# BIOTHERMODYNAMIC DATA CAPTURE

**Example: Solubilities of biomaterials in solution**

**Data source:** Carta, R. *J. Chem. Thermodyn.*, **1998**, *39*, 1038-1048.

**General Experiment Description:** Solubilities of L-cystine, L-tyrosine, L-leucine, and glycine in sodium chloride solutions at various pH values determined gravimetrically.

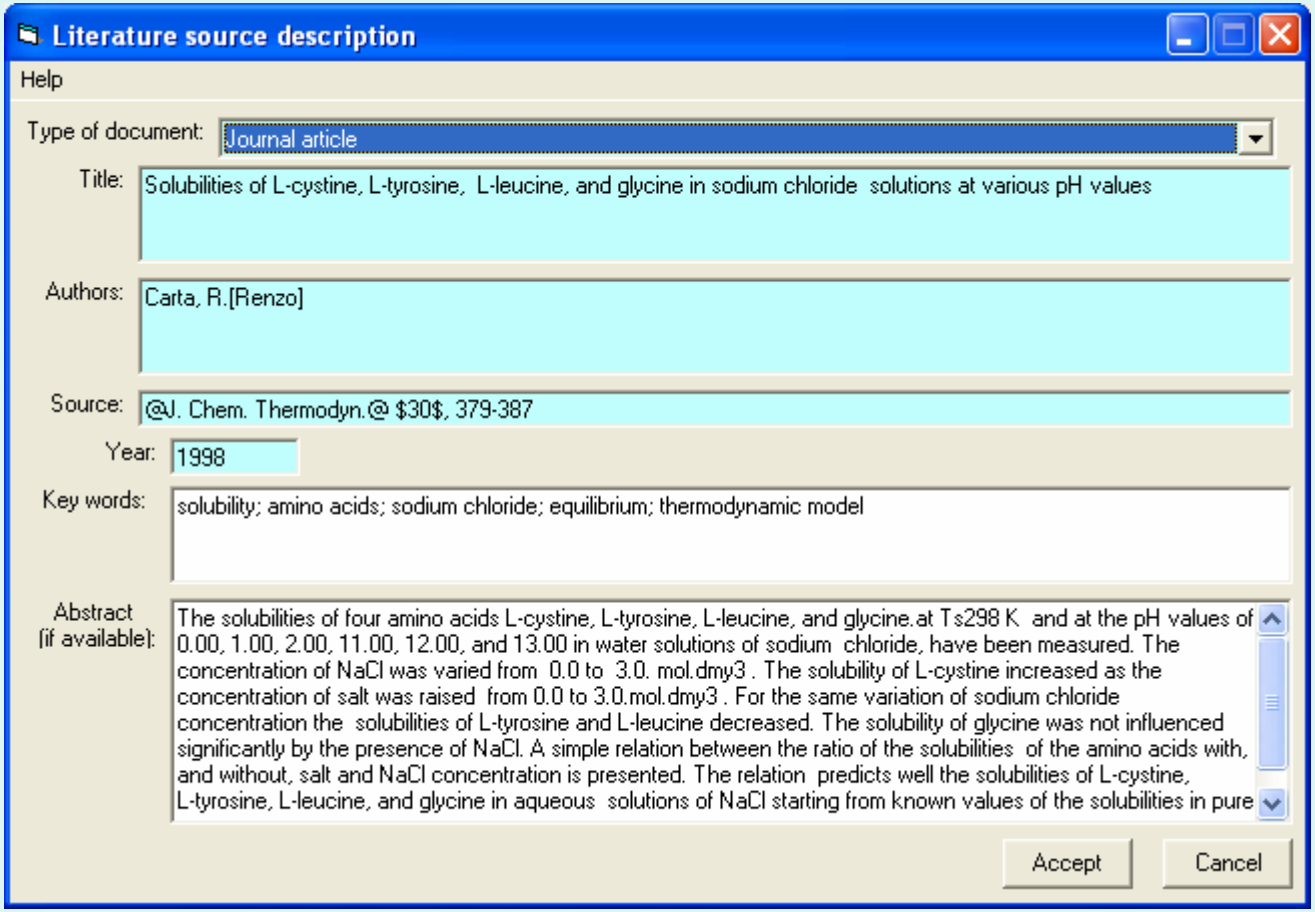
**Target Properties for the example:** Molarities of L-cystine in a complex solution.

# Bibliographic information:

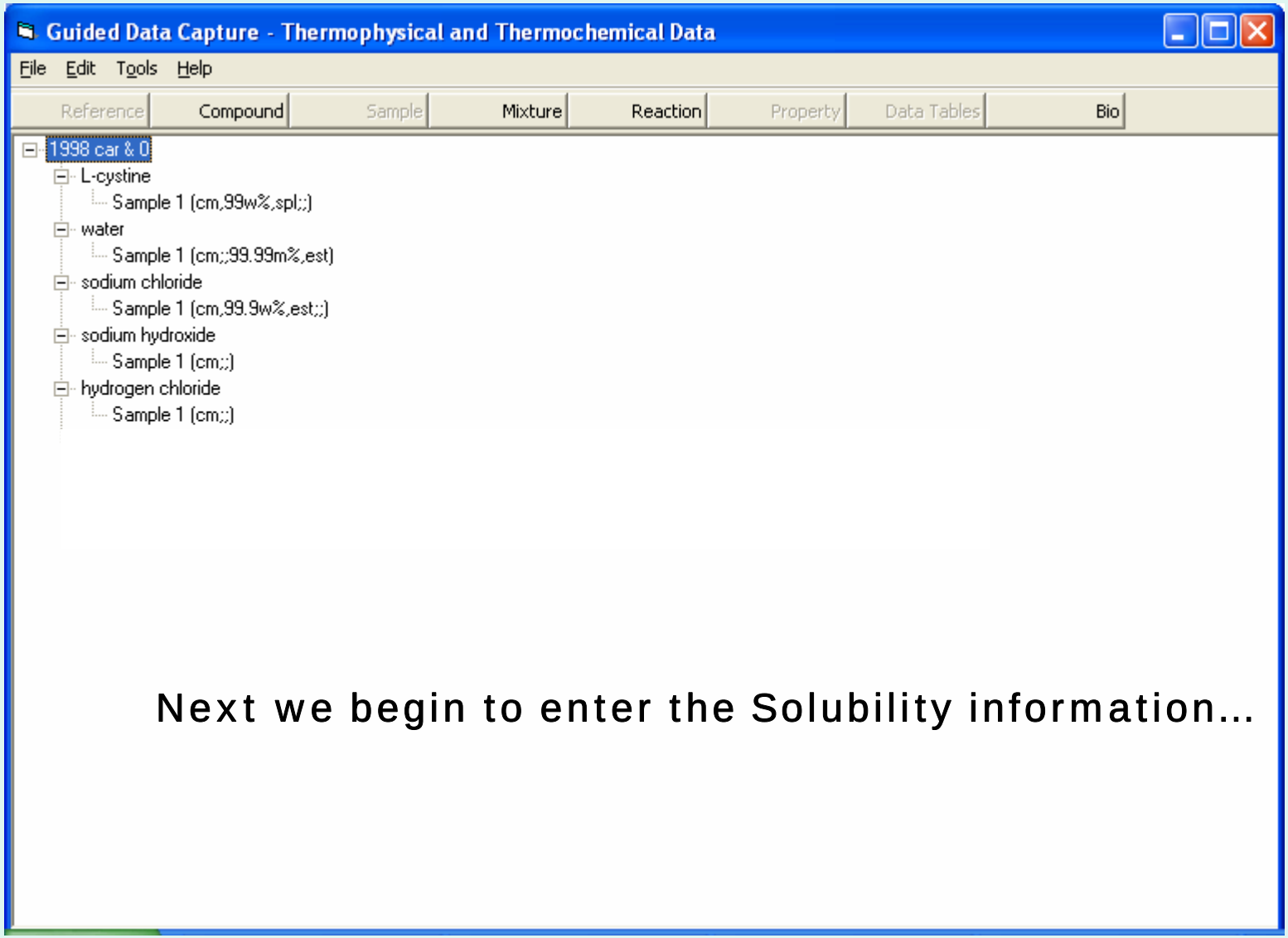
***No new additions were made to GDC for biothermodynamic data.***

**See: http://www.trc.nist.gov/GDC.html for general help.**
**See: http://www.trc.nist.gov/helpdocs/basic/BIBLIOGRAPHICinfo.pdf for specific help on entering bibliographic information.**

**Here is the captured bibliographic information for the example:**

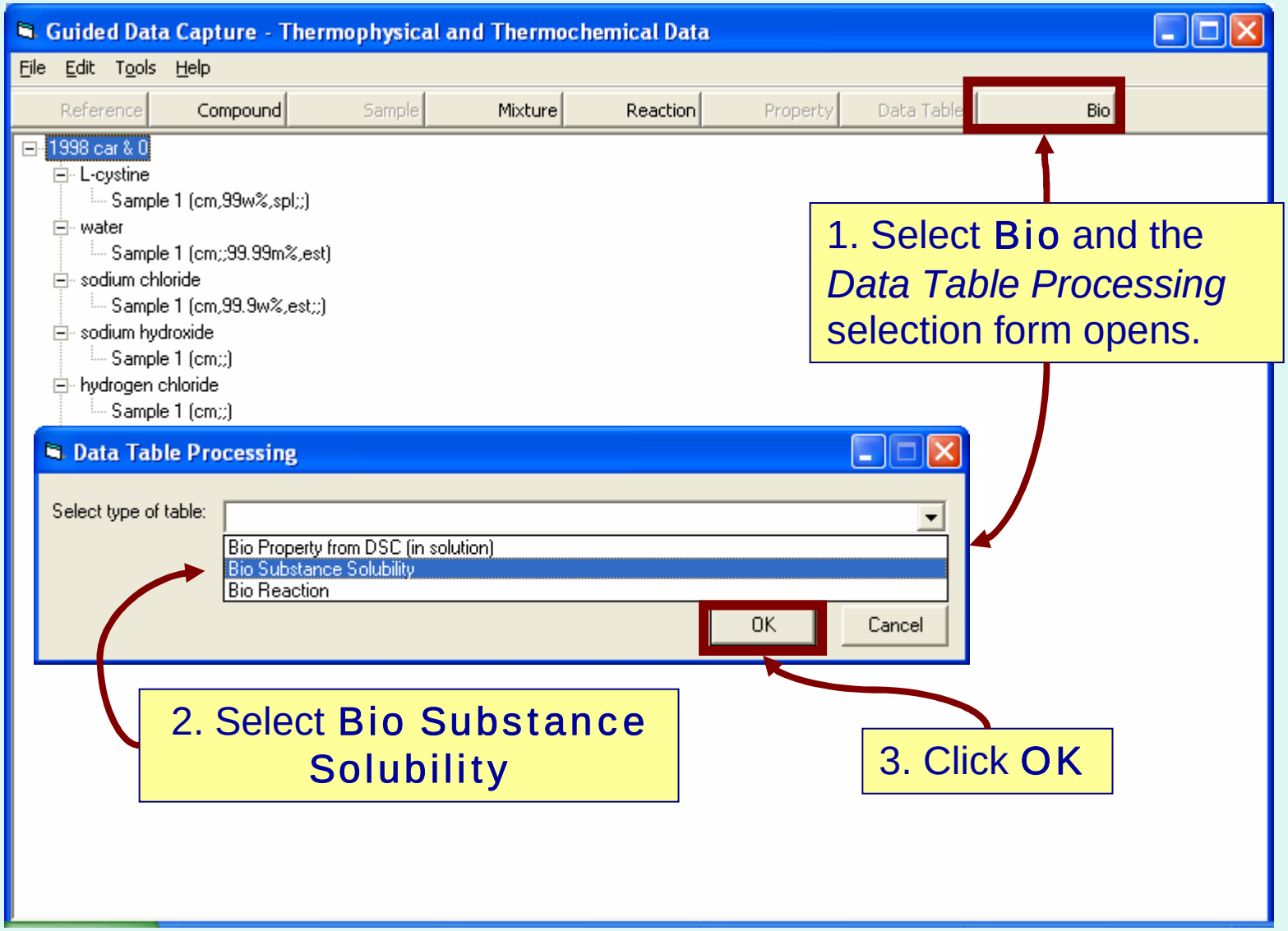


**After capture of bibliographic info and specification of the reaction components, the Main GDC form looks like this…**



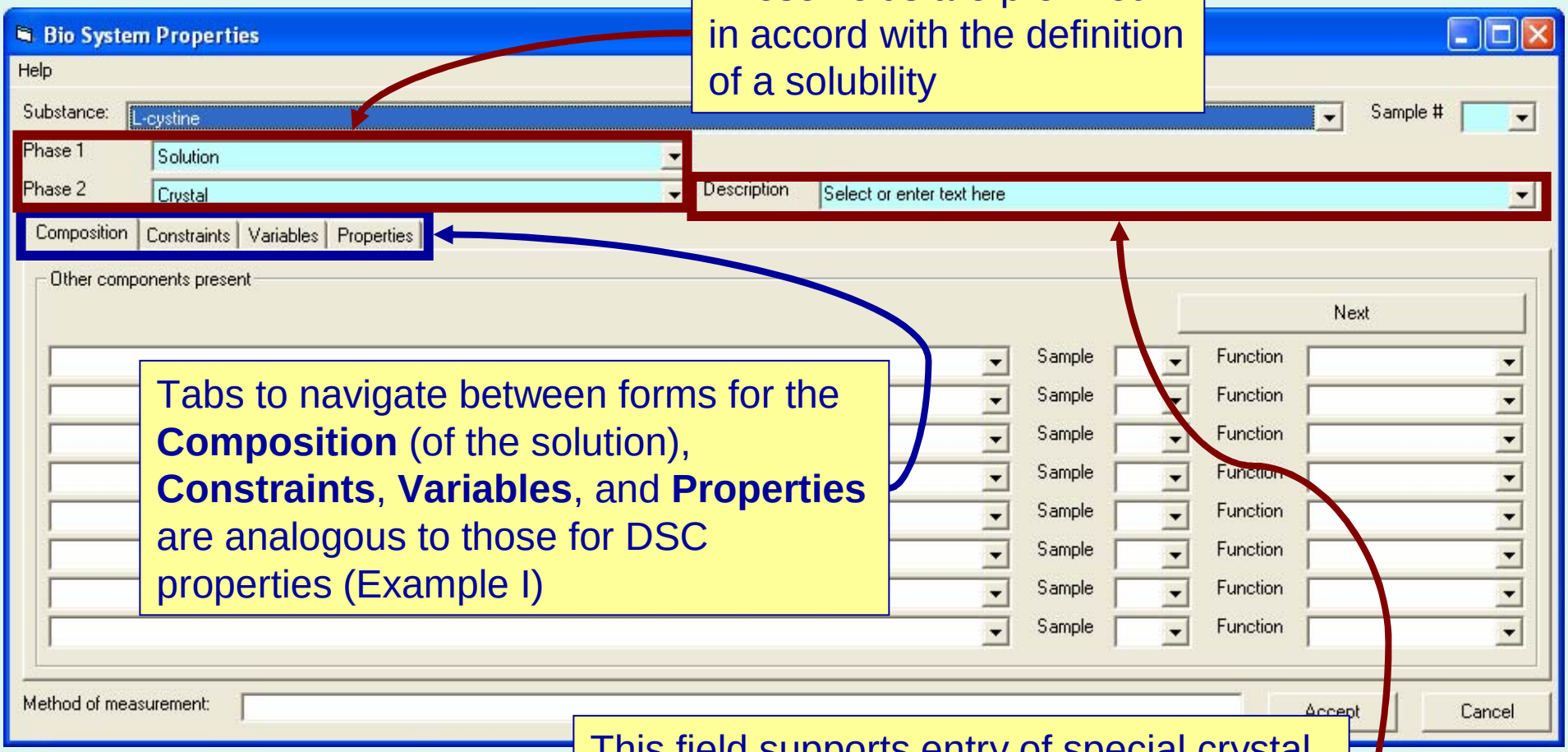

Next we begin to enter the Solubility information...

## Initiation of Bio Substance Solubility property capture…




Next…

## The Bio System Properties form appears for Solubilities…

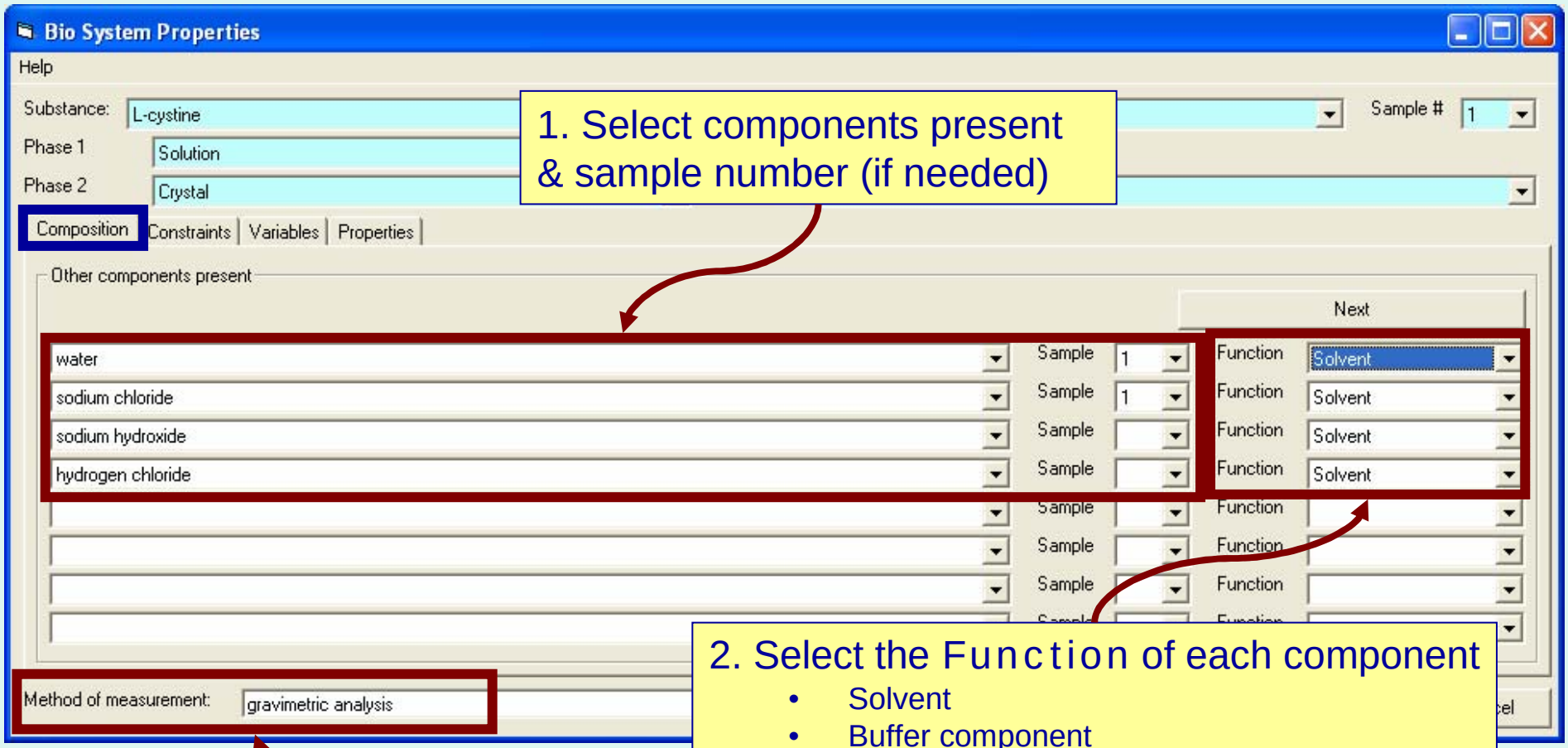



These fields are pre-filled in accord with the definition of a solubility

Tabs to navigate between forms for the **Composition** (of the solution), **Constraints**, **Variables**, and **Properties** are analogous to those for DSC properties (Example I)

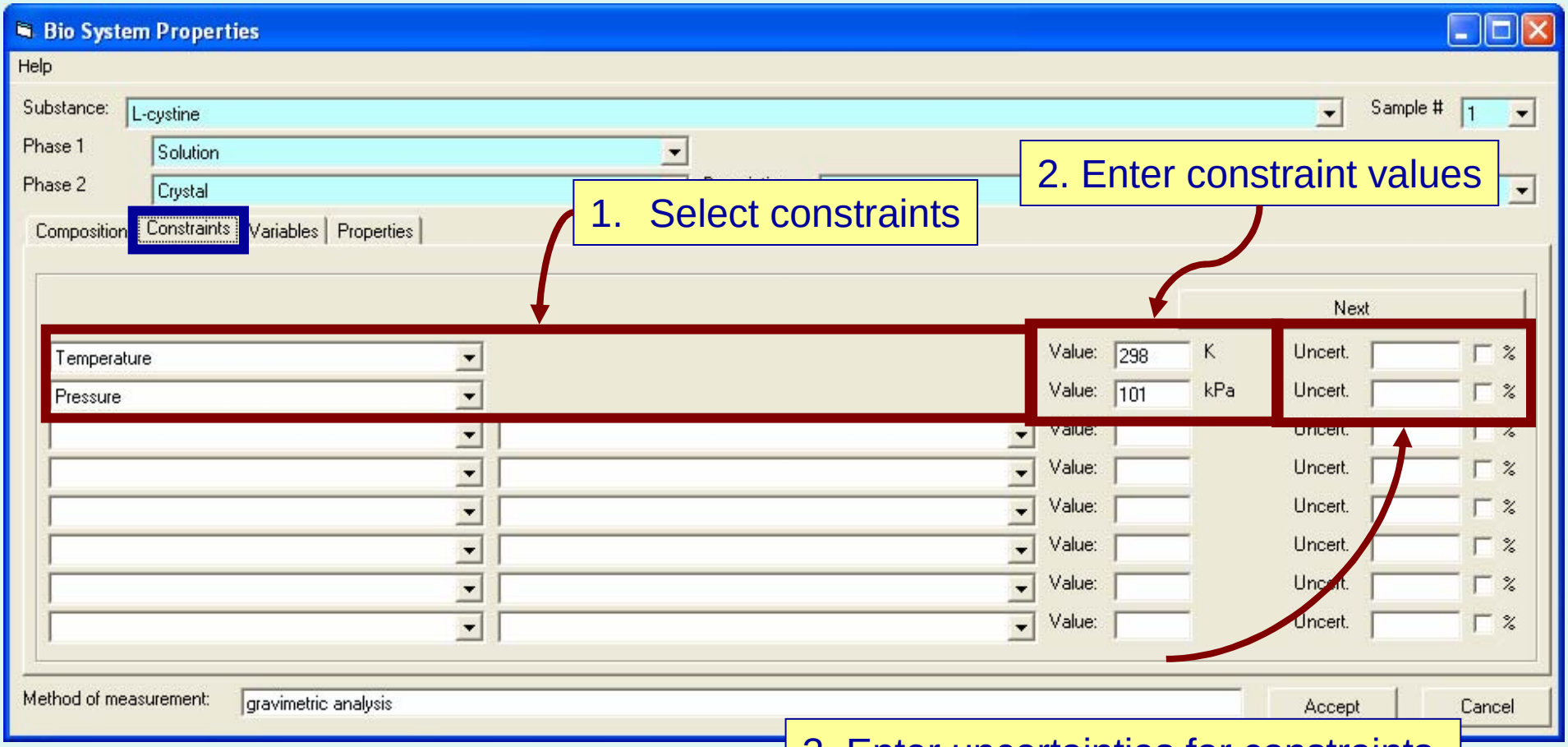
This field supports entry of special crystal descriptors, such as *alpha, beta, monoclinic, amorphous*, etc. At present, these are entered as text strings.

# Define the Composition (of the solution):



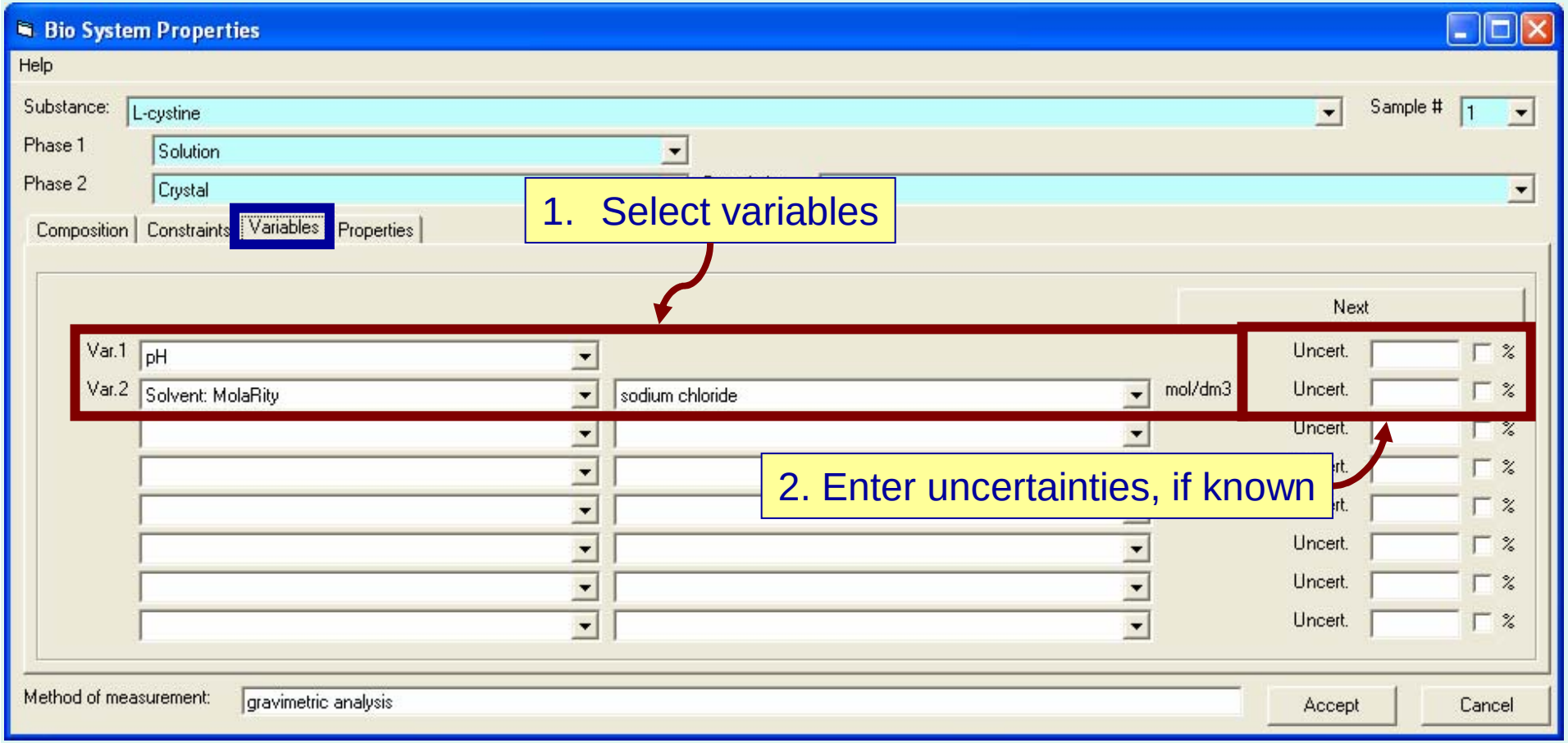

Next...

# Define the Constraints:



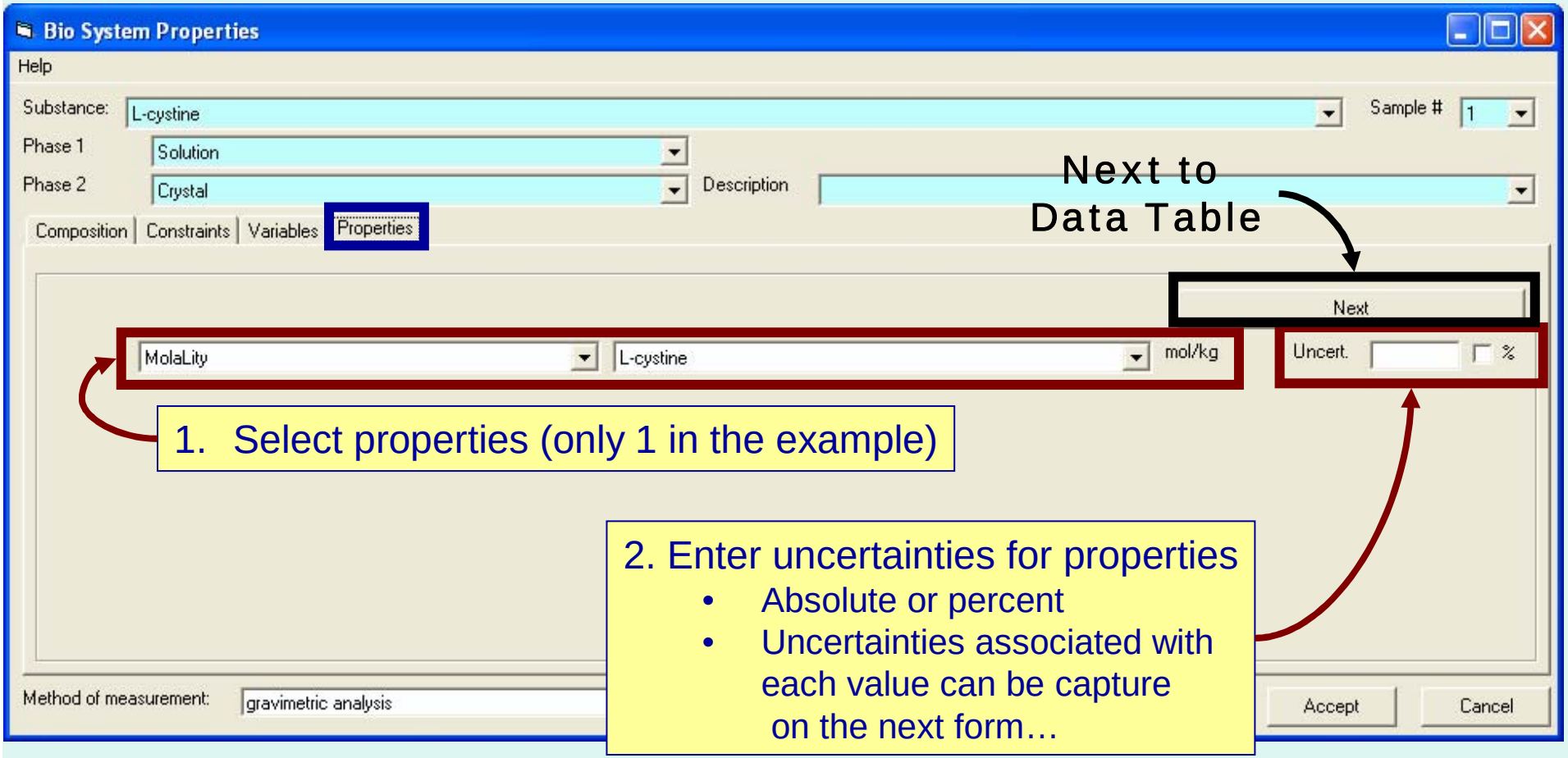

Next tab...

# Define the Variables:



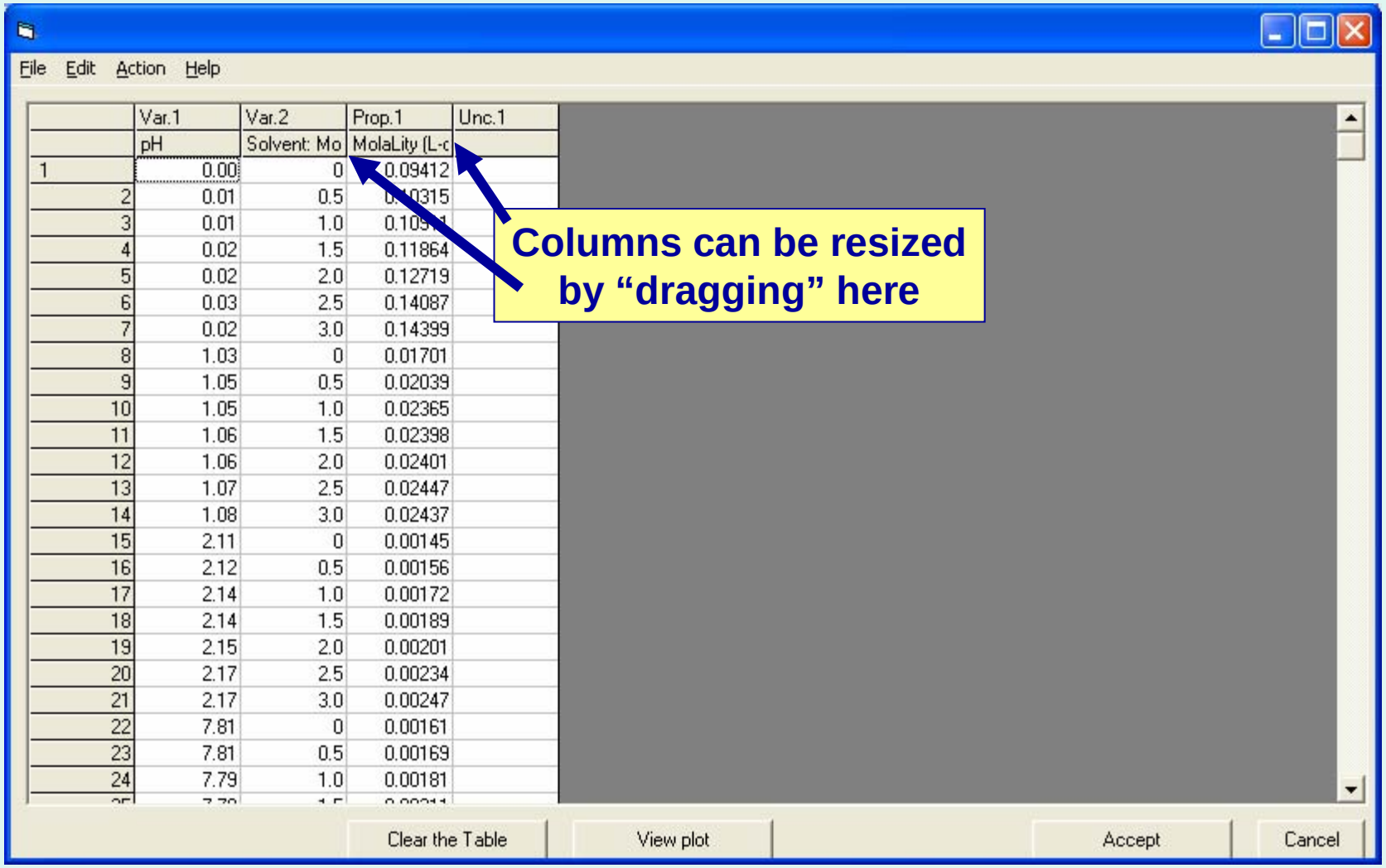

Next tab...

# Define the Properties:

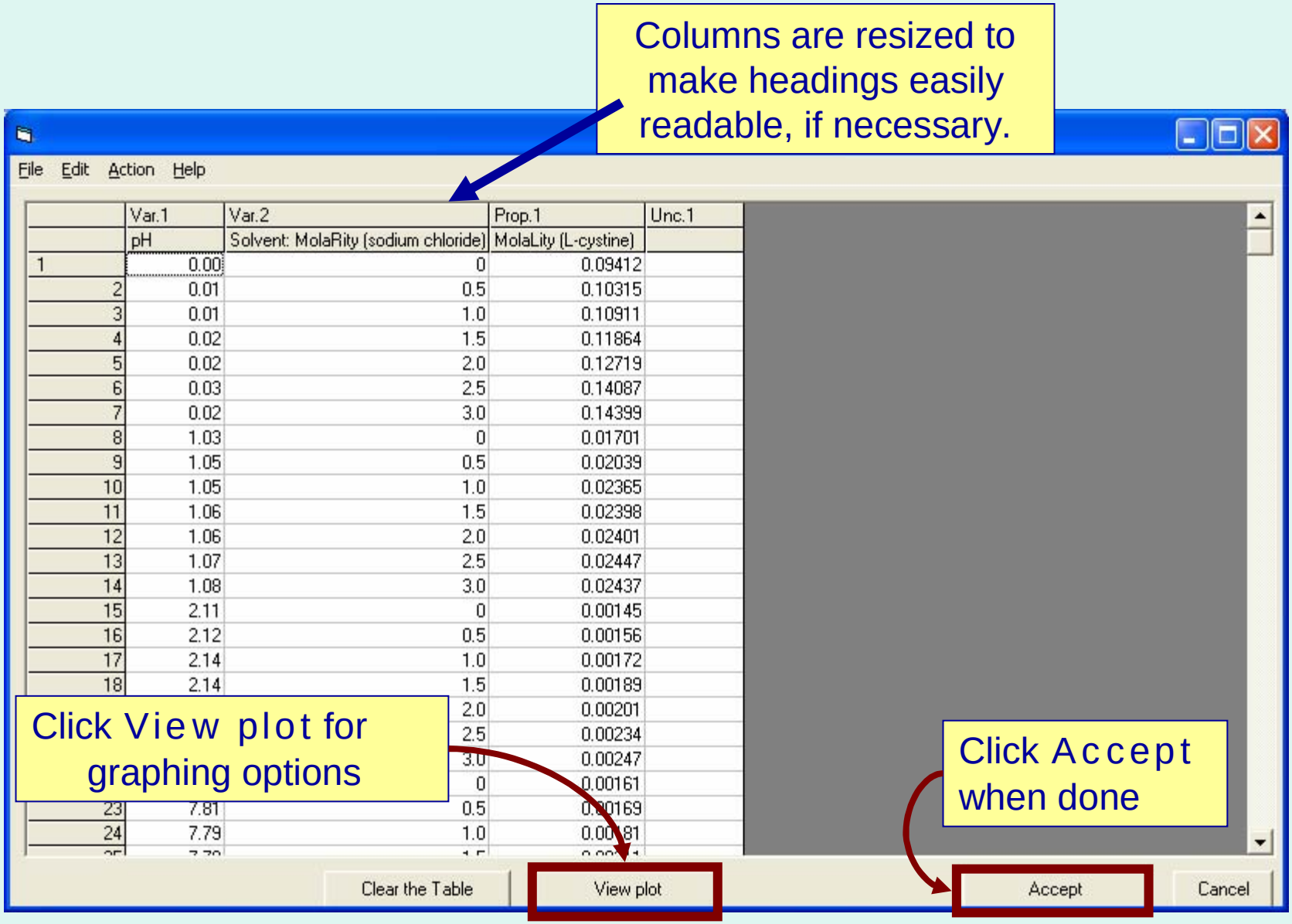


# Enter numerical values for *Variables* and *Properties*:

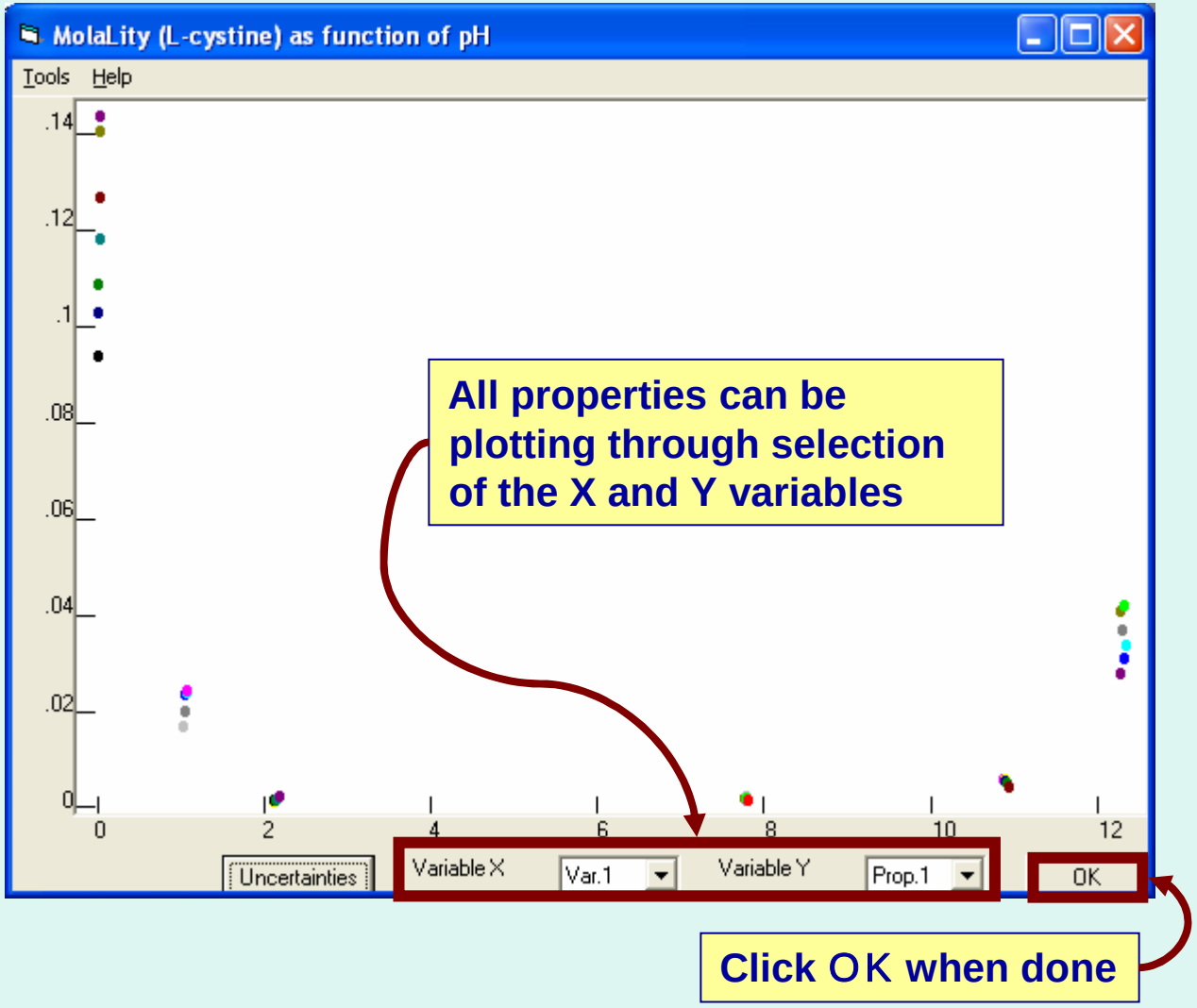
See page 382 of the example article pdf.




See next page...

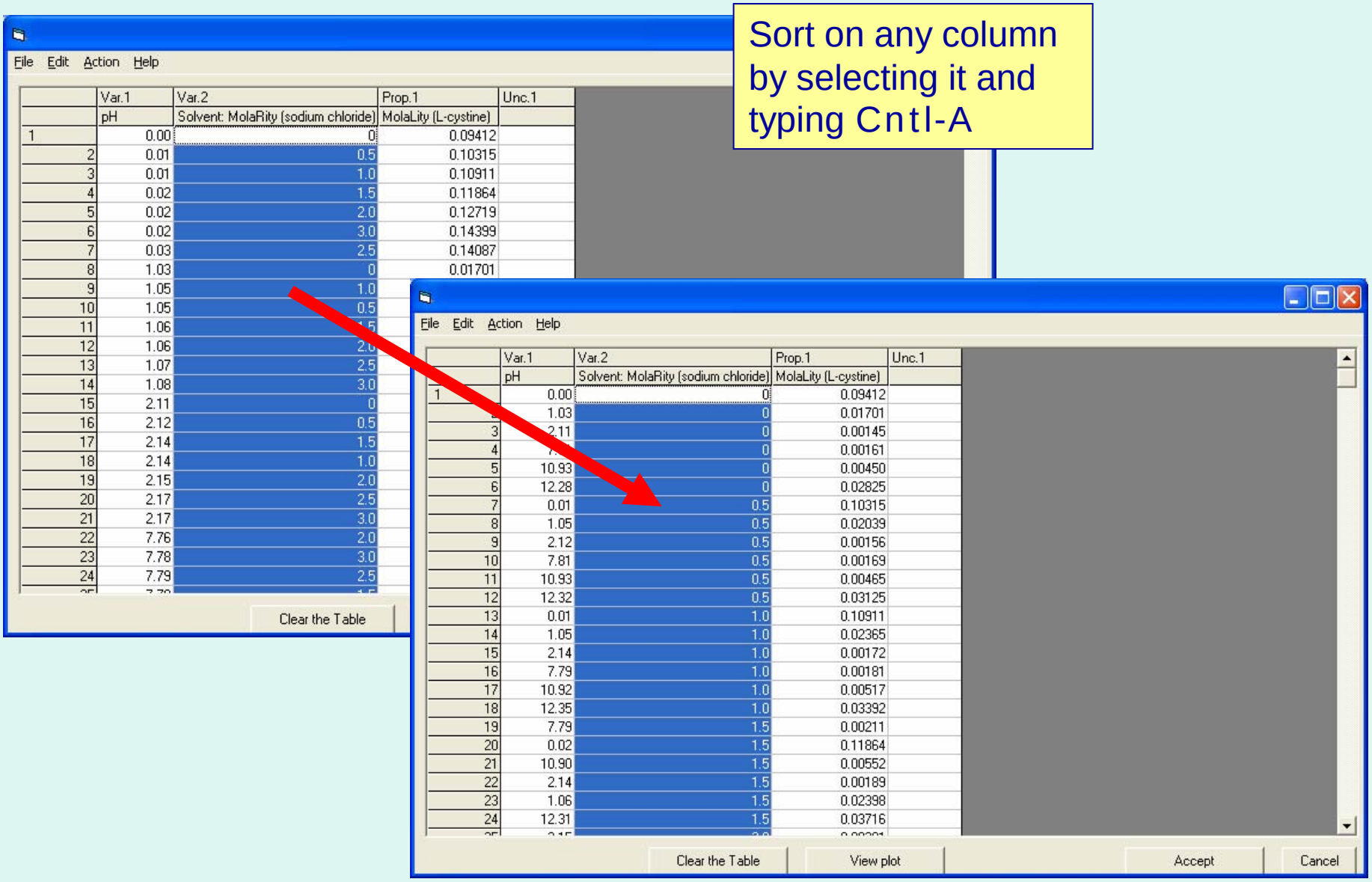

Columns are resized to make headings easily readable, if necessary.
File Edit Action Help
Var.1 pH
Var.2 Solvent: MolaRity (sodium chloride)
Prop.1 MolaLity (L-cystine)
Unc.1
1 0.00 0 0.09412
2 0.01 0.5 0.10315
3 0.01 1.0 0.10911
4 0.02 1.5 0.11864
5 0.02 2.0 0.12719
6 0.03 2.5 0.14087
7 0.02 3.0 0.14399
8 1.03 0 0.01701
9 1.05 0.5 0.02039
10 1.05 1.0 0.02365
11 1.06 1.5 0.02398
12 1.06 2.0 0.02401
13 1.07 2.5 0.02447
14 1.08 3.0 0.02437
15 2.11 0 0.00145
16 2.12 0.5 0.00156
17 2.14 1.0 0.00172
18 2.14 1.5 0.00189
2.0 0.00201
2.5 0.00234
3.0 0.00247
0 0.00161
23 7.81 0.5 0.00169
24 7.79 1.0 0.00181
Click View plot for graphing options
Click Accept when done
Clear the Table
View plot
Accept
Cancel

# Plotting Options: Plot any property against any variable (2-d only)

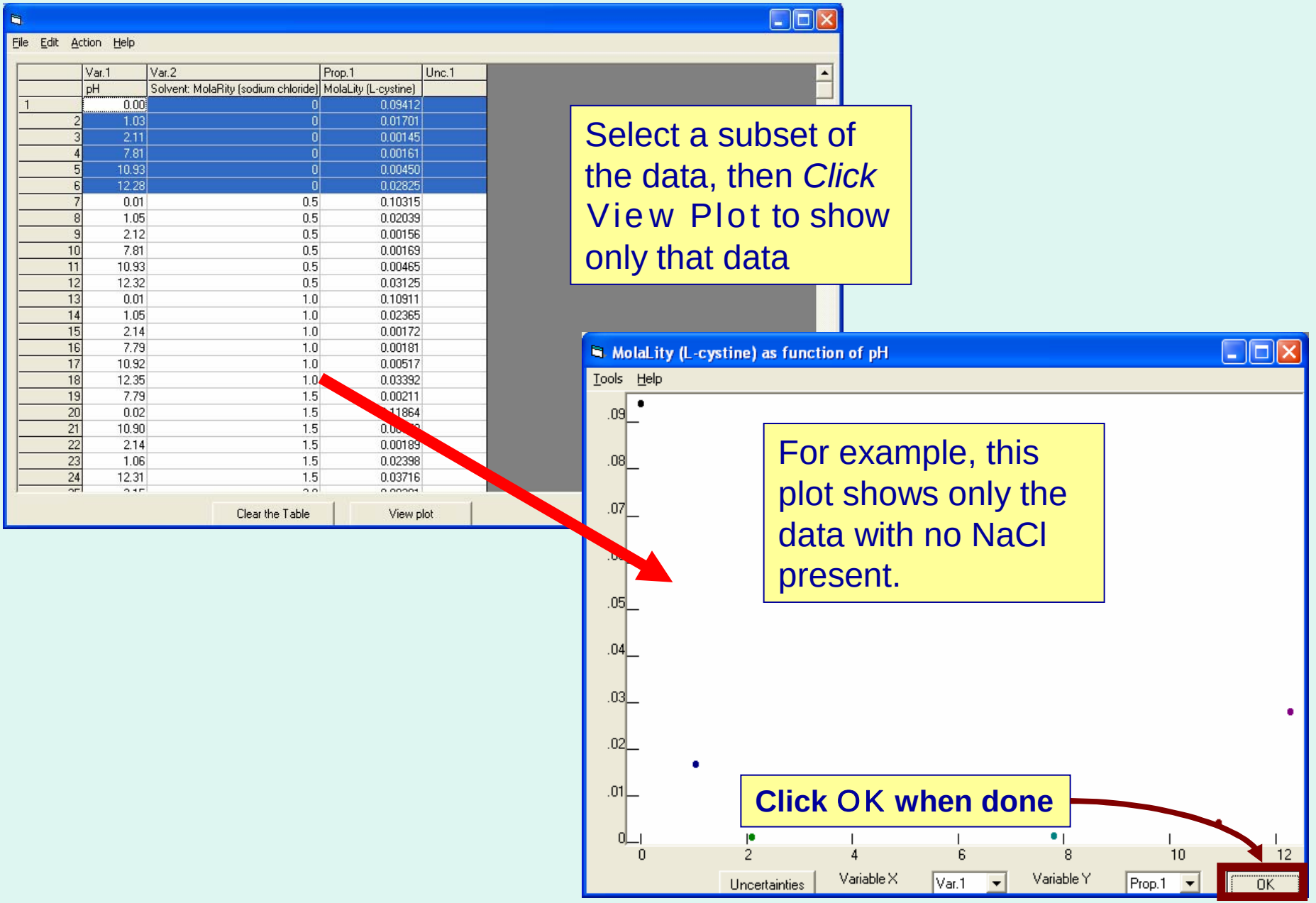


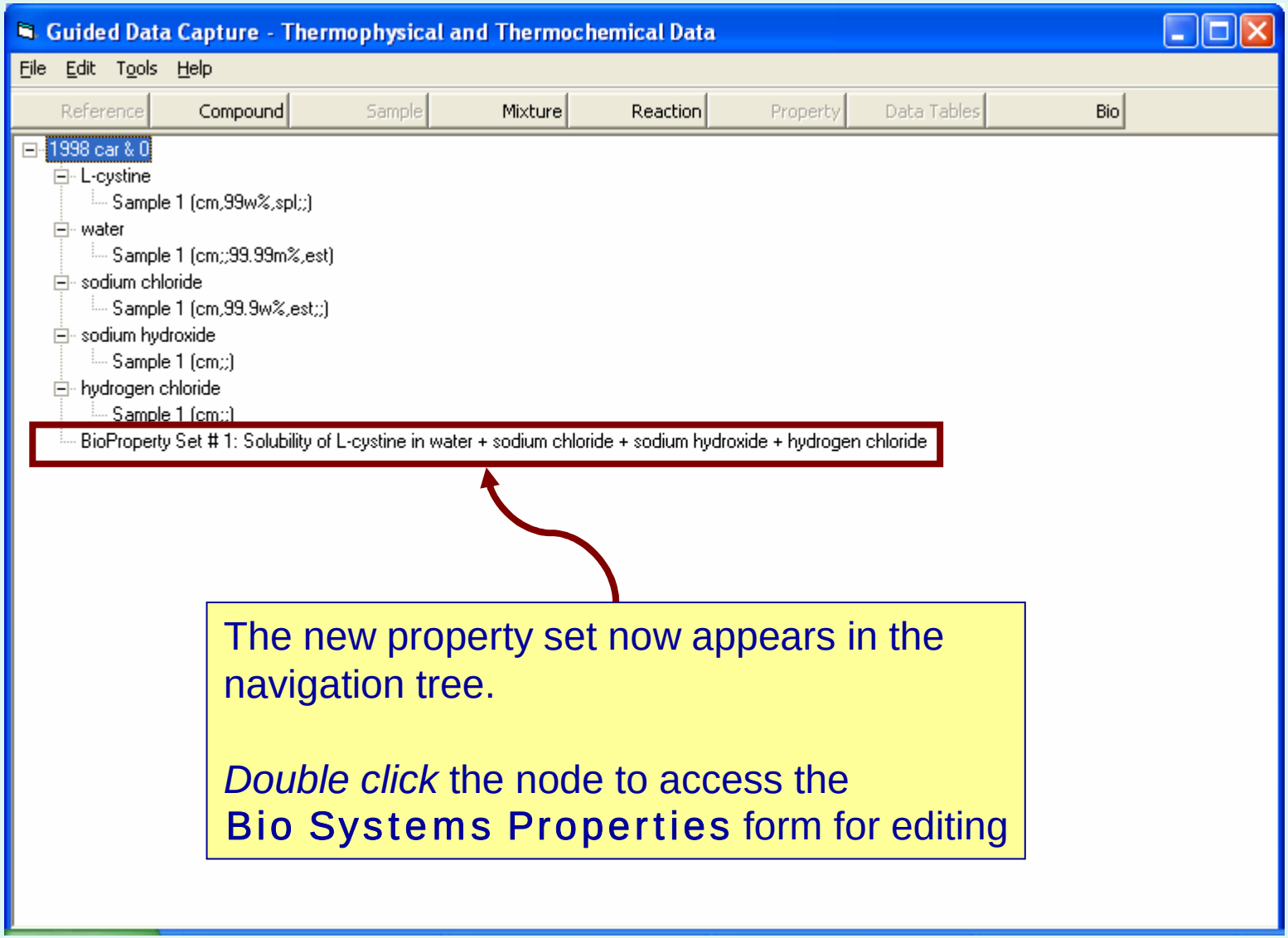
# Some additional useful features of GDC plotting

Sort on any column by selecting it and typing Cntl-A



# Some additional useful features of GDC plotting




Guided Data Capture - Thermophysical and Thermochemical Data
File Edit Tools Help
Reference Compound Sample Mixture Reaction Property Data Tables Bio
1998 car & O
L-cystine
Sample 1 (cm,99w%,spl;;)
water
Sample 1 (cm;;99.99m%,est)
sodium chloride
Sample 1 (cm,99.9w%,est;;)
sodium hydroxide
Sample 1 (cm;;)
hydrogen chloride
Sample 1 (cm;;)
BioProperty Set # 1: Solubility of L-cystine in water + sodium chloride + sodium hydroxide + hydrogen chloride
The new property set now appears in the navigation tree.
*Double click* the node to access the **Bio Systems Properties** form for editing