannot be used as word separators. Use only spaces.
4. When more than one search word is used, rule 1 applies only to one of the words. Other search words can be brackets, Greek letters spelled out, primes, semicolons, numbers, braces...
5. Any name fragment can be used. To find "Cyclohexylamine", one may type, in the LIGAND SEARCH WORDS dialog box:
   a. Cyclohexylamine
   b. CYCLOHEXYLAMINE
   c. yclo amin
   d. CYCLO AMINE
   e. amine yclo hexyl
   f. AMINE C6 N1

Response a. will find <u>Cyclohexylamine</u> unequivocally.

Response b. will find <u>Cyclohexylamine</u> first, but further paging will show additional hits such as Di<u>cyclohexylamine</u> and N,N-Dimethyl<u>cyclohexylamine</u>. This case-insensitive string search was initiated by using all capital letters.

Response c. finds about 61 matching names (such as trans-1,2-C<u>yclo</u>hexylenediiminodipropanedioic acid and 1,5-diazac<u>yclo</u>octane-N,N'-diacetic acid) before stepping to C<u>yclo</u>hexyl<u>amin</u>e. All compounds are cyclic amines and were found because their names contain the word fragment "yclo" and their indexes contain the fragment "amin".

Response d. finds hits C<u>yclo</u>propyl<u>amine</u>, C<u>yclo</u>pentyl<u>amine</u>, C<u>yclo</u>hexyl<u>amine</u> (the desired ligand), C<u>yclo</u>hexylmethyl<u>amine</u>,Tri<u>cyclo</u>[3.1.1.1(3,7)]decan-1-<u>amine</u>,... Each ligand found has an upper or lower case "cyclo" and "amine" in its name. This case-insensitive string search was initiated by using all capital letters.

Response e. illustrates that the order in which the word fragments are entered is immaterial. For this combination Cyclohexylamine is found immediately. There are other matches.

Response f. is an example whereby a case-insensitive (all caps) amine containing six carbon atoms and one nitrogen is sought. There are 16 hits, but Cyclohexylamine comes up second. If the "1" were left off, a redundant all-nitrogen-containing ligand search would be made, and many more unwanted hits would result.

The initial setting for this Ligand search words dialog box is set for (EDTA) as the initial default search word. Many common acronyms in the database are surrounded by ( ). Try (NTA) vs. NTA.
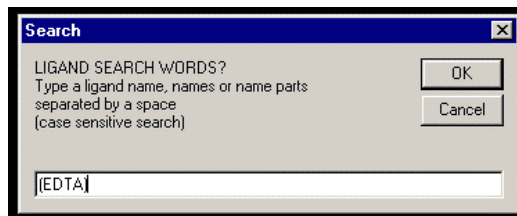
D. LIGAND SEARCHING BY FORMULA

The Formula command (Search menu) brings up a formula dialog box which allows direct ligand search by empirical formula. This dialog box looks very similar to the previous by-name dialog box. "Formula" is one or more terms separated by spaces. Each formula term is case sensitive and

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often consists of an element symbol followed by a fused multiplier. However formula terms may be anything expected in the sought ligand's name. Examples:

> a. C12 H22 O11
> b. O11 C12 H22
> c. N4
> d. N4 PYRID
> e. 3,3,4
> f. H3 P1 O4
> g. [14]
> h. [14] O3

Response a,b. These examples illustrate the most common usage of the FORMULA command and will locate Sucrose and several other disaccharides regardless of ordering if space delimited.

Response c. Will locate any 4 nitrogen ligand.

Response d. Will locate a 4 nitrogen pyridine derivative. It may also find a compound such as [14]aneN4 with a higher than 4 N count.

Response e. Will locate 3,3,4-Tet (thermospermine or 1,5,9,14-tetraazatetradecane.)

Response f. Will find phosphoric acid, but not as a first hit.

Response g. Will find all 14-membered macrocyclic ring containing ligands.

Response h. Will find all 14-membered macrocyclic ring ligands with 3 oxygens in the ligand. The oxygens are not necessarily in the ring.

E. SEARCHING FOR LIGANDS SEQUENTIALLY

The BROWSE command (Search menu) is useful for sequential paging forward (Next command) and backward (Previous command) through groups of similar ligands. The optional parameter N for the dialog box is the serial number of the ligand on which browsing starts. Without the parameter the browsing starts at the last ligand displayed. The ligands N≤4708 are the main body for which numeric data are available. Ligands>4708 are "Other Ligands" for which the metals studied and bibliography has been compiled, but no data are included. The largest allowed BROWS parameter is 6166. (There is no Ligand #1)

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The Table at the end of this section lists other broad values of the browse N parameter. Examples of this parameter are:

        a. 2
        b. 683
        c. 4810

Response a. Starts BROWSE at the first ligand. (There is no ligand 1. The 1st record is reserved for internal file information.)

Response b. Starts Browse at ligand 683, Diglycine, the first of the peptide ligands for which critical data were compiled.

Response c. Starts browse at ligand 4810, at the beginning of "other ligands" cis-2-Aminocyclohexanecarboxylic acid.

Response d. No parameter was entered therefore the last ligand displayed becomes available as starting point for browsing either forward (Next) or backward (Previous).

Table of Optional Parameters for the Browse Command (Search Menu)

CRITICALLY SELECTED LIGANDS (blue and red data windows)

2	Amino Acids
181	secondary N
286	tertiary N
335	Aza macrocycles with carboxylic acids
425	Iminodiacetic acid and derivatives
463	NTA and derivatives
574	EDTA and derivatives
683	Peptides
875	tripeptides
961	polypeptides
1110	Aniline carboxylic acids
1187	Pyridine carboxylic acids
1228	Aliphatic amines
1565	secondary N
1718	tertiary N
1825	Cyclic amines
1877	Aza-macrocycles
2051	oxa
2172	oxo
2249	thia
2277	Pyrroles (azoles)
2418	Pyridines (azines)

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2655	Quinolines
2687	Bipyridines
2721	Phenanthrolines
2734	Tripyridines
2754	Pyrimidines
2802	Purines
2856	phosphates
2890	Aminophosphorus acids
3042	Carboxylic acids
3219	hydroxy
3280	keto
3321	oxy
3366	thio
3473	diacids
3553	hydroxy
3651	polyacids
3705	Organophosphorus and arsenic acids
3806	Phenols
3871	salicylic acids
3946	Catechols
3995	fuchsons
4031	Naphthols
4131	Ketones (oxo ligands)
4175	cyclic
	Miscellaneous ligands
4231	alcohols and sugars
4285	crown ethers
4313	sulfides
4346	mercaptans
4391	hydrocarbons
4482	sulfonic acids
4498	hydroxamic acids
4577	amides
4635	ureas, hydrazides, amidines
4708	Inorganic ligands

LIGANDS NOT SELECTED (green data windows only)

4810	First Ligand
6166	Last Ligand

F. SEARCHING FOR LIGAND WITH A METAL

There is no direct way to search for a metal ion. This would be impractical, since most metal ions appear too often. Instead, with the Metal command (Search menu) a dialog is established to specify the metal element (case sensitive) and metal oxidation states (case sensitive) of interest. The choice of metal is then locked on so that any

Selected Metal Species:
Fe/2+

Previous   Data

Ligand, Formula, or Browse will show ligand matches containing the specified metal ion. A large information box is shown to remind the user which metal ion is specified from the displayed table. To select a species, type the species exactly. To select all the metal species with a given metal, simply click OK. These queries are case-sensitive, e.g. Fe works, FE or fe does not work.

G. SEARCHING THE LITERATURE

The Author command (Search menu) starts a case-sensitive, binary indexed, chronological search for bibliographic information based on author's names entered into the search dialog box. Enter words, names, numbers, etc. separated by a space. If a match is found, the citation is shown with the ligands and metals studied. Examples:

    a. Smith
    b. smith
    c. SMITH
    d. mit
    e. mann
    f. Mann
    g. Schwarzen 1947 Acker
    h. Martell 198
    i. bach G.

Response a. Will find the first occurrence of Smith with an option to continue searching for more references. It will also locate Smithson.

Response b. Because the first letter is not capitalized, no hits are possible except in the middle of some name.

Response c. No hits possible because all caps. This is not to be confused with the case insensitivity obtained by capitalizing the entire query on the Ligand Search command
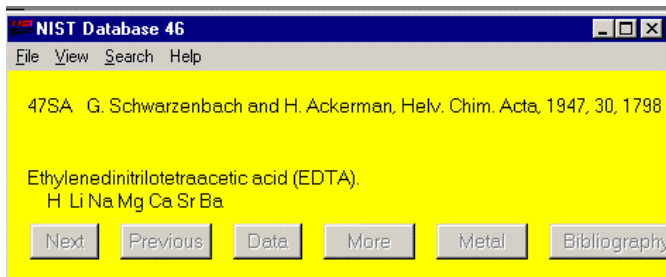
Response d. Smith will be found first, but that is lucky.

Response e. Shumann will be found first, but not Mann.

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Response f. Mannweiler will be found first.

Response g. Typical suggested query, in this case one is looking for a paper by Schwarzenbach and Ackerman published in 1947. Order of words is unimportant. Here's the first reference found:

Response h. A suggestion to find all papers published by A.E. Martell in the 80's.

Response i. A suggestion to find Gerald Schwarzenbach if you are unsure of the spelling.

H. DISPLAY WINDOW SUMMARY

All stability and thermodynamic constant data are shown directly on the data display window. In addition, the bibliographic data can be accessed from these windows. Each window can take on one of three colors: BLUE, RED or GREEN. For a given ligand pressing Data button originally accesses this window.

1. BLUE DATA WINDOW is the usual stability constant display. The values listed are always presented as logarithms of quotients shown. For each ligand the highest protonation constant is listed on the first page. When data are available under several conditions, the values at 0.100 ionic strength are listed first and those at 0 are listed last.

2. RED DATA WINDOW is the thermodynamic constant display. The ΔH values are given in both kcal/mol and kJ/mol together with the defining quotient, and on a subsequent page the calculated ΔS values are given in cal/deg/mole and J/deg/mole.

3. GREEN WINDOW allows quick realization that the ligand or metal ion has no critical data associated with it. However, the metals studied with this ligand are shown. The bibliographic information of the non-critical studies is also in the database. For example, the ligand 4-nitrophenylazocatechol is a ligand for which there are no critical data.
The data fields are marked by a star symbol (*) for the non critical metal/ligand combinations.

Common to all three data display windows are the following commands:
　　Data Handling (Command buttons)
　　　a.　More　　　　　　Lists next page of data records
　　　b.　Metal　　　　　　Jump and lock onto particular ion
　　　　　　　　　　　　　　unlocks ion when nothing is entered
　　　c.　Bibliography　　Bibliography displayed
　　　d.　Footnotes　　　Footnotes displayed (if any)
　　Printing Commands (File menu)
　　　e.　Print Data　　　Print data with displayed ligand
　　　　　　　　　　　　　　Print data with displayed metal (see b. Metal)
　　　f.　Print Bibliography　Print reference of displayed metal
　　Resume search Commands
　　　g.　Next　　　　　　Next Ligand (button)
　　　h.　Previous　　　　Search in opposite direction (button)
　　　i.　Help　　　　　　Help (menu bar)
　　　j.　Exit　　　　　　Quit the program (File menu)

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GETTING STARTED

Install the program on the hard disk according to the directions. Then double click icon to start the program and read the opening window which contain useful and legal information.

On the menu bar, click Help and read the items in reverse order:
    About,
    Specifications
    Disclaimer
    Generic Instructions: Study this abbreviated summary carefully
    Help: Scroll through for future reference of all details.

On the menu bar, click Search then Author:
(This will not find any constants, but allows studying the bibliography)
    Enter some author names or parts of names. One of the parts must be longer than literal characters. Note the case sensitive search.
    Try the above examples on page 15: "G. Searching the Literature."

On the menu bar, click Search then Ligand.
    In the dialog box (EDTA) appears as a default. Click OK. A black window with the EDTA structural formula appears. Clicking the command button Next indicates that no more (EDTA)'s are in the database. Click on the button Data to view a page of log protonation constant for EDTA. Click on the button More to see a red page of heats corresponding to the first protonation constant. Click on the button More again to see a red page of entropies for the first protonation equilibrium. Click on More again to see the page of log second protonation constant.

    Click the button Metal to see the menu of metals studied with EDTA. Type Fe/2, click OK and see ferrous stability constants with EDTA. Click on Metal and this time enter Fe/3 and view the ferric EDTA complexes.

    Try clicking on the Bibliography button. This will display the references to the displayed ligand/metal pair.
    Click on the Footnotes button to see any footnotes.

On the menu bar choose the command Print Data (File menu) and OK the selection. Inspect the printed matter.

On the menu bar choose the command Print Bibliography (File menu) and OK the selection. Inspect the printed matter.
On the menu bar, click on Browse (Search menu).
    This should show a black EDTA window, if that was the last displayed ligand. Click the button Next a few times to see various EDTA analogs

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displayed in succession. Click the button Previous a few times to revisit the scrolled by ligands in backward order. If you want, you may examine any data by clicking the button Data.

On the menu bar click on Ligand (Search menu).
Try each of the following and with the button Next inspect the various hits as they come up:
a. Glycine
b. glycine
c. ane [ ] C20
d. Cyclo amine ene
e. amine N' N'' (two single apostrophes)
f. ulfur
g. osph
h. osph C6
i. S P C N acid

On the menu bar, click on Formula (Search menu).
Try the following formulas and with the button Next inspect the various hits as they come up:
a. C8
b. C8 N4
c. N4 C8
d. Cl2
e. C7 N1

On the menu bar, click on Metal (Search menu).
We will look for any catechol ligand with aluminum constants. From the displayed elements block, type in Al (case sensitive). At the species menu type in Al or simply click OK to select all of the Al species. Now click on Browse (Search menu) and type in a parameter like 3580 (catechols, from table in Help (Help menu)).

Try all the commands to become familiar with the mechanics of data display and metal selection.

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Appendix A

SELECTION CRITERIA

A. OUTLINE OF CRITERIA[1]

When several workers are in close agreement on a particular value, the average of their results has been selected for that value. Values showing considerable scatter have been eliminated. In cases where the agreement is poor and few results are available for comparison, more subtle methods were needed to select the best value. This selection was often guided by a comparison with values obtained for other metal ions with the same ligand and with values obtained for the same metal ion with similar ligands.

While established trends among similar metal ions and among similar ligands were valuable in deciding between widely varying values, such guidelines were used cautiously, so as not to overlook occasionally unexpected real examples of specificity or anomalous behavior.

When there was poor agreement among published values and comparison with other metal ions and ligands did not suggest the best value, the results of more experienced research groups who had supplied reliable values for other ligands were selected. When such assurances were lacking, it was sometimes possible to give preference to values reported by an investigator who had published other demonstrably reliable values obtained by the same experimental method.

Values reported by only one investigator are included in these tables unless there was some reason to doubt their validity. It is recognized that some of these values may be in error, and that such errors will probably not be detected until the work is repeated by other investigators. Some values have been omitted because of serious questions about the composition of their complexes, and the formulation of the equilibrium quotients.

A bibliography for each ligand is included so that the user may determine the completeness of the literature search employed in the determination of critical values. The user may also employ these references to make his or her own evaluation if he or she has any questions or reservations concerning this compilation.

Papers deficient in specifying essential reaction conditions (e.g., temperature, ionic strength, nature of supporting electrolyte) were not employed in this compilation. Also used as a basis for disqualification of published data is lack of information on the purity of the ligand. Frequent deficiencies are lack of calibration of potentiometric apparatus, and failure to define the equilibrium quotients reported in the paper. Papers in which both temperature and ionic strength are not controlled have been omitted from the bibliography.

B. PRESENTATION CONVENTIONS

The values in the database are considered to be the most reliable of the ones available. Values considered to be of questionable validity are enclosed in parentheses. Values having considerable doubt have been omitted.

The range of other values considered reliable is given by + or- quantities in parentheses, describing the difference in the last digit between the other values and the selected value. The range ±0 indicates one or more values which agree exactly with the stated value. Ranges above ±10 are rounded to the nearest ten. Uncertainties of the numbers in the database are indicated by the number of significant figures employed. The larger the numbers of significant figures, the more reliable are the numbers in the database.

All equilibria are expressed as concentration constants. Mixed protonation constants were converted to concentration constants using hydrogen ion activity coefficients. Protonation constants determined at pH values above 12 or below 2 are questioned because of their reduced accuracy. Enthalphy values determined from temperature variation are also questioned. Data set in parentheses represents the questioned values.

Equilibrium constants are given for 25°C unless other temperatures were used and an enthalphy value was not available for conversion to 25°C. Equilibrium data in the database are listed to the nearest 0° or 5° except for 12°, 18°, 22°, 27°, and 37°. Values at 37° and 0.15 ionic strength are included where available. Temperature ranges for enthalphy calculations from temperature variation are rounded to the nearest ten.

Equilibrium data in the database are listed at the most commonly used values of ionic strength: 0.1, 0.5, 0.7, 1.0, 2.0, 3.0, etc. Thus 0.1 represents values from 0.05 to 0.24 and 0.5 include those from 0.25 to 0.60.

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Log K values at ionic strengths greater than zero and less than 0.05 are not used.

C. MINIMUM REQUIREMENTS FOR EQUILIBRIUM DATA[2,3]

1. The equilibrium quotients and each term in the equilibrium quotient should be carefully defined.
2. The purity of ligands, reagents and solvents, and the procedures followed in their purification must be described.
3. The ionic strength, the composition of the solution, and other relevant factors including the range of metal and ligand concentrations investigated must be included.
4. The pH range over which measurements have been made, the titrant used, and the K_w value used must be stated.
5. The pH meter, electrode, and other instruments such as spectrophotometer, etc., used in the experimental studies and an explicit description of the method of calibration must be described.
6. The temperature and temperature range must be stated.
7. The number of data points used per titration (or elsewhere as appropriate), and the number of replicate measurements must be recorded.
8. The computer program, or the method of calculation used to derive the results from experimental values must be included. Previously unpublished programs and calculation procedures should be described in terms of the stepwise logic involved.
9. The final results should include the range together with the standard deviation, the sources of error, and the methods used in establishing parameters.
10. The assumptions made in working up and modeling the data as well as any problems encountered during the determinations or calculations should be clearly set forth.

D. REFERENCES

1. Martell, A. E.; R. M. Smith, Critical Stability Constants, Vols. 1-6, Plenum Press, New York, 1974, 1975, 1977, 1976, 1982, 1989.
2. Tuck, D. G. Pure Appl. Chem. 1989, 61, 1161.
3. Martell, A. E.; Motekaitis, R. J., The Determination and Use of Stability Constants, 2nd Edition, VCH Publishers, Deerfield Beach, FL, 1992.

Appendix B CONTACTS

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NOTE: The author would appreciate an e-mail of errors found.
Indicate the Ligand by number and the nature of the error found.
    Ex.:#694 The name should be Picolyl-L-histidine.

1. Indicate the page by providing the three internal index numbers.
   Ex.: The bibliography on screen 59426 59427 59478 is missing a reference to our work.
   J. L. Messer and B.T. Wasser, J. Kin. Meas. 1987, 20, p 199-201.
2. Indicate AUTHOR screens by providing the bibliographic symbol.
3. Ex.: In Reference 53RQa there is no mention of H. Only metals are given.

If you have questions or comments about the database, Standard Reference Data would like to hear from you. Also, if you have any problems with the diskettes or installation, please let us know by contacting:

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