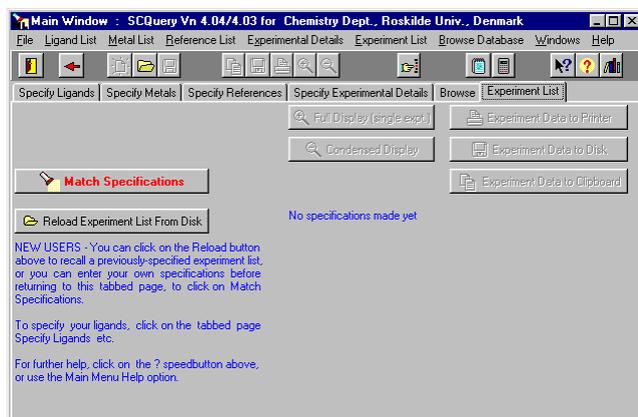
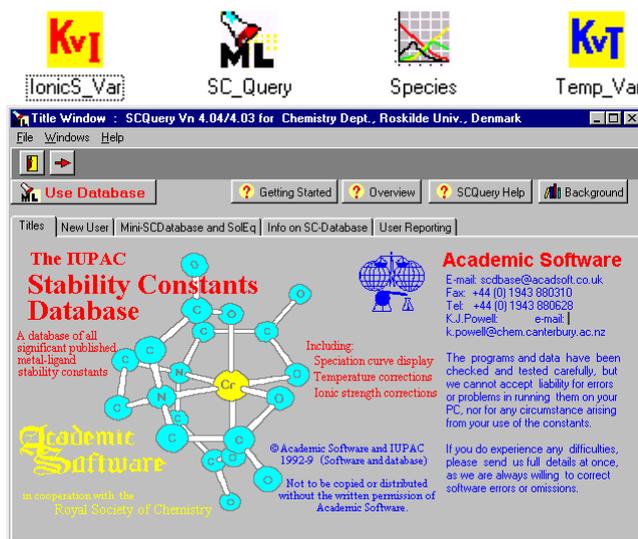


How to use Stability Constants Data base.

SCDbase is basically an almost complete compilation of stability data for coordination compounds (metal complexes) from the literature. This programme has a number of facilities of presenting such data in graphs, which illustrate such equilibria very clearly. Here is a short manual on how to extract data from the database and how to use the display facilities.

Use SCDbase

- On the Windows desktop you will find a folder called SCDbase. Open it by a double click.
- In the folder there are four ikons for four programmes; SC_Query us used for extracting data from the database, Species is used for drawing grafs, and the variation of the stability constants with ionic strength and temperature can be calculated by using IonicS_Var and Temp_Var.
- To extract data click on the ikon for SC_Query. This will result in the window shown to the right. Now click the "Use Database" button.
- The window now open has a number of entrances to be used for different purposes. You may look for data for specified ligands, specified metal ions or data obtained under specified experimental conditions or data in a specified reference. When you have specified what data you look for, you click the "Match Specification" button. The programmes return a list over the experiments in the base, corresponding to your specifications.



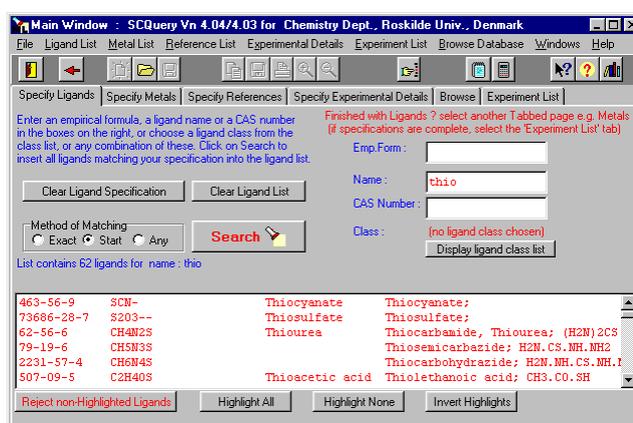
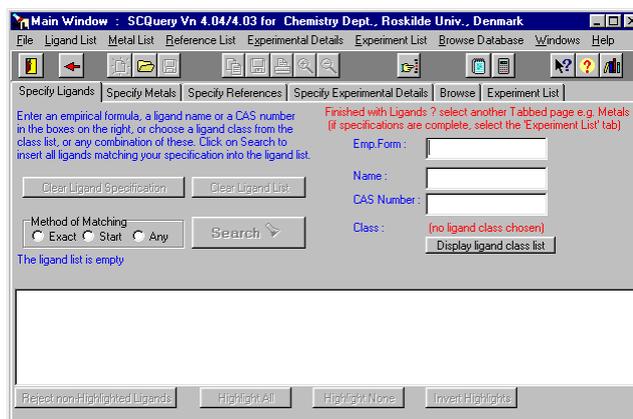
How to specify

In the following a step by step procedure is given to find a specified coordination compound. As an example we look for stability constants for the complex formation between Fe^{3+} and SCN^- . We will get a number of studies, where the stability constants have been determined. In order not to get too many answers the conditions have to be specified as much as possible. As an example we will look for experiments conducted at 25°C . The steps are:

- 1) Choose the ligand (SCN^-), 2) choose the metal ion (Fe^{3+}), 3) specify the experimental conditions (the temperature is 25°C).

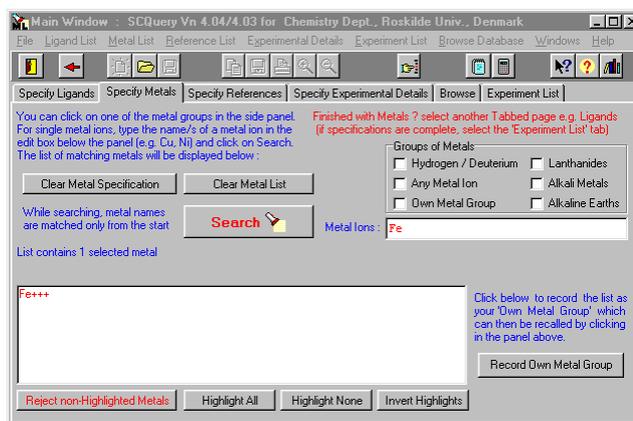
The choice of ligand

- Click on "Specify Ligands".
- Enter the formula, name or CAS number of the ligand in the corresponding square; Emp. Form, Name and CAS Number. It is not necessary to enter one of the ways to represent a ligand. If you use the name you should observe to enter the name of the neutral compound to which the ligand is derived from, e.g. enter glycine (or 2-aminoethanoic acid). for the ligand glycinate. We use here the start of the name (thio).
- The name can be entered exactly or as a part of the name. Chose the appropriate "Method of Matching" Here we use Start. We look for ligander with a name beginning with "thio".
- Now click the "Search" button.
- As a result we get a list of ligands with "thio" as the first letters in their names. To exclude all but SCN⁻, we click on it. Clicking the "Reject non-Highlighted Ligands" button removes all other ligands from the list. In this example only thiocyanate is left.
If you want to look for data describing complex formation of different ligands e.g. with the same metal ion you may have more ligands on the list.



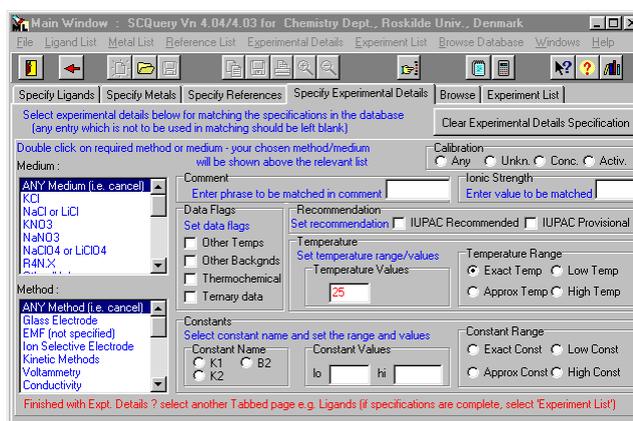
The choice of metal ion

- Click on "Specify Metals".
- Enter the metal ion in the square "Metal ions". You may enter more metal ions if you want to look for stability data for the complex formation between different metal ions with the same ligand. In the square the symbols of the metals should be entered separated with a comma. In the present example we enter Fe.
- Now start the search by clicking the "Search" button.
- As a result we get a list of possible metal ions. In the present example it is Fe(0), Fe(IV), Fe⁺, Fe²⁺ and Fe³⁺. Now, exclude all other forms than those in question (here Fe³⁺) by clicking on the relevant forms in the list and then the "Reject non-Highlighted Ligands" button. You may add more metal ions to the list.



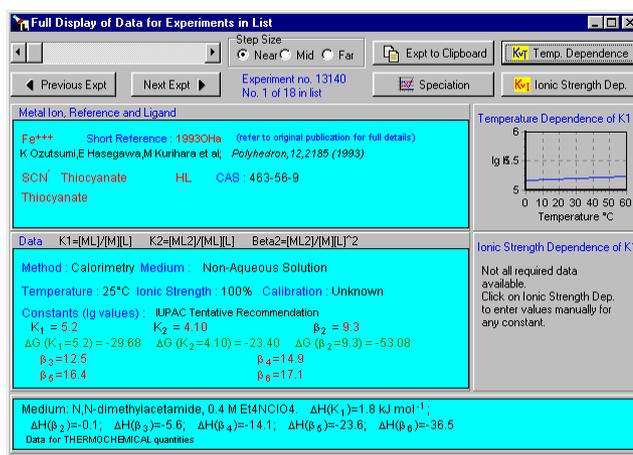
Specifying experimental details

- Click on "Specify Experimental Details".
- You may reduce the number of results by specifying the experimental details. If you are only interested in data for complex formation at a specific temperature or in a specified medium, or determined by a specific method, then the number of matching results will probably be smaller. This implies that you should study and choose among less data. In the present example the temperature is set to 25°C. If you want to specify "Medium" or "Method" you should double click on the relevant detail on the list. These details will then appear in red next to "Medium:" and "Method:".



The search and its result

- Click on "Experiment List".
- Now, search by clicking the "Match Specification" button. You will get two windows on the screen: one lying behind showing all the entries in the database which match the search profile, and a second in front, showing the first result. To the left is shown the window in front giving the first matching data.
- Some important information is given: the values of the stability constants, experimental details, the reference (authors, journal etc.) and the internal number in the database for the particular data (in this case Experiment no. 13140). In some cases graphs are given for the dependence on temperature and/or ionic strength (further details: click on the buttons  and/or ).
- A useful option is to get graphs showing the concentration of the different species as a function of pH or ligand concentration. By clicking the button "Speciation" you start this programme (which can be used independently).



The programme Speciation

- The programme opens the window shown to the right.
- By choosing "Reactants" you may enter values for the concentration of the metal ion and ligand. These numbers are used for the calculation of the distribution curves for the coordination compounds.
- By choosing "Constants" values of stability constants may be entered or altered. In the present Fe^{3+} - SCN^- example $\log \beta_3$ to $\log \beta_6$ obtained from the search has been entered as seen below to the right.

- With the buttons **pH** and **pX** you may choose between graphs showing the dependence on pH or ligand concentration. In the present case is shown the distribution curves of the thiocyanatoiron(III)-complexes as a function of ligands concentration.
- How to do: Click on **pX**. Now pH has to set, and the ligand concentration range has to be entered. In the example pH is set to 7 and the pX range to between 0 and 12. The programme automatically indicates the scale on the x-axis in tenths of the whole range. Accordingly, the ranges 0-10 or 2-12 gives integers on the x-axis scale.

With the relevant value and range entered press

 **Calculate** and then  **Graphs**. This gives you a graphical representation.

- You may add a text on the graph. Use the  button.
- You may add scale lines on the graph. Use the  buttons.
- You may enlarge the graph by using . If you want to get back to original size, press the  again.
- You may see the effect of a changed $\log \beta$ value. Use the **Change B etc.** button in the bottom left corner,
- Printing the graphs: Set landscape or portrait format in Windows control panel before you print.

