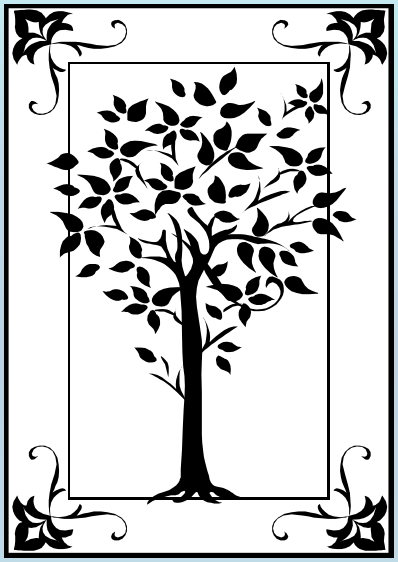
METADATA AND NUMERICAL DATA CAPTURE:
DENSITY for a saturated solution
(2-component solvent + 1 crystal phase)

Guided Data Capture (GDC)



This tutorial describes
METADATA AND NUMERICAL DATA CAPTURE:
for **saturated solution (liquid + crystal)**
DENSITY (kg/m^3)
with the Guided Data Capture (GDC) software.

NOTE:

The tutorials proceed sequentially to ease the descriptions. It is not necessary to enter *all* compounds before entering *all* samples, etc.

Compounds, samples, properties, etc., can be added or modified at any time.

However, the hierarchy must be maintained (i.e., a property cannot be entered, if there is no associated sample or compound.)

The experimental data used in this example is from:

J. Chem. Eng. Data **2001**, *46*, 175−176

Solubility and Density of the Disodium Salt Hemiheptahydrate of Ceftriaxone in Water + Ethanol Mixtures

Ming Zhu

Zhejiang Provincial Institute for Drug Control, Hangzhou, 310004, P. R. China

The solubilities of the disodium salt hemiheptahydrate of ceftriaxone in water + ethanol at (10, 20, and 30) °C are presented by using the gravimetrical method. The densities of the saturated solutions are also determined with a digital densimeter (Anton Paar, model DMA 45) at 30 °C. The solubility of the disodium salt hemiheptahydrate of ceftriaxone increases with temperature but decreases with increasing concentration of ethanol in the solution.

DENSITY of a saturated solution of a *salt* in a 2-component solvent (*water* + *ethanol*): 3 components total

Table 2. Densities ρ (g/cm^3) of the Saturated Solutions of the Disodium Salt Hemihydrate of Ceftriaxone in Water + Ethanol at 30 °C

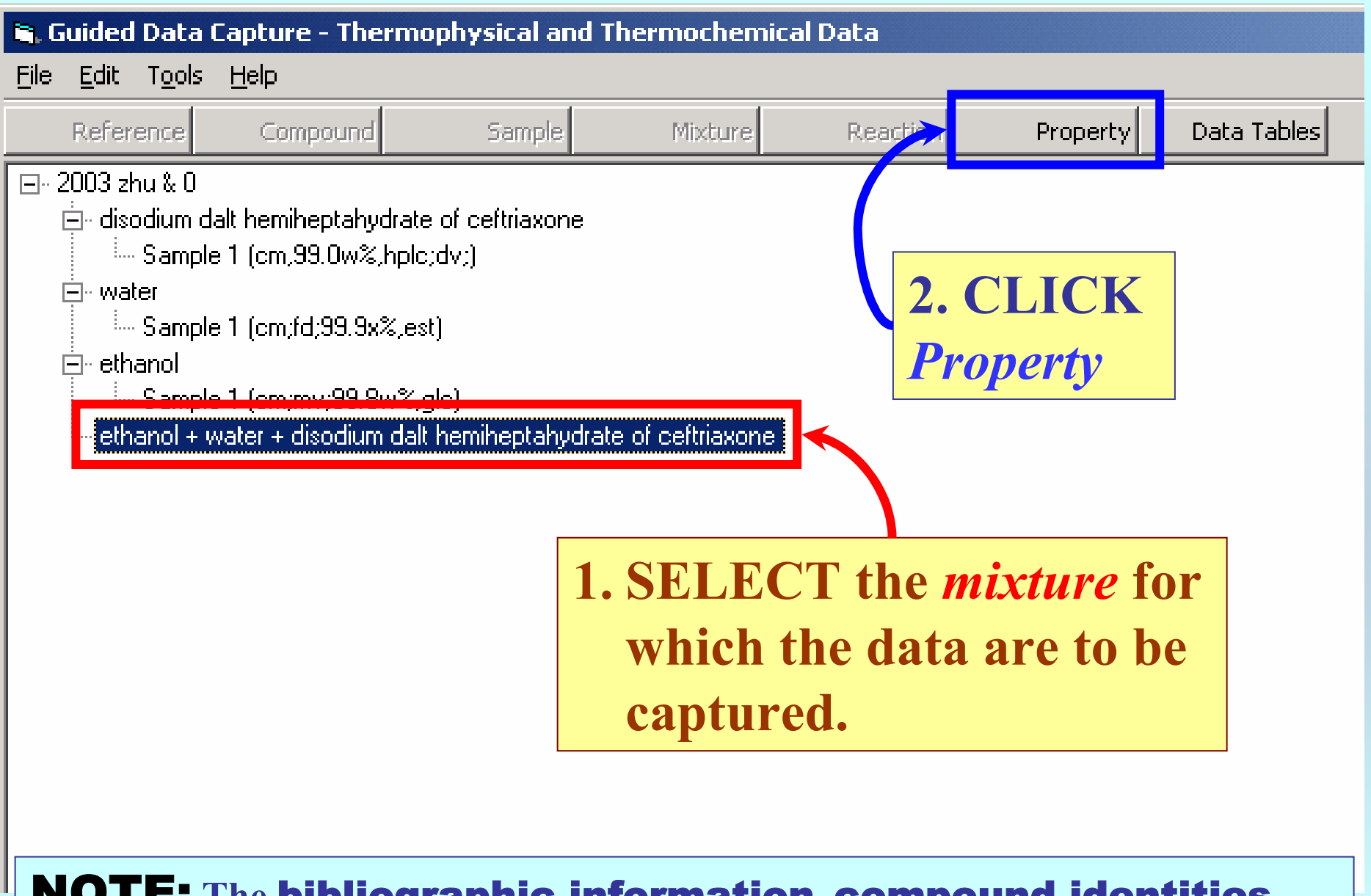
ethanol wt %	ρ/(g/cm^3)			
	pure solvents	10 °C	20 °C	30 °C
28.72	0.9528 ± 0.0003	0.9769 ± 0.0031	0.9995 ± 0.0052	1.0218 ± 0.0044
39.84	0.9324 ± 0.0002	0.9493 ± 0.0038	0.9684 ± 0.0040	0.9864 ± 0.0040
50.35	0.9101 ± 0.0003	0.9222 ± 0.0064	0.9344 ± 0.0049	0.9490 ± 0.0056
59.86	0.8883 ± 0.0003	0.8960 ± 0.0123	0.9039 ± 0.0085	0.9157 ± 0.0051
68.44	0.8683 ± 0.0002	0.8731 ± 0.0106	0.8774 ± 0.0152	0.8854 ± 0.0089
80.20	0.8399 ± 0.0003	0.8408 ± 0.0276	0.8422 ± 0.0300	0.8453 ± 0.0214
84.48	0.8292 ± 0.0002	0.8297 ± 0.0292	0.8306 ± 0.0274	0.8315 ± 0.0225
88.95	0.8177 ± 0.0002	0.8181 ± 0.0315	0.8190 ± 0.0333	0.8197 ± 0.0324

These data are considered here.

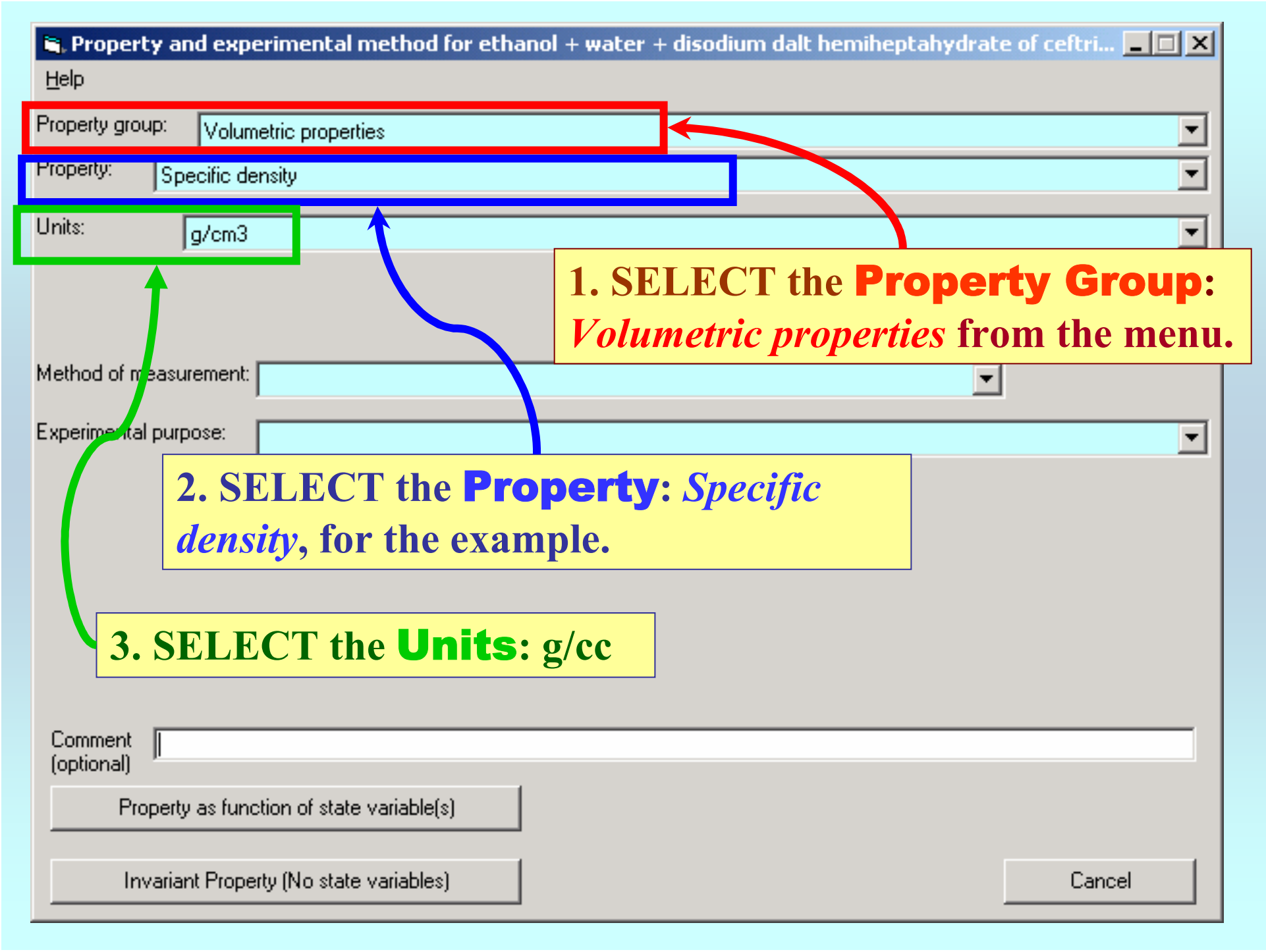
Results are reported for 3 temperatures with pressure constrained to p = 101.3 kPa.

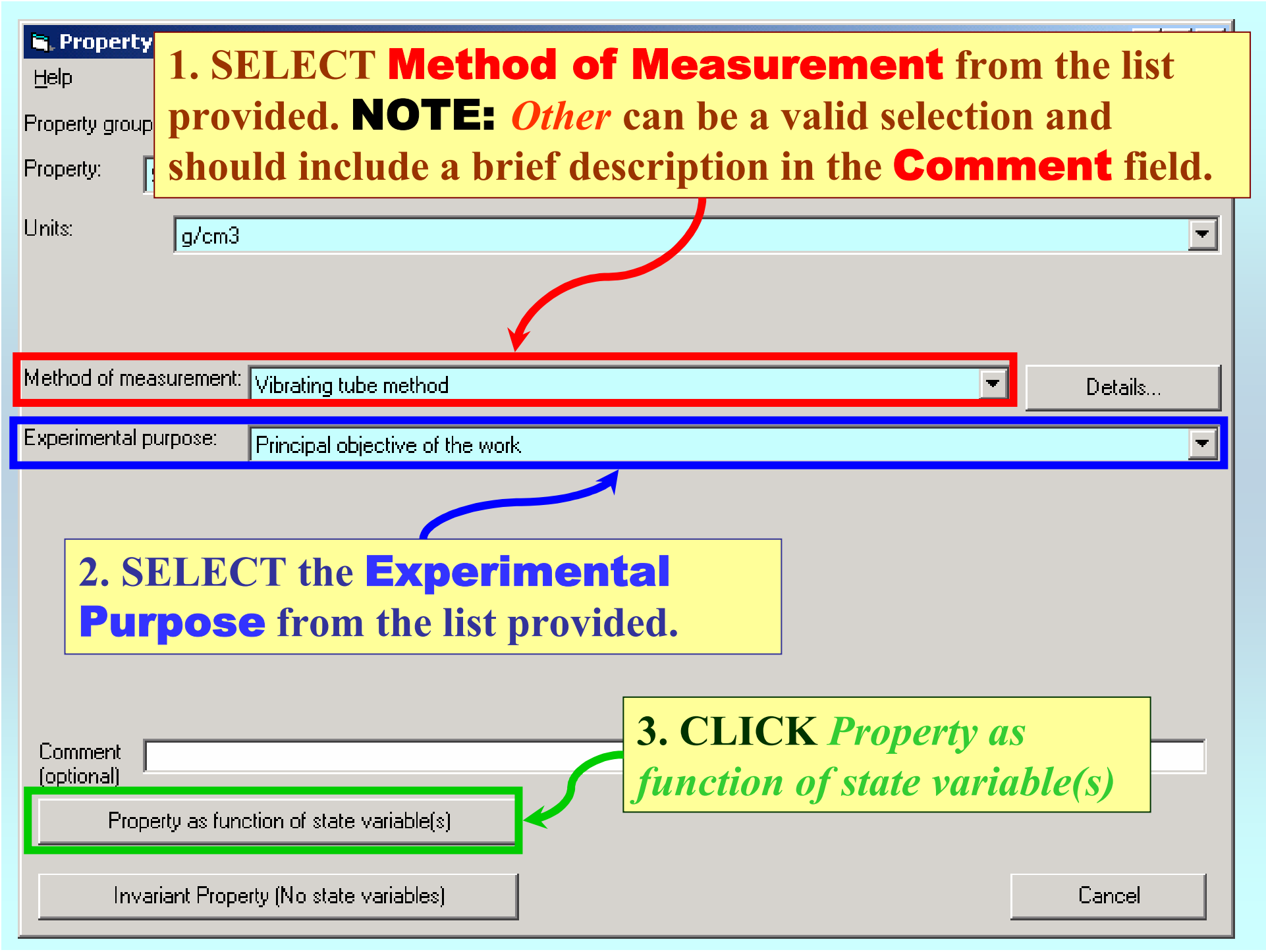
Experimental Method Info:

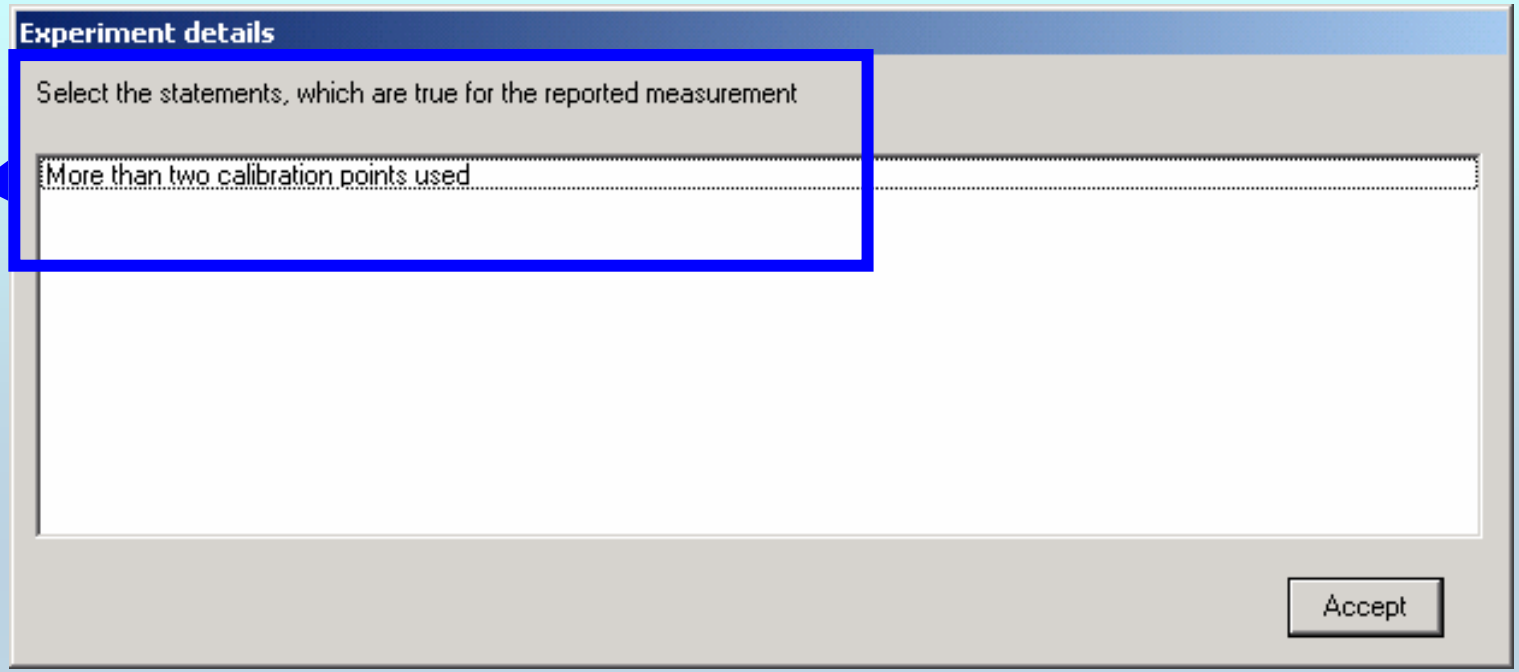
Vibrating-tube densimeter



NOTE: The **bibliographic information**, **compound identities**, **sample descriptions**, and **mixture** were entered previously. (There are separate tutorials, which describe capture of this information, if needed.)

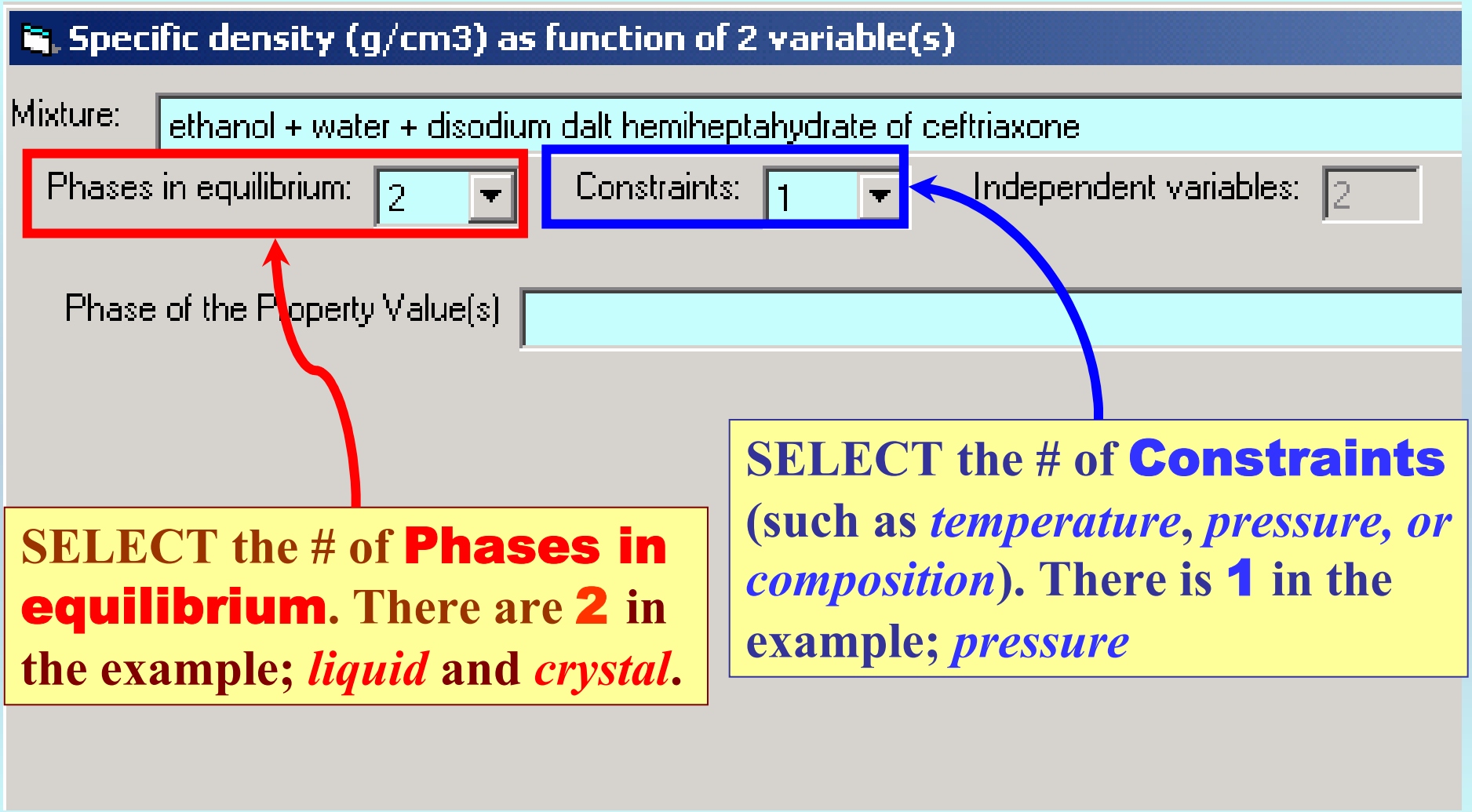

Property and experimental method for ethanol + water + disodium dalt hemiheptahydrate of ceftri...
Help
Property group:
Volumetric properties
Property:
Specific density
Units:
g/cm3
1. SELECT the Property Group: Volumetric properties from the menu.
Method of measurement:
Experimental purpose:
2. SELECT the Property: Specific density, for the example.
3. SELECT the Units: g/cc
Comment (optional)
Property as function of state variable(s)
Invariant Property (No state variables)
Cancel


Property
Help
Property group
Property:
Units:
g/cm3
1. SELECT Method of Measurement from the list provided. NOTE: Other can be a valid selection and should include a brief description in the Comment field.
Method of measurement:
Vibrating tube method
Details...
Experimental purpose:
Principal objective of the work
2. SELECT the Experimental Purpose from the list provided.
3. CLICK Property as function of state variable(s)
Comment (optional)
Property as function of state variable(s)
Invariant Property (No state variables)
Cancel



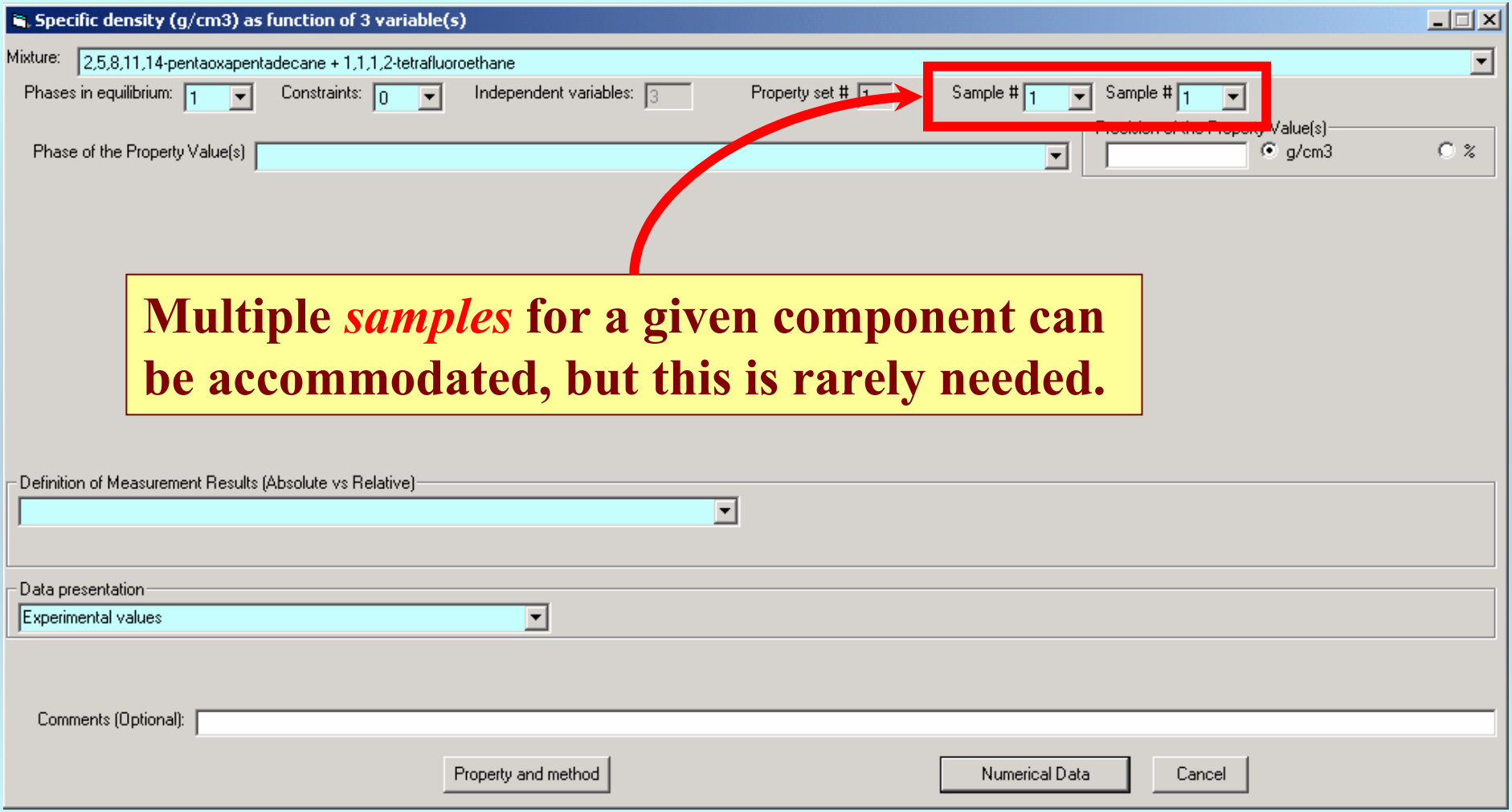
NOTE: For some methods, additional information is requested.

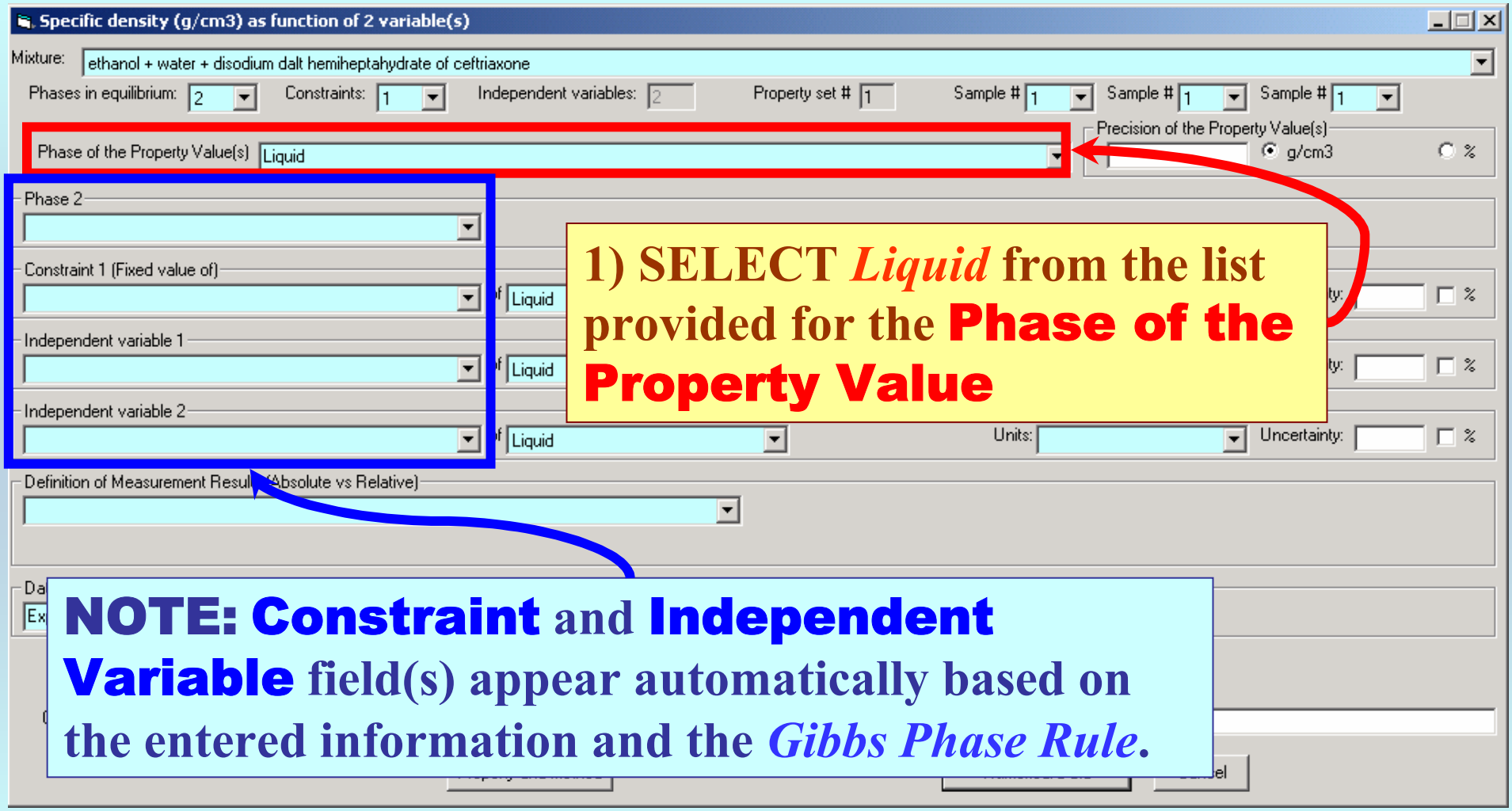
SELECTION of # of Phases in Equilibrium and # of Constraints

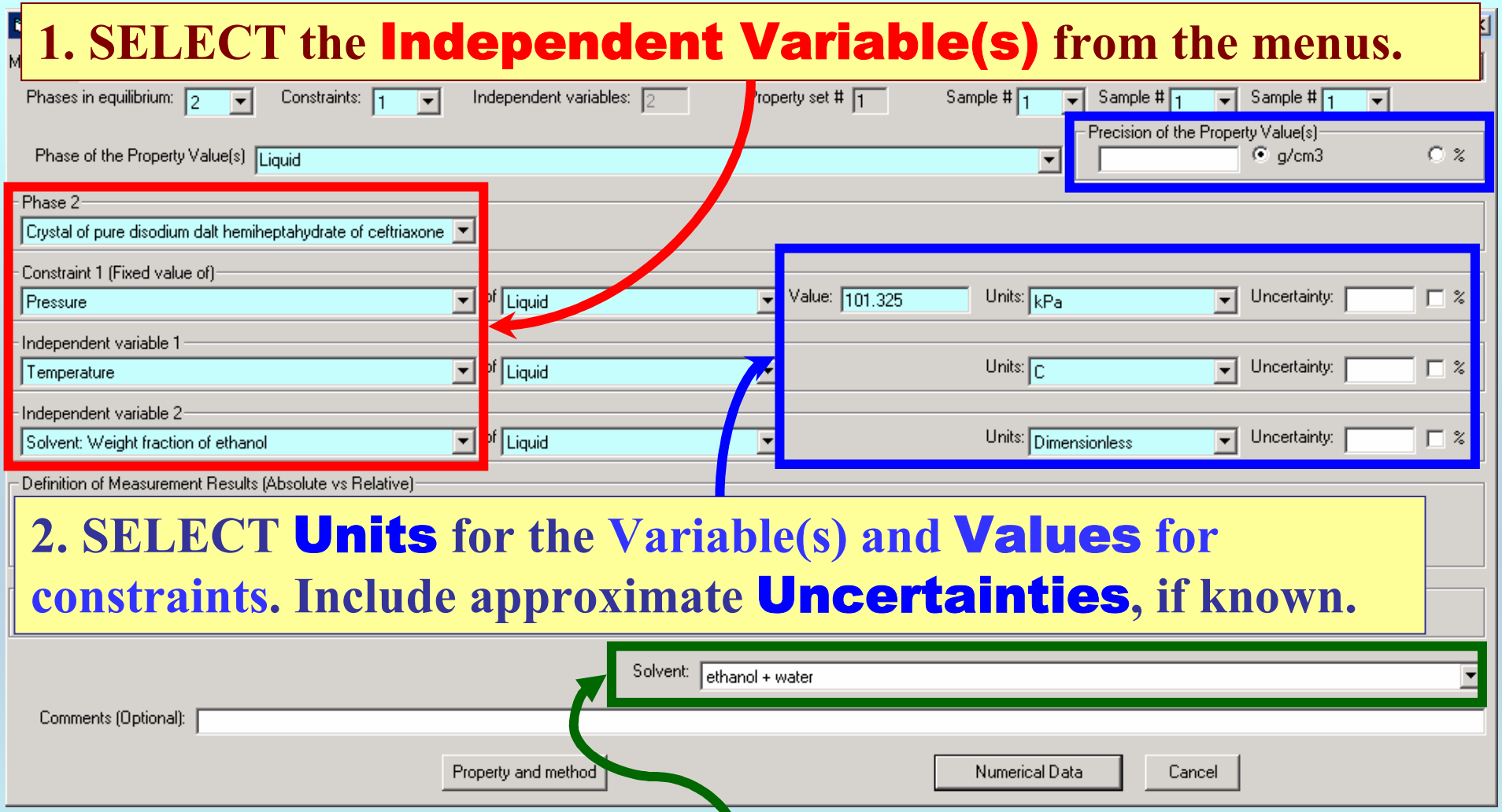


SELECT the # of **Phases in equilibrium**. There are **2** in the example; *liquid* and *crystal*.

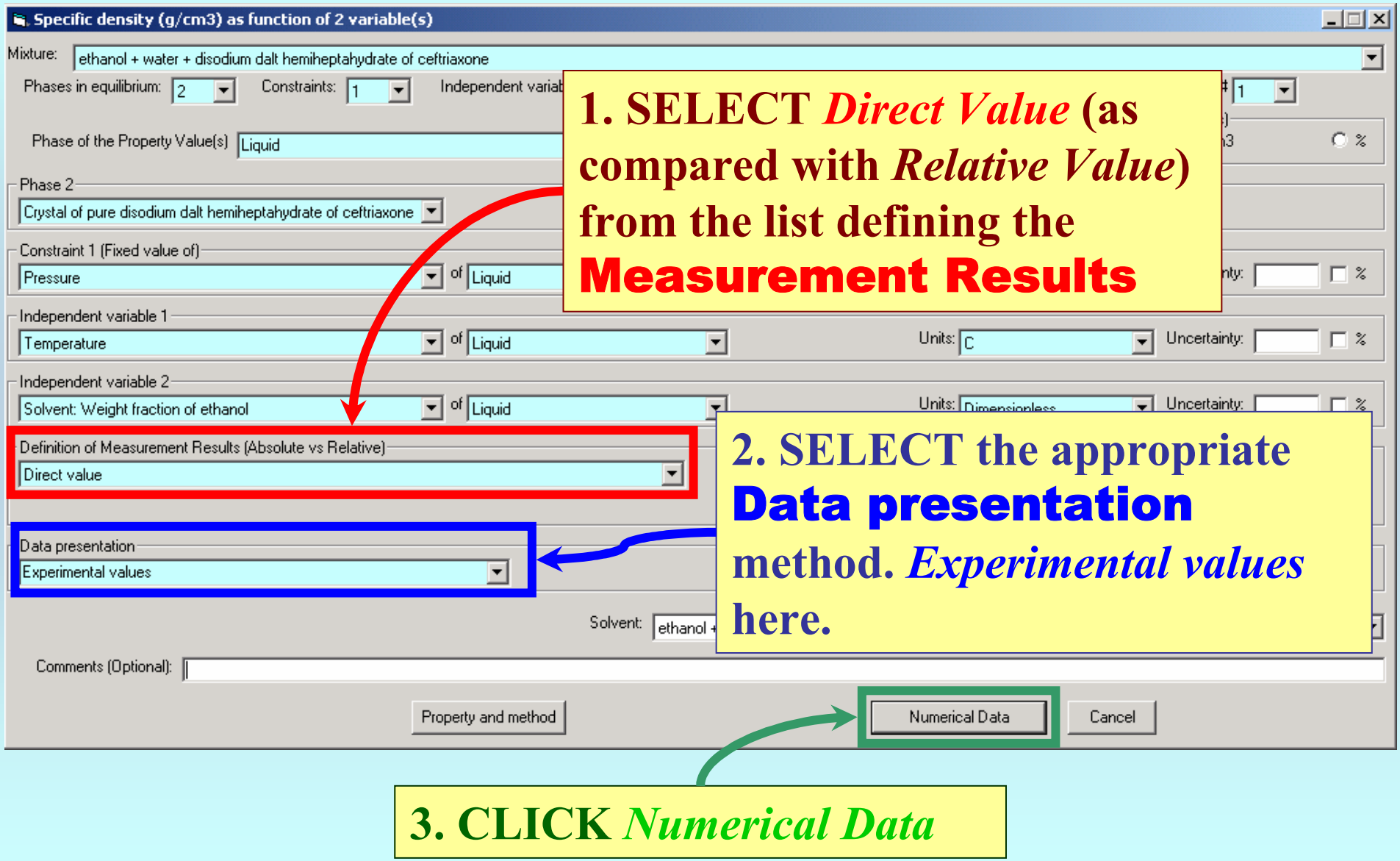
SELECT the # of **Constraints** (such as *temperature*, *pressure*, *or composition*). There is **1** in the example; *pressure*


Specific density (g/cm3) as function of 3 variable(s)
Mixture:
2,5,8,11,14-pentaoxapentadecane + 1,1,1,2-tetrafluoroethane
Phases in equilibrium:
1
Constraints:
0
Independent variables:
3
Property set #
Sample #
1
Sample #
1
Phase of the Property Value(s)
g/cm3
%
Multiple samples for a given component can be accommodated, but this is rarely needed.
Definition of Measurement Results (Absolute vs Relative)
Data presentation
Experimental values
Comments (Optional):
Property and method
Numerical Data
Cancel


Specific density (g/cm3) as function of 2 variable(s)
Mixture:
ethanol + water + disodium dalt hemiheptahydrate of ceftriaxone
Phases in equilibrium:
2
Constraints:
1
Independent variables:
2
Property set #
1
Sample #
1
Sample #
1
Sample #
1
Phase of the Property Value(s)
Liquid
Precision of the Property Value(s)
g/cm3
%
Phase 2
Constraint 1 (Fixed value of)
Independent variable 1
Independent variable 2
Liquid
Liquid
Liquid
Units:
Uncertainty:
%
Definition of Measurement Result (Absolute vs Relative)
1) SELECT Liquid from the list provided for the Phase of the Property Value
NOTE: Constraint and Independent Variable field(s) appear automatically based on the entered information and the Gibbs Phase Rule.



Note- *Solvent: Weight fraction of ethanol* **is one of the variables. With this selection, the Solvent field appears and the solvent must be defined. Here it is** *ethanol + water*.


Specific density (g/cm3) as function of 2 variable(s)
Mixture: ethanol + water + disodium dalt hemiheptahydrate of ceftriaxone
Phases in equilibrium: 2
Constraints: 1
Phase of the Property Value(s): Liquid
Phase 2
Crystal of pure disodium dalt hemiheptahydrate of ceftriaxone
Constraint 1 (Fixed value of)
Pressure
of Liquid
Independent variable 1
Temperature
of Liquid
Units: C
Uncertainty:
Independent variable 2
Solvent: Weight fraction of ethanol
of Liquid
Definition of Measurement Results (Absolute vs Relative)
Direct value
Data presentation
Experimental values
Solvent:
Comments (Optional):
Property and method
Numerical Data
Cancel
1. SELECT Direct Value (as compared with Relative Value) from the list defining the Measurement Results
2. SELECT the appropriate Data presentation method. Experimental values here.
3. CLICK Numerical Data

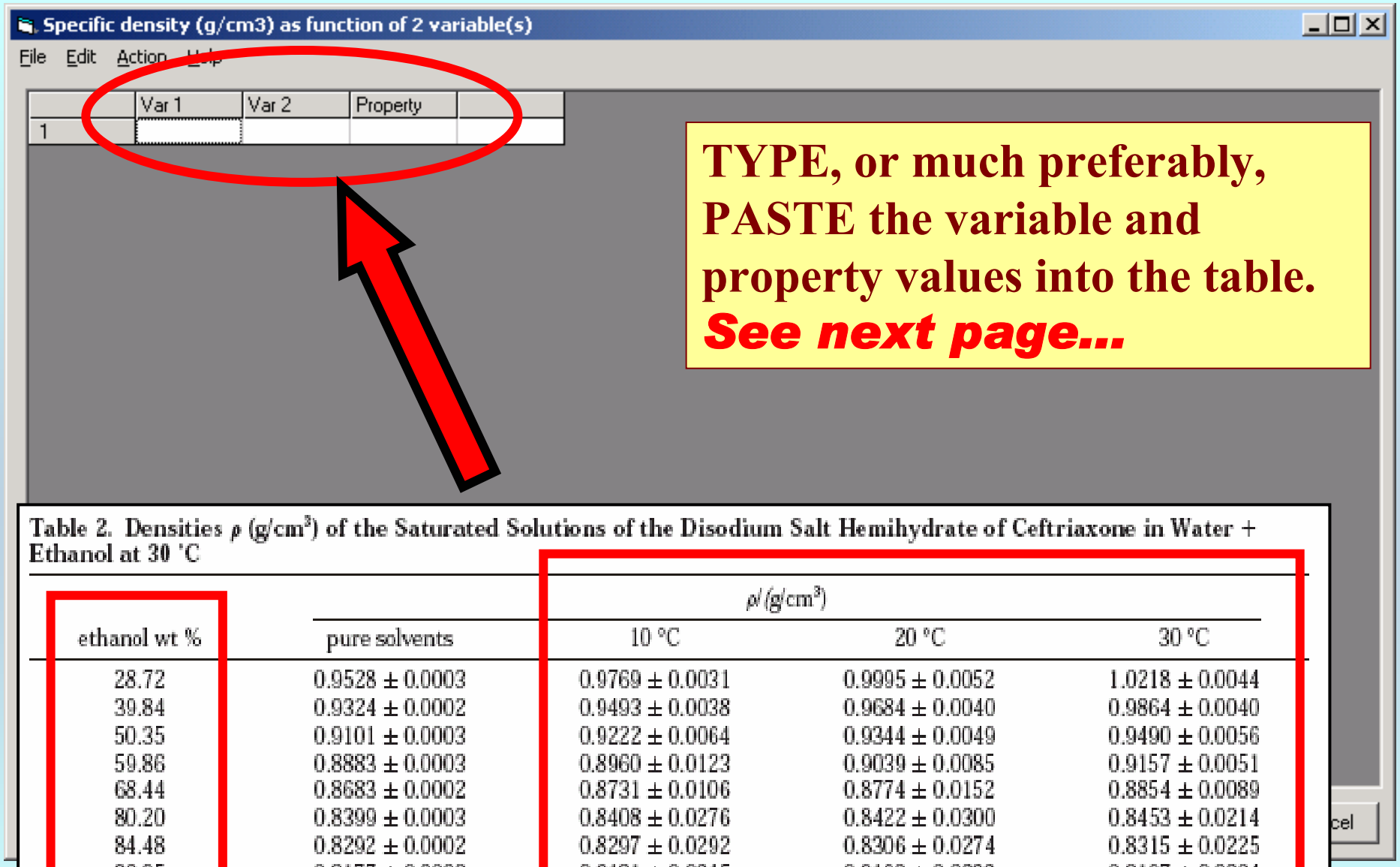


Table 2. Densities ρ (g/cm^3) of the Saturated Solutions of the Disodium Salt Hemihydrate of Ceftriaxone in Water + Ethanol at 30 °C

ethanol wt %	pure solvents	ρ/(g/cm^3) 10 °C	20 °C	30 °C
28.72	0.9528 ± 0.0003	0.9769 ± 0.0031	0.9995 ± 0.0052	1.0218 ± 0.0044
39.84	0.9324 ± 0.0002	0.9493 ± 0.0038	0.9684 ± 0.0040	0.9864 ± 0.0040
50.35	0.9101 ± 0.0003	0.9222 ± 0.0064	0.9344 ± 0.0049	0.9490 ± 0.0056
59.86	0.8883 ± 0.0003	0.8960 ± 0.0123	0.9039 ± 0.0085	0.9157 ± 0.0051
68.44	0.8683 ± 0.0002	0.8731 ± 0.0106	0.8774 ± 0.0152	0.8854 ± 0.0089
80.20	0.8399 ± 0.0003	0.8408 ± 0.0276	0.8422 ± 0.0300	0.8453 ± 0.0214
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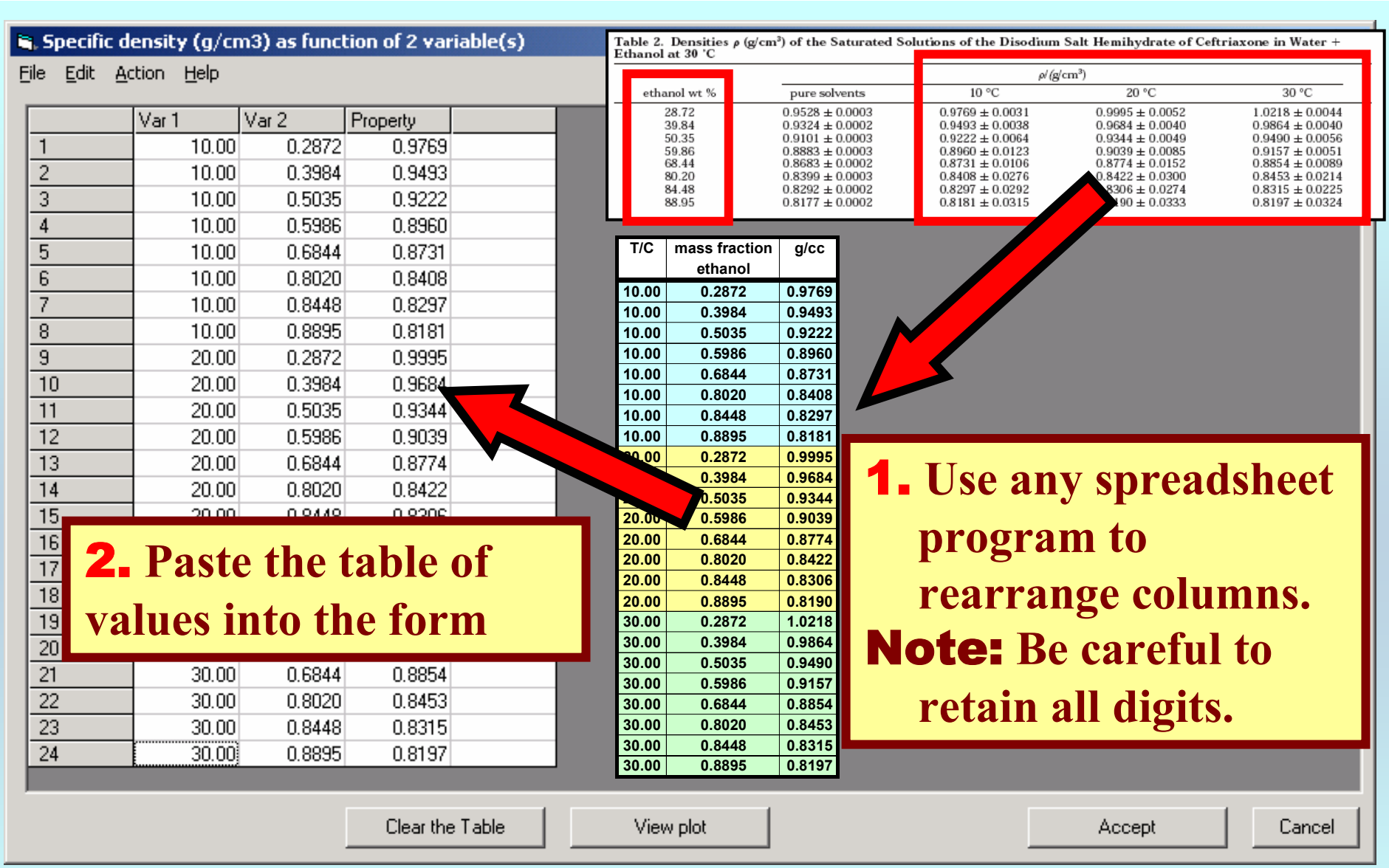
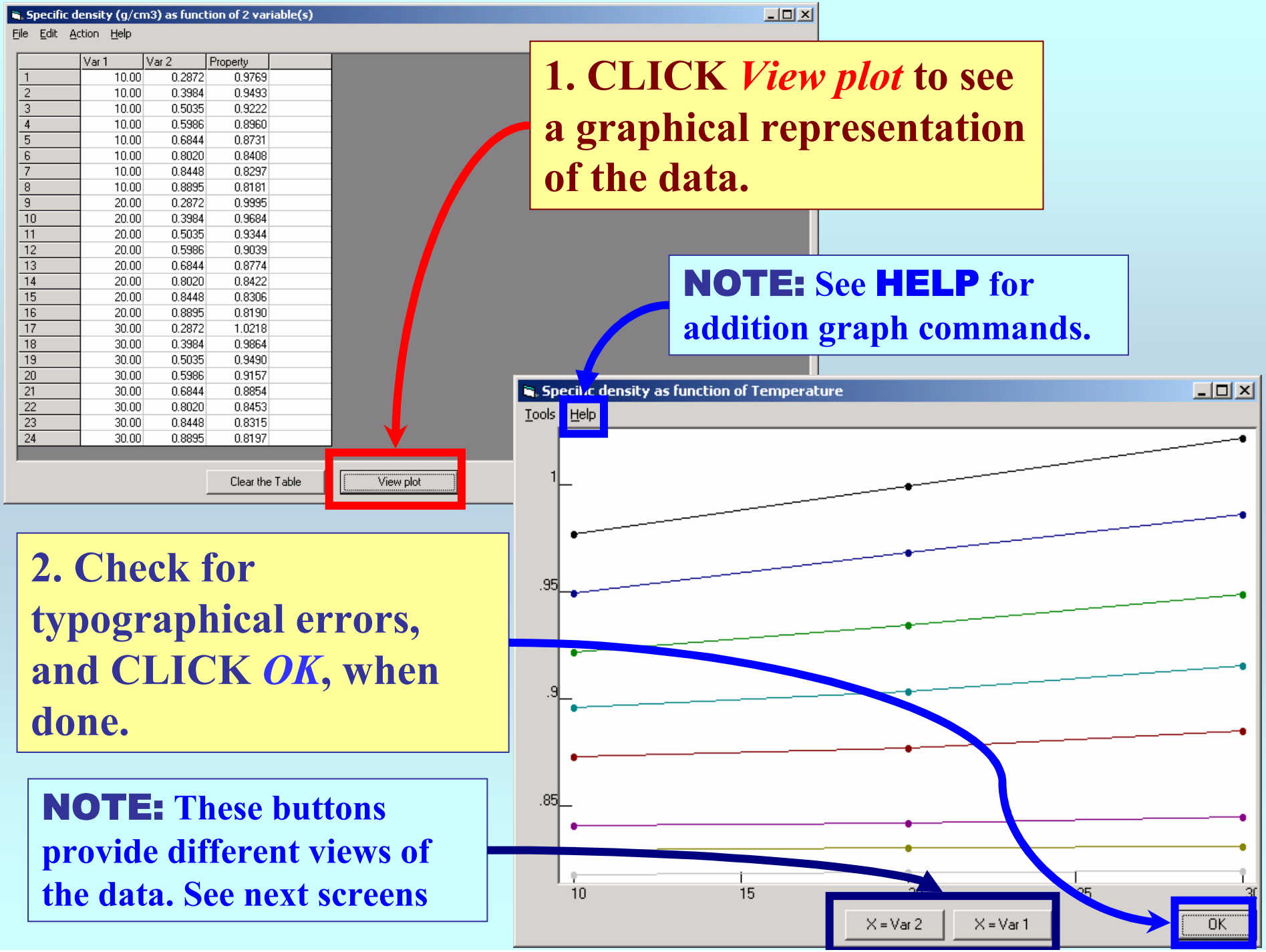
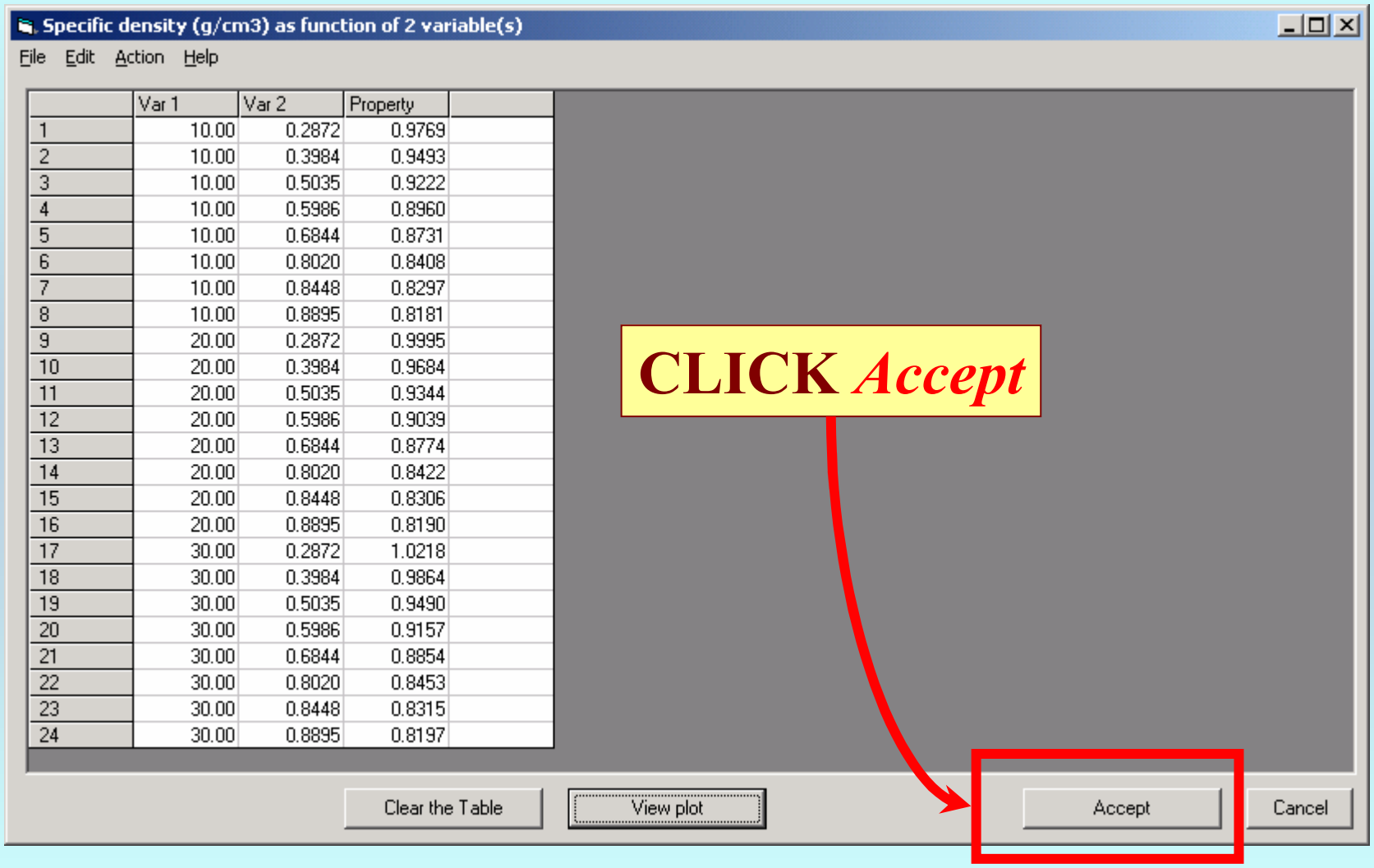
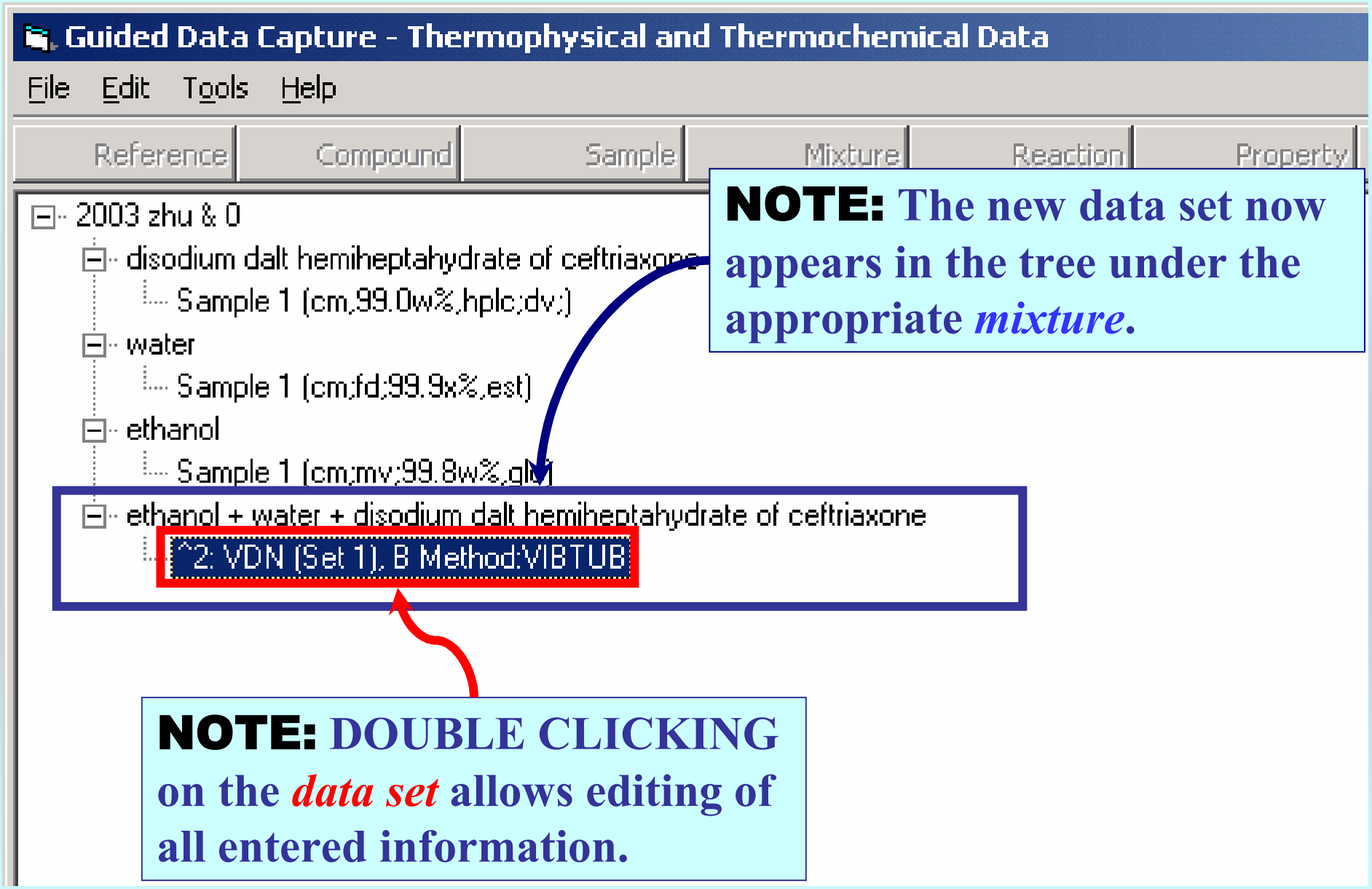
88.95	0.8177 ± 0.0002	0.8181 ± 0.0315	0.8190 ± 0.0333	0.8197 ± 0.0324



NOTE: Simple CUT/PASTE procedures can be used within the table to convert the original table into the required number of columns. (This can also be done externally in spreadsheet software, e.g., EXCEL.)


Specific density (g/cm3) as function of 2 variable(s)
File Edit Action Help
Var 1 Var 2 Property
1 10.00 0.2872 0.9769
2 10.00 0.3984 0.9493
3 10.00 0.5035 0.9222
4 10.00 0.5986 0.8960
5 10.00 0.6844 0.8731
6 10.00 0.8020 0.8408
7 10.00 0.8448 0.8297
8 10.00 0.8895 0.8181
9 20.00 0.2872 0.9995
10 20.00 0.3984 0.9684
11 20.00 0.5035 0.9344
12 20.00 0.5986 0.9039
13 20.00 0.6844 0.8774
14 20.00 0.8020 0.8422
15 20.00 0.8448 0.8306
16 20.00 0.8895 0.8190
17 30.00 0.2872 1.0218
18 30.00 0.3984 0.9864
19 30.00 0.5035 0.9490
20 30.00 0.5986 0.9157
21 30.00 0.6844 0.8854
22 30.00 0.8020 0.8453
23 30.00 0.8448 0.8315
24 30.00 0.8895 0.8197
Clear the Table
View plot
1. CLICK View plot to see a graphical representation of the data.
NOTE: See HELP for addition graph commands.
Specific density as function of Temperature
Tools Help
1
.95
.9
.85
10
15
X = Var 2
X = Var 1
OK
2. Check for typographical errors, and CLICK OK, when done.
NOTE: These buttons provide different views of the data. See next screens


Specific density (g/cm3) as function of 2 variable(s)
File Edit Action Help
Var 1 Var 2 Property
1 10.00 0.2872 0.9769
2 10.00 0.3984 0.9493
3 10.00 0.5035 0.9222
4 10.00 0.5986 0.8960
5 10.00 0.6844 0.8731
6 10.00 0.8020 0.8408
7 10.00 0.8448 0.8297
8 10.00 0.8895 0.8181
9 20.00 0.2872 0.9995
10 20.00 0.3984 0.9684
11 20.00 0.5035 0.9344
12 20.00 0.5986 0.9039
13 20.00 0.6844 0.8774
14 20.00 0.8020 0.8422
15 20.00 0.8448 0.8306
16 20.00 0.8895 0.8190
17 30.00 0.2872 1.0218
18 30.00 0.3984 0.9864
19 30.00 0.5035 0.9490
20 30.00 0.5986 0.9157
21 30.00 0.6844 0.8854
22 30.00 0.8020 0.8453
23 30.00 0.8448 0.8315
24 30.00 0.8895 0.8197
CLICK Accept
Clear the Table
View plot
Accept
Cancel


Guided Data Capture - Thermophysical and Thermochemical Data
File Edit Tools Help
Reference Compound Sample Mixture Reaction Property
2003 zhu & 0
disodium dalt hemiheptahydrate of ceftriaxone
Sample 1 (cm,99.0w%,hplc;dv;)
water
Sample 1 (cm;fd;99.9x%,est)
ethanol
Sample 1 (cm;mv;99.8w%,gl
ethanol + water + disodium dalt hemiheptahydrate of ceftriaxone
^2: VDN (Set 1), B Method:VIBTUB
NOTE: The new data set now appears in the tree under the appropriate mixture.
NOTE: DOUBLE CLICKING on the data set allows editing of all entered information.

END

Continue with other compounds, samples, properties, reactions, etc...

***or* save your file and exit the program, if all properties have been captured.**