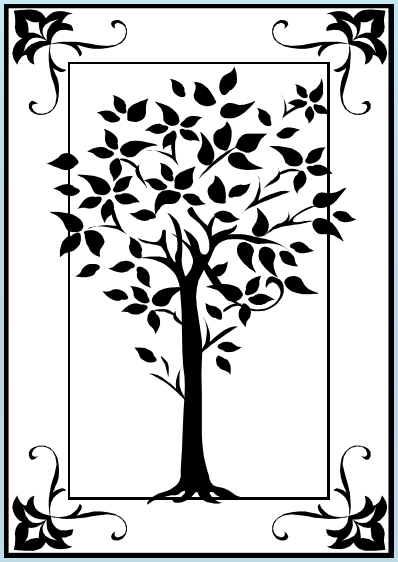
METADATA AND NUMERICAL DATA CAPTURE:
VLE (Txy) data
(3 components)

Guided Data Capture (GDC)



This tutorial describes
METADATA AND NUMERICAL DATA CAPTURE:
for **VLE (Txy) data**
Composition at phase equilibrium
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:

JE0301460

VLE ($Tx_1x_2y_1y_2$) for a 3-component mixture (*ethanol + cyclohexane + water*)

Table 2 VLE data for ethanol(1)–cyclohexane(2)–water(3) system

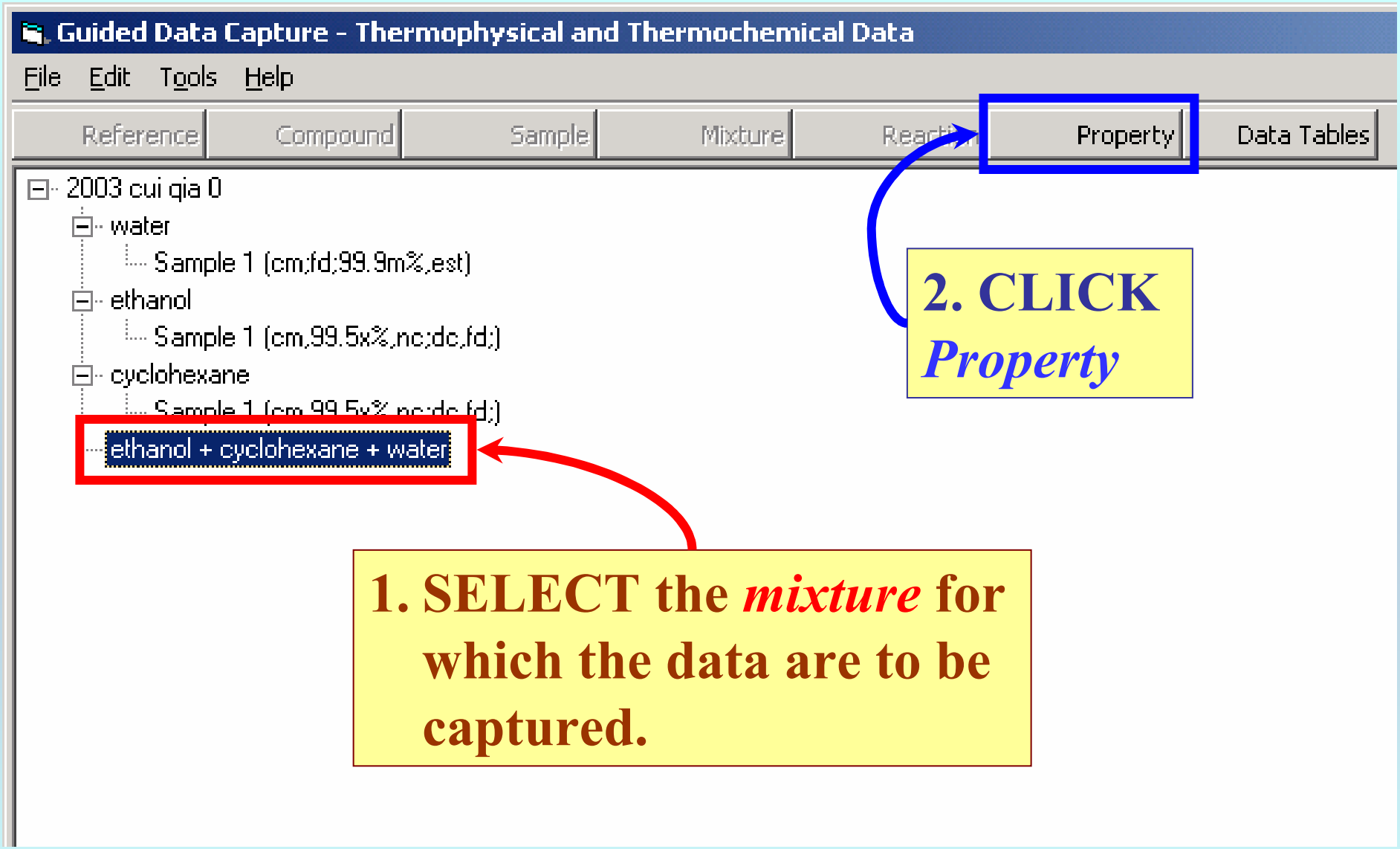
t/°C	mole fraction in liquid phase x_1	x_2	mole fraction in vapor phase y_1	y_2
	0.5096	0.4257	0.2948	0.6352
	0.5776	0.3814	0.3269	0.6251
	0.5972	0.3589	0.3201	0.6325
	0.6675	0.2752	0.3381	0.6116
35	0.7155	0.2137	0.3369	0.6095
	0.7066	0.1073	0.3213	0.5809
	0.8100	0.0973	0.4101	0.5302
	0.8457	0.0678	0.4795	0.4640
	0.4790	0.0046	0.4651	0.2965
	0.4902	0.4886	0.3887	0.5754
	0.5542	0.4095	0.3881	0.5668
	0.5825	0.3746	0.3861	0.5588
	0.6411	0.3065	0.3957	0.5503
	0.6885	0.2439	0.4043	0.5344
50	0.7703	0.1121	0.4274	0.4915
	0.8324	0.0766	0.5229	0.4075
	0.6749	0.1437	0.3603	0.5513
	0.6753	0.0682	0.4049	0.4525
	0.5982	0.0263	0.4332	0.3647
	0.4644	0.0103	0.3796	0.4190
	0.8276	0.0786	0.5584	0.3672
	0.6822	0.0603	0.4141	0.4379
	0.8650	0.0405	0.6221	0.3027
	0.8060	0.1113	0.5175	0.4174
65	0.8098	0.1288	0.5057	0.4418
	0.7160	0.2370	0.4572	0.4957
	0.6124	0.3523	0.4271	0.5244
	0.5653	0.4041	0.4204	0.5327

These data are considered here.

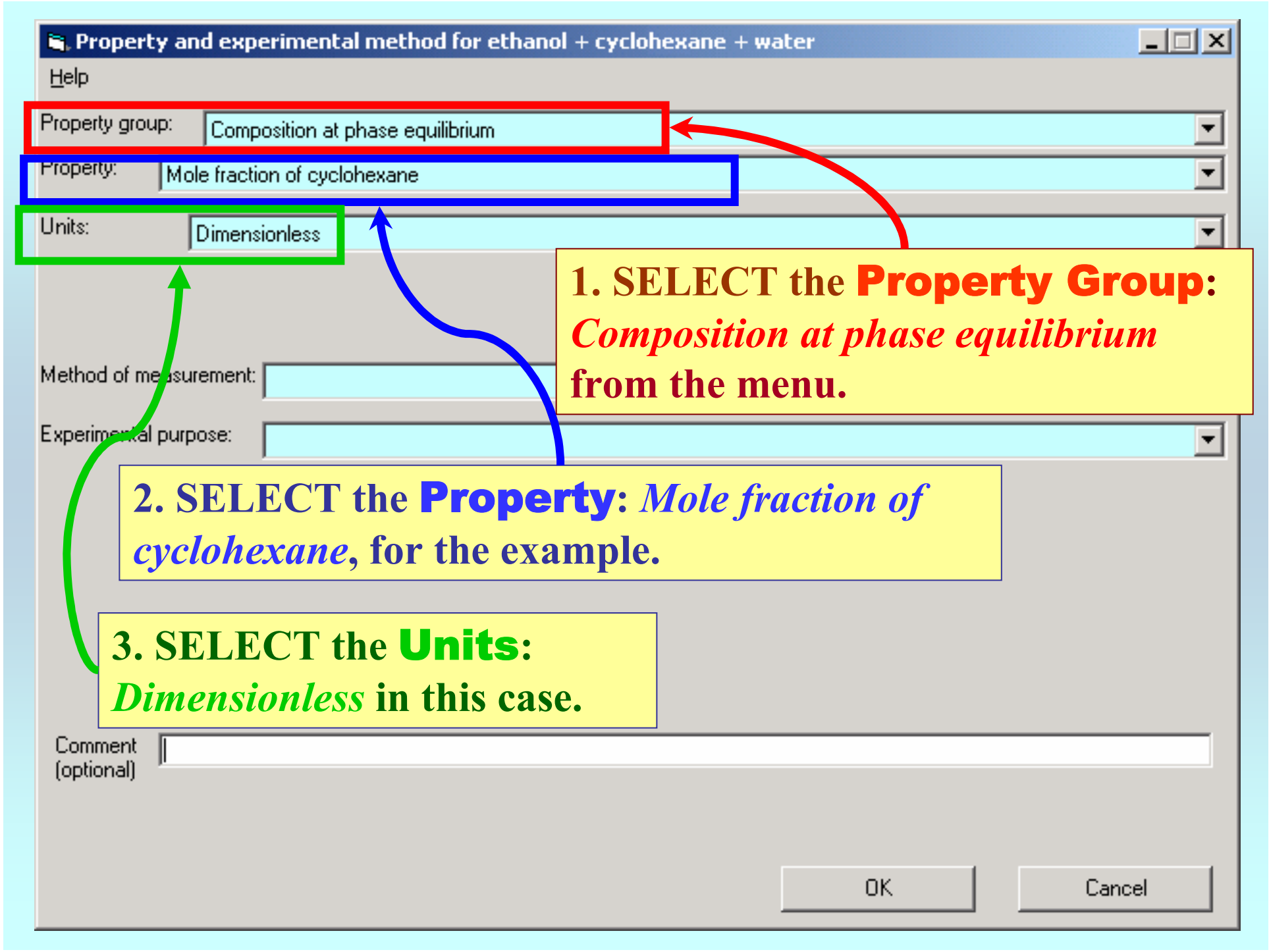
Results are reported for 3 temperatures.

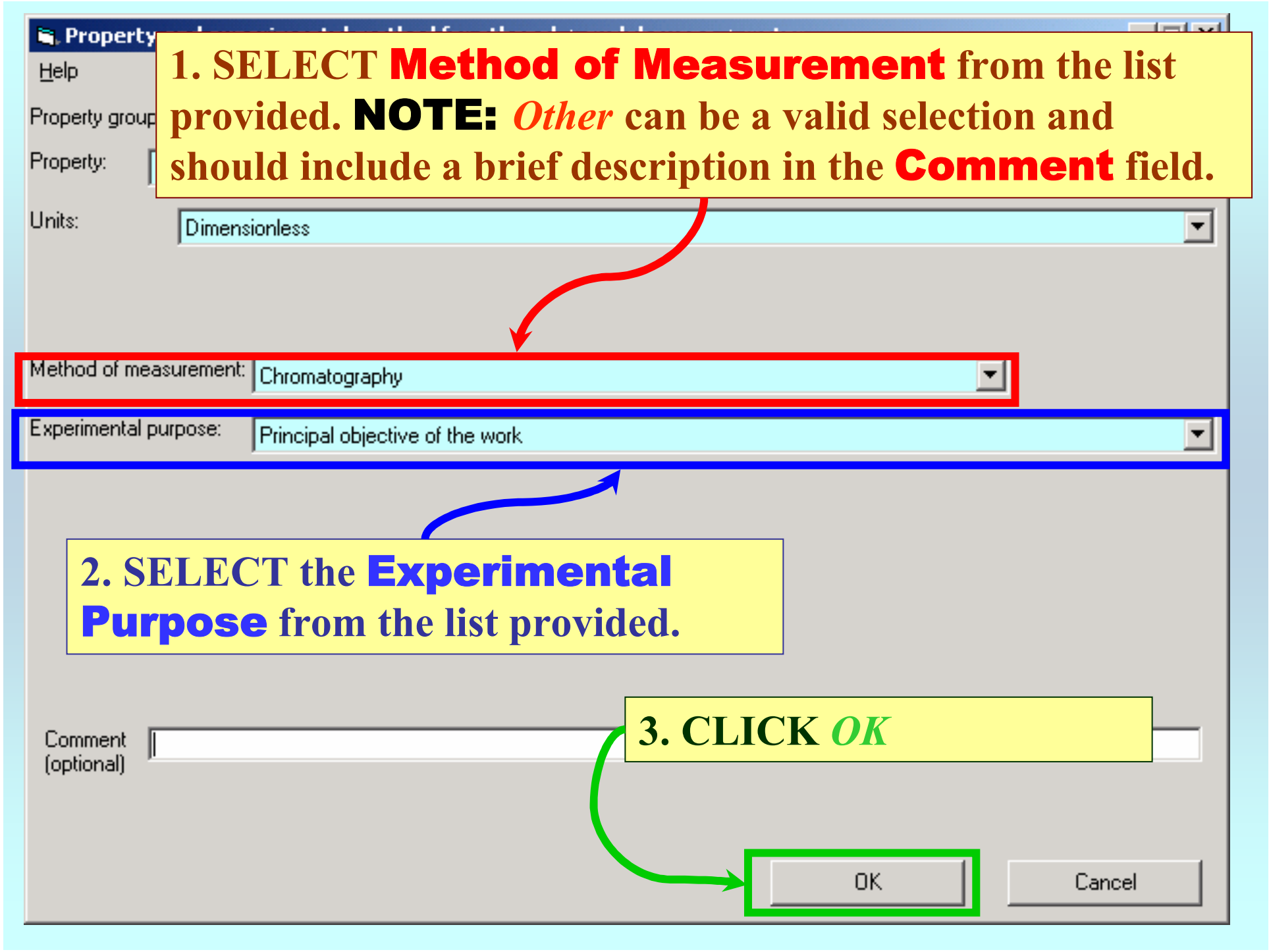
Experimental Method Info:

Compositions are determined by gas chromatography

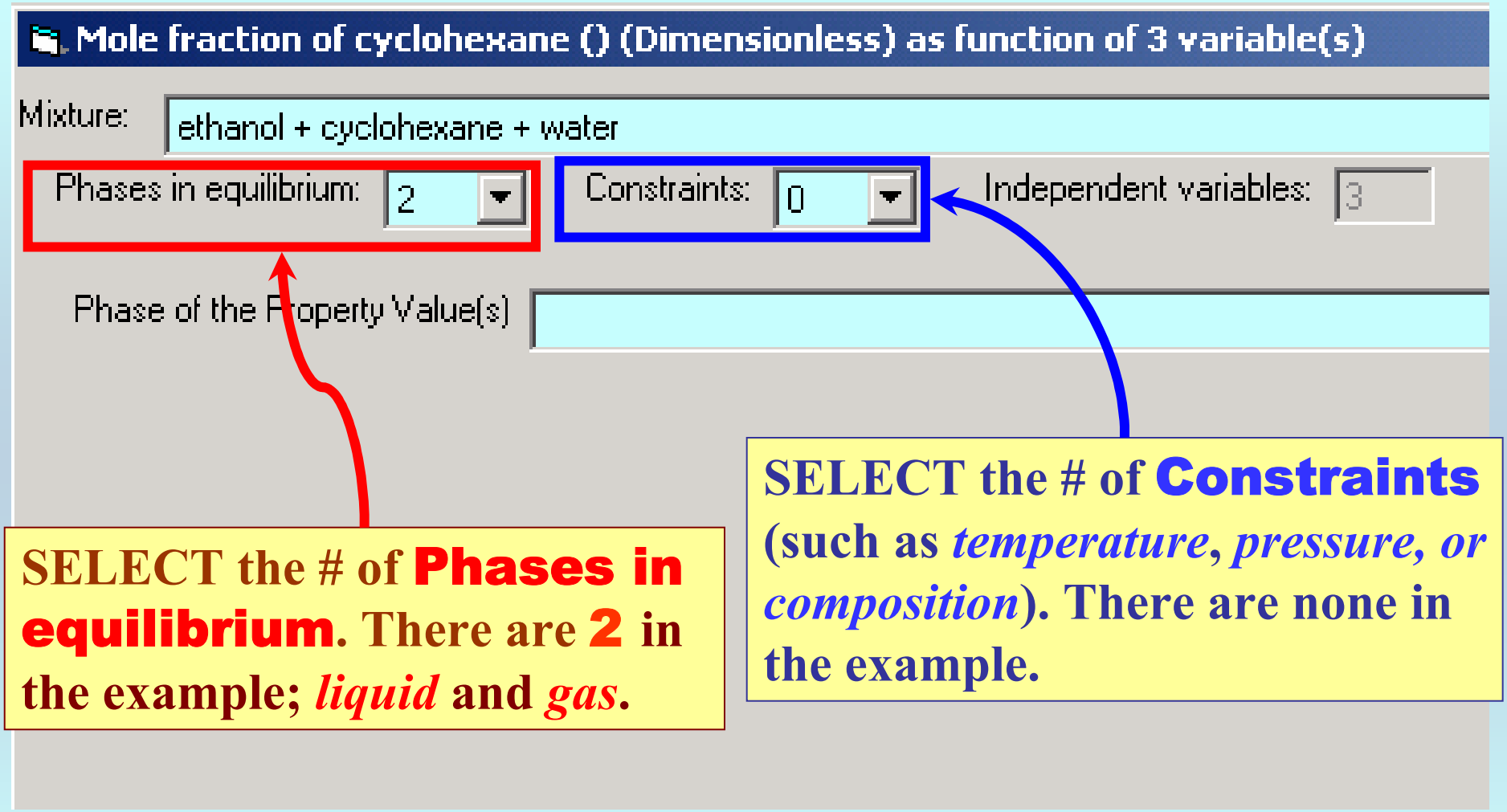


NOTE: The **bibliographic information**, **compound identities**, **sample descriptions**, and **mixture** were entered previously. (There are separate tutorials, which describe capture of this information, if needed.)


Property and experimental method for ethanol + cyclohexane + water
Help
Property group:
Composition at phase equilibrium
Property:
Mole fraction of cyclohexane
Units:
Dimensionless
Method of measurement:
Experimental purpose:
1. SELECT the Property Group: Composition at phase equilibrium from the menu.
2. SELECT the Property: Mole fraction of cyclohexane, for the example.
3. SELECT the Units: Dimensionless in this case.
Comment (optional)
OK
Cancel

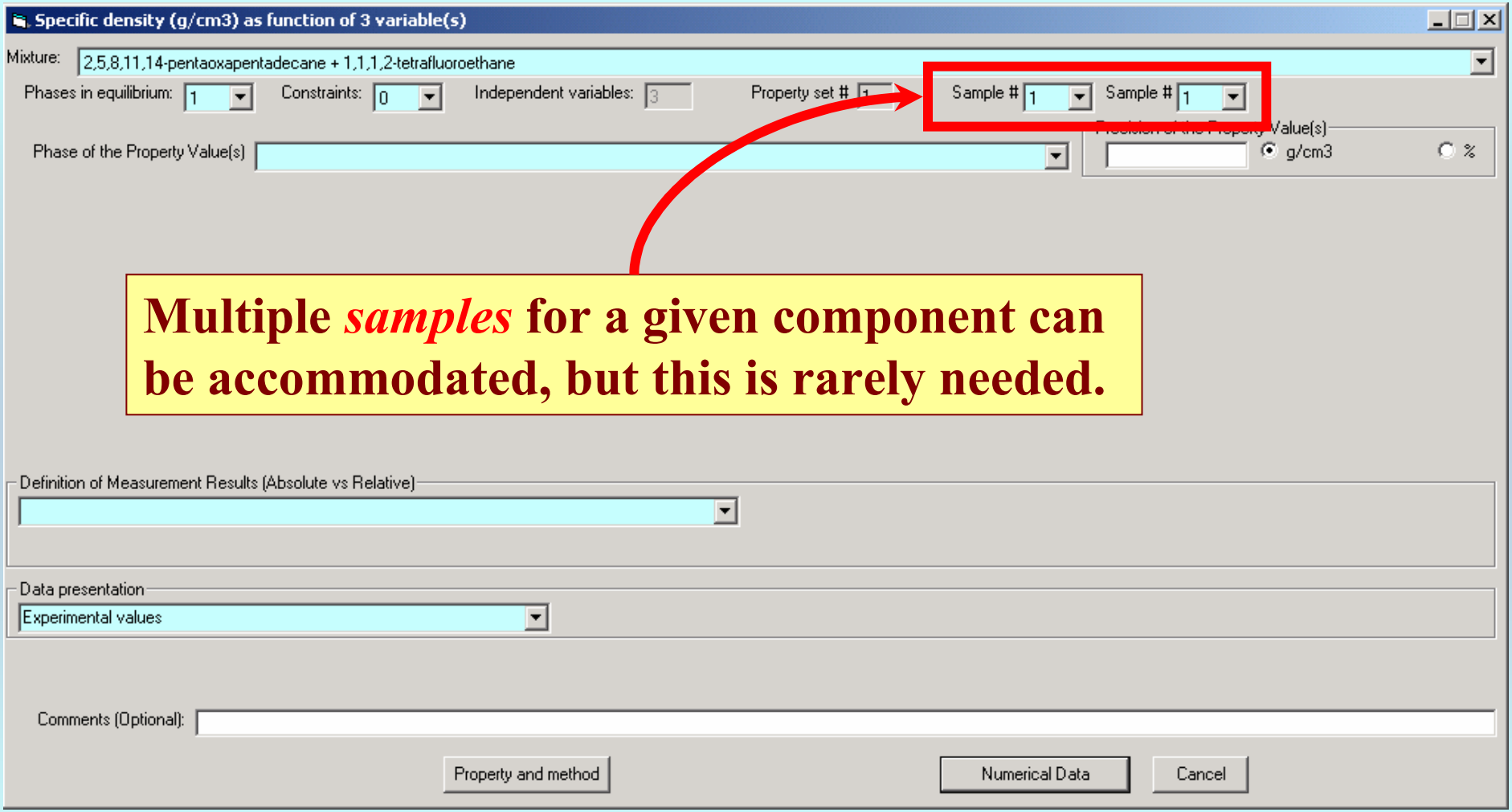

Property
Help
Property group
Property:
Units:
Dimensionless
1. SELECT Method of Measurement from the list provided. NOTE: Other can be a valid selection and should include a brief description in the Comment field.
Method of measurement:
Chromatography
Experimental purpose:
Principal objective of the work
2. SELECT the Experimental Purpose from the list provided.
Comment (optional)
3. CLICK OK
OK
Cancel

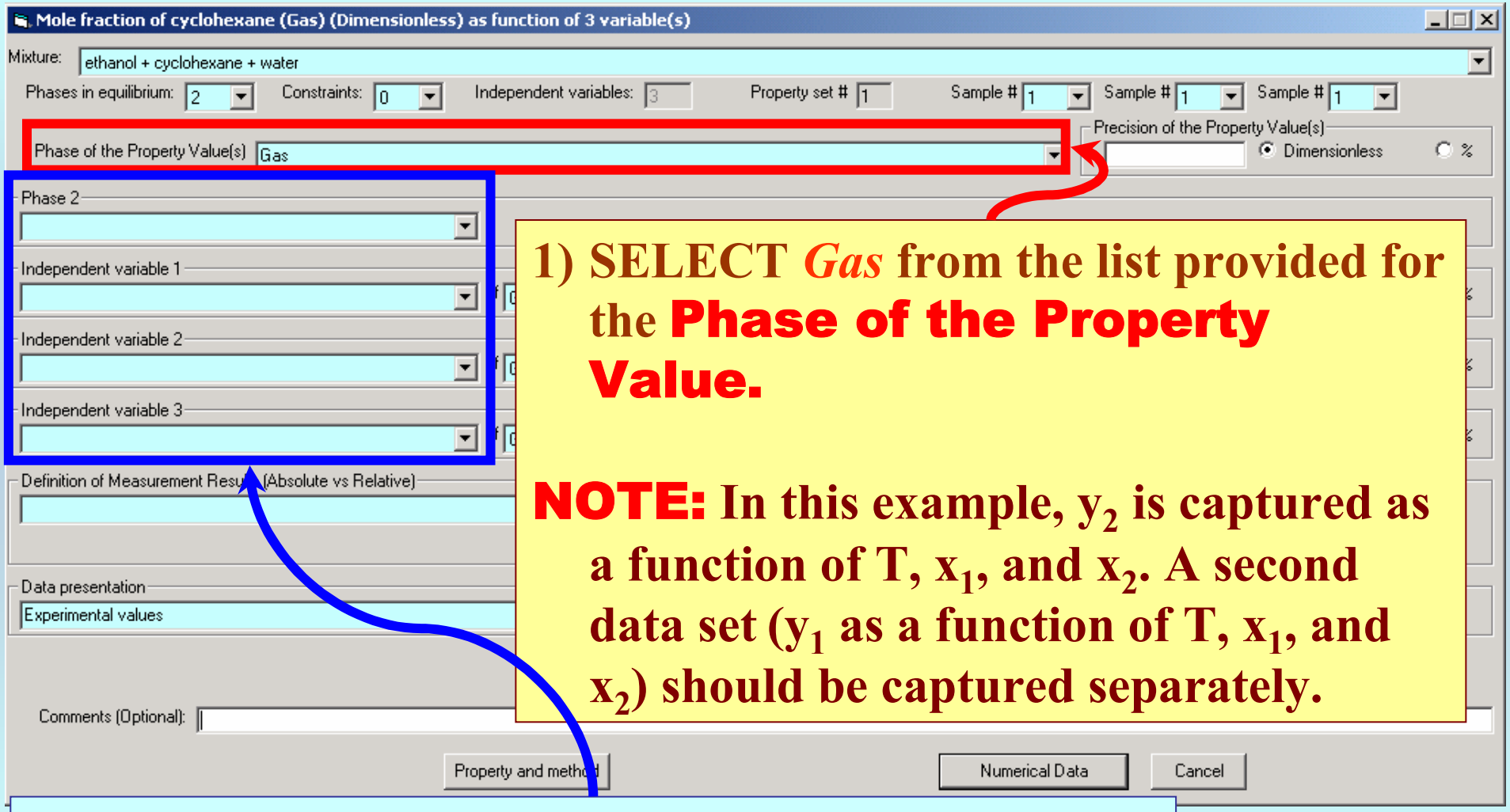
SELECTION of # of Phases in Equilibrium and # of Constraints



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

SELECT the # of **Constraints** (such as *temperature*, *pressure, or composition*). There are none in the example.


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

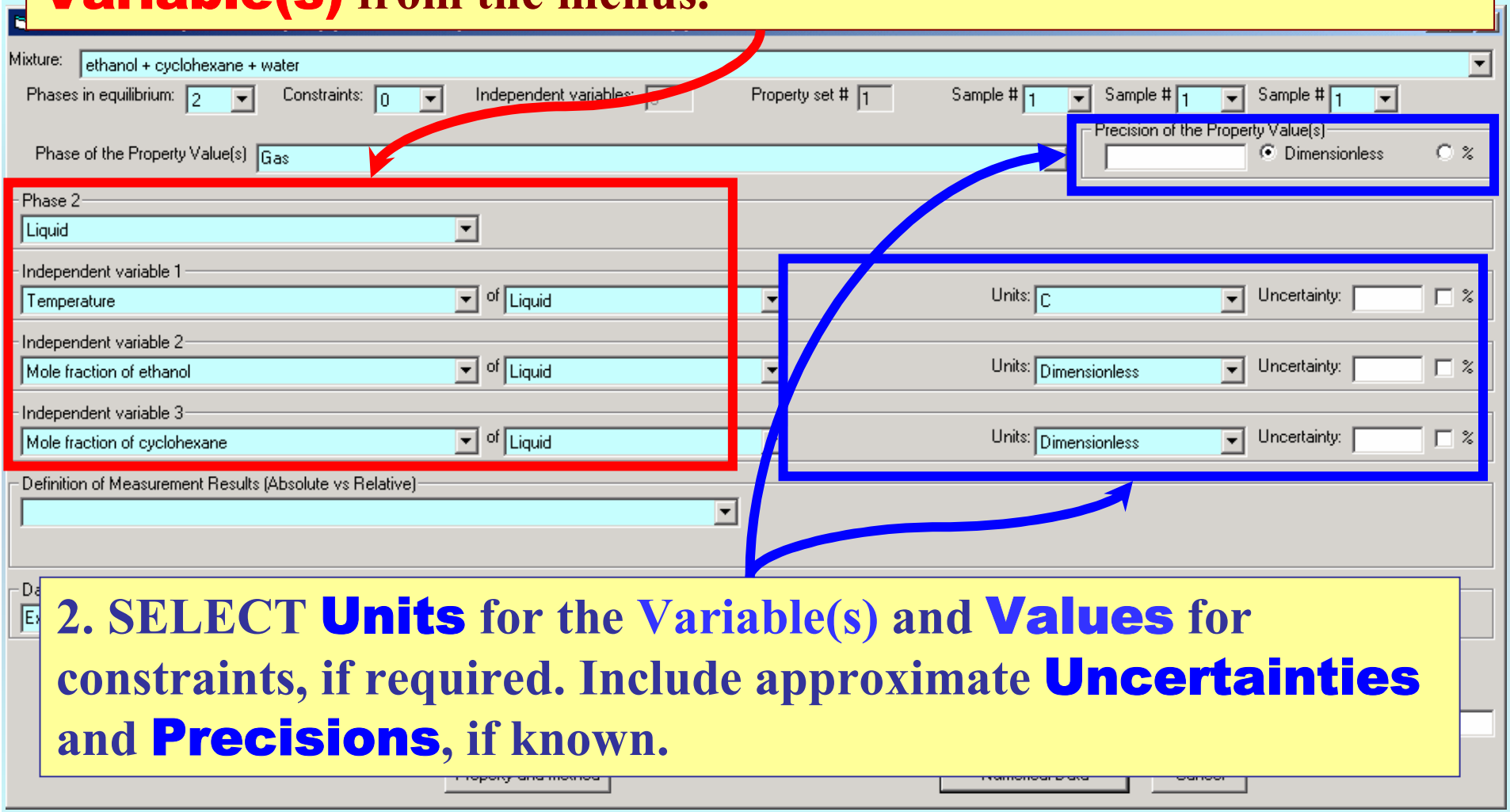


1) SELECT *Gas* from the list provided for the **Phase of the Property Value.**

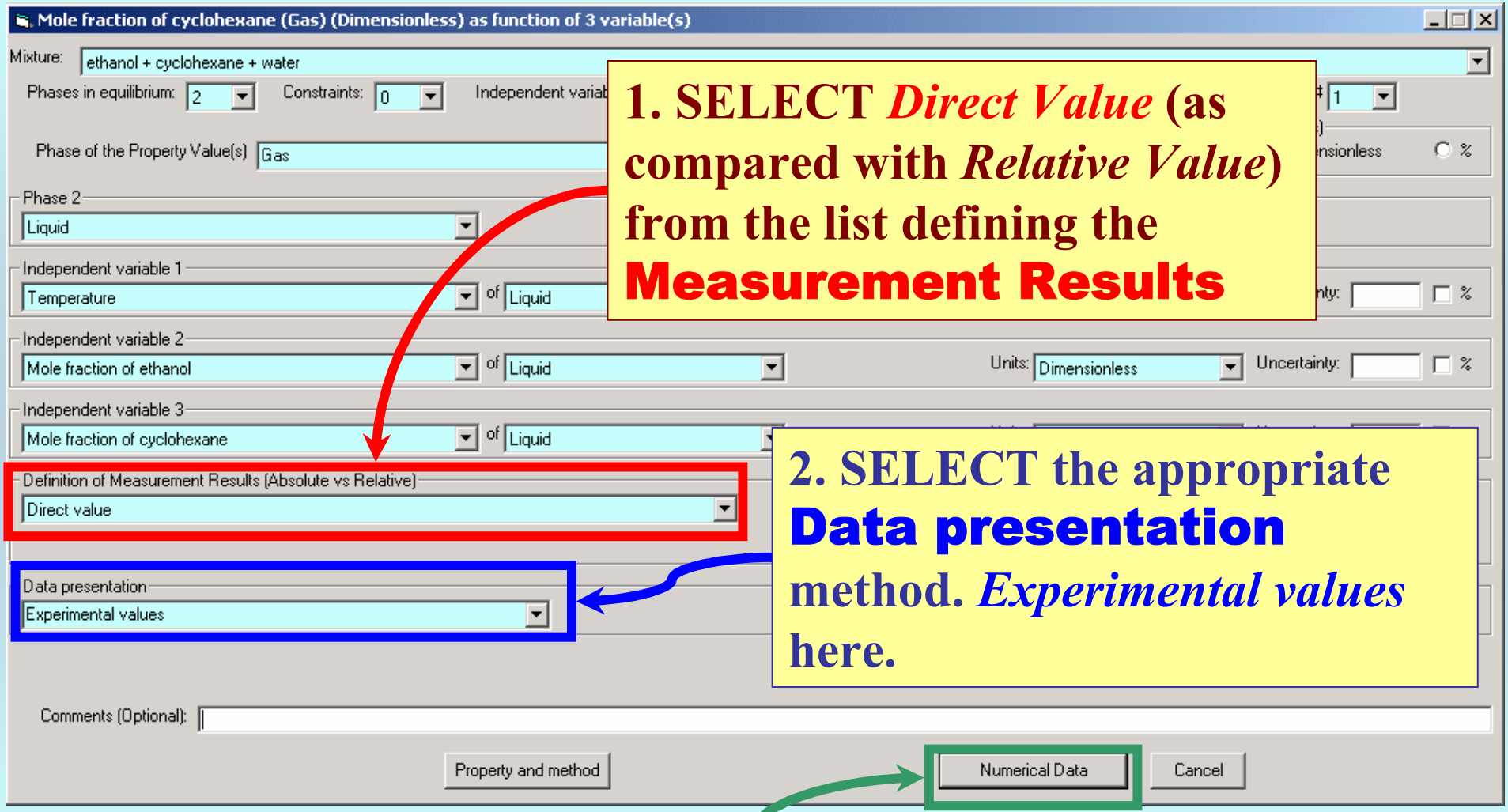
NOTE: In this example, y_2 is captured as a function of T, x_1, and x_2. A second data set (y_1 as a function of T, x_1, and x_2) should be captured separately.

NOTE: Constraint and **Independent Variable** field(s) appear automatically based on the entered information and the *Gibbs Phase Rule*.

1. SELECT **Phase 2**, *Liquid*, and the **Independent Variable(s)** from the menus.



2. SELECT **Units** for the Variable(s) and **Values** for constraints, if required. Include approximate **Uncertainties** and **Precisions**, if known.


Mole fraction of cyclohexane (Gas) (Dimensionless) as function of 3 variable(s)
Mixture: ethanol + cyclohexane + water
Phases in equilibrium: 2
Constraints: 0
Phase of the Property Value(s): Gas
Phase 2
Liquid
Independent variable 1
Temperature
of Liquid
Independent variable 2
Mole fraction of ethanol
of Liquid
Units: Dimensionless
Uncertainty:
Independent variable 3
Mole fraction of cyclohexane
of Liquid
Definition of Measurement Results (Absolute vs Relative)
Direct value
Data presentation
Experimental values
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

Mole fraction of cyclohexane (Dimensionless) as function of 3 variable(s)

File Edit Action Help

	Var 1	Var 2	Var 3	Property	
2					
3					
4					
5					
6					
7					
8					
9					
10					

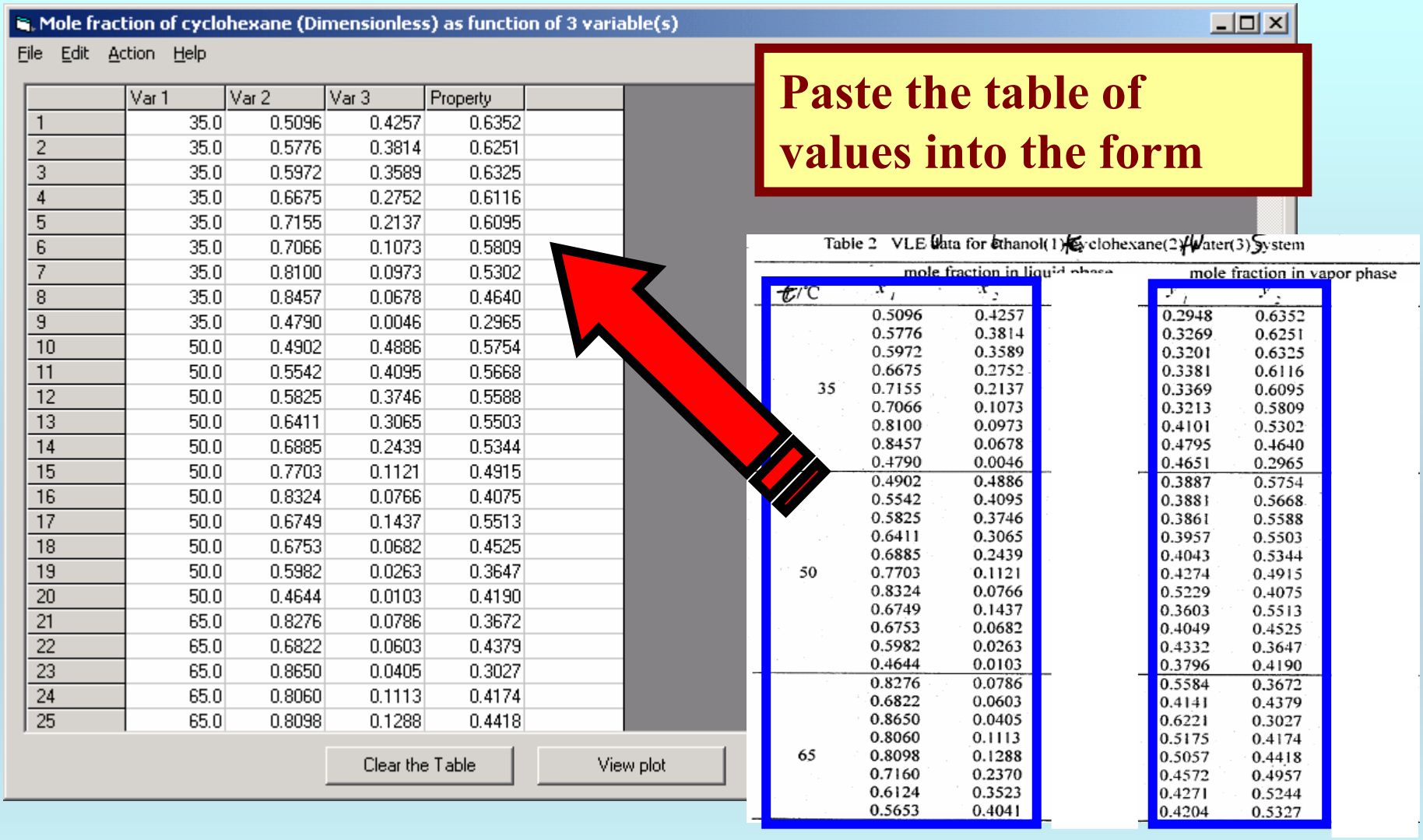
Clear the Table

TYPE, or much preferably, PASTE the variable and property values into the table.

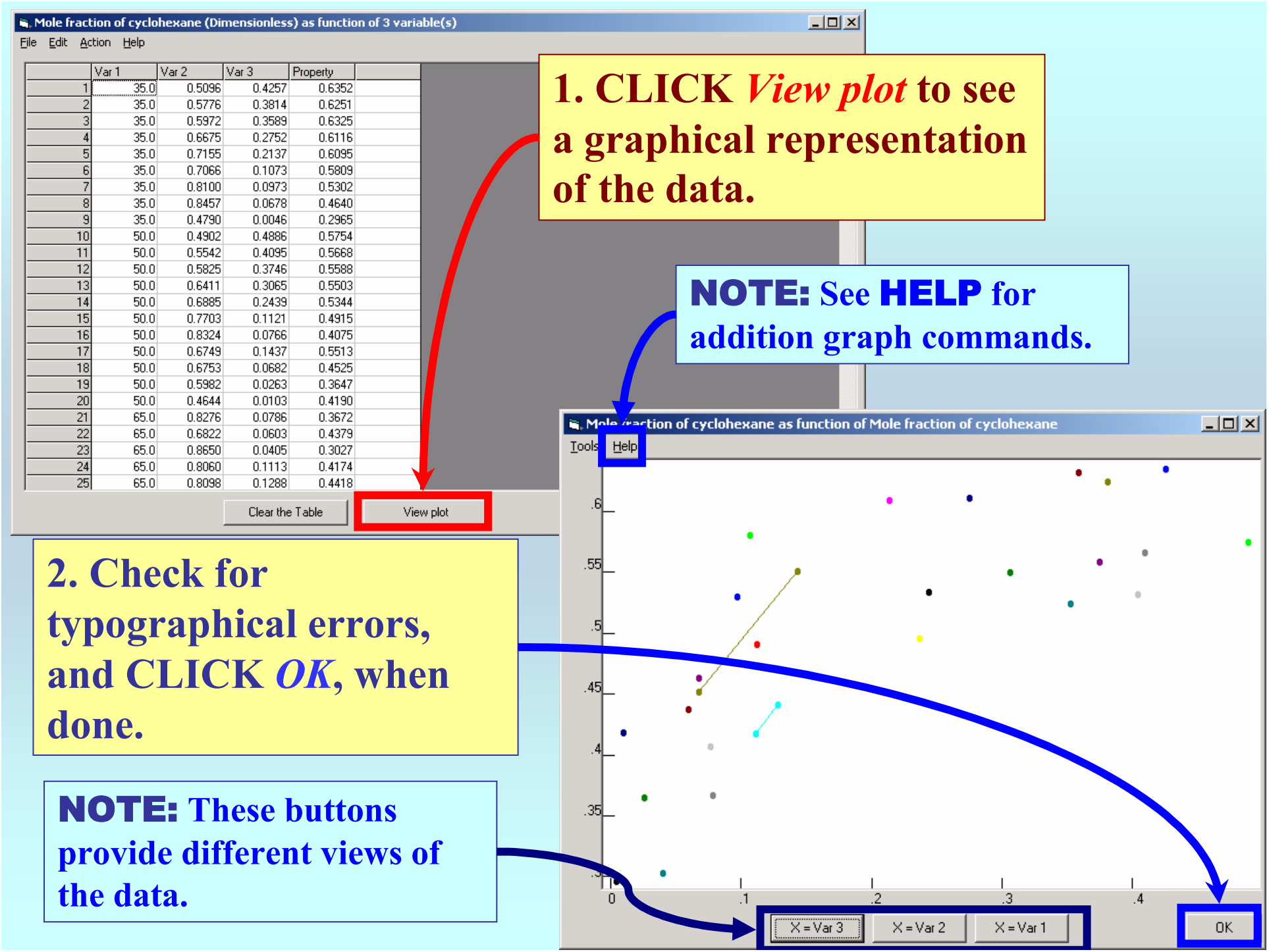
See next page...

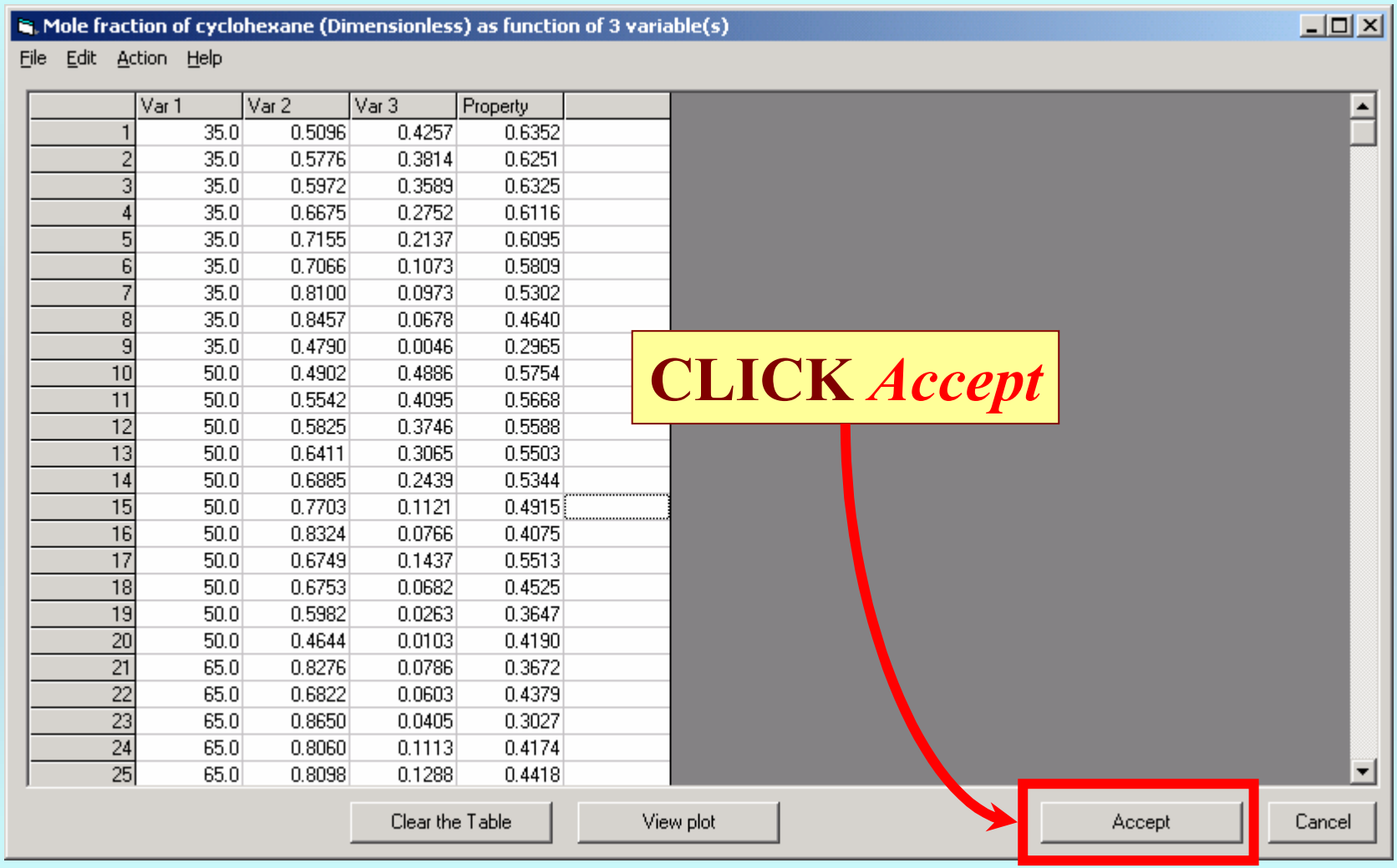
Table 2 VLE data for ethanol(1)–cyclohexane(2)–water(3) system

t/°C	mole fraction in liquid phase x_1	x_2	mole fraction in vapor phase y_1	y_2
35	0.5096	0.4257	0.2948	0.6352
	0.5776	0.3814	0.3269	0.6251
	0.5972	0.3589	0.3201	0.6325
	0.6675	0.2752	0.3381	0.6116
	0.7155	0.2137	0.3369	0.6095
	0.7066	0.1073	0.3213	0.5809
	0.8100	0.0973	0.4101	0.5302
	0.8457	0.0678	0.4795	0.4640
	0.4790	0.0046	0.4651	0.2965
50	0.4902	0.4886	0.3887	0.5754
	0.5542	0.4095	0.3881	0.5668
	0.5825	0.3746	0.3861	0.5588
	0.6411	0.3065	0.3957	0.5503
	0.6885	0.2439	0.4043	0.5344
	0.7703	0.1121	0.4274	0.4915
	0.8324	0.0766	0.5229	0.4075
	0.6749	0.1437	0.3603	0.5513
	0.6753	0.0682	0.4049	0.4525
	0.5982	0.0263	0.4332	0.3647
	0.4644	0.0103	0.3796	0.4190
65	0.8276	0.0786	0.5584	0.3672
	0.6822	0.0603	0.4141	0.4379
	0.8650	0.0405	0.6221	0.3027
	0.8060	0.1113	0.5175	0.4174
	0.8098	0.1288	0.5057	0.4418
	0.7160	0.2370	0.4572	0.4957
	0.6124	0.3523	0.4271	0.5244
	0.5653	0.4041	0.4204	0.5327



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.)


Mole fraction of cyclohexane (Dimensionless) as function of 3 variable(s)
File Edit Action Help
Var 1 Var 2 Var 3 Property
1 35.0 0.5096 0.4257 0.6352
2 35.0 0.5776 0.3814 0.6251
3 35.0 0.5972 0.3589 0.6325
4 35.0 0.6675 0.2752 0.6116
5 35.0 0.7155 0.2137 0.6095
6 35.0 0.7066 0.1073 0.5809
7 35.0 0.8100 0.0973 0.5302
8 35.0 0.8457 0.0678 0.4640
9 35.0 0.4790 0.0046 0.2965
10 50.0 0.4902 0.4886 0.5754
11 50.0 0.5542 0.4095 0.5668
12 50.0 0.5825 0.3746 0.5588
13 50.0 0.6411 0.3065 0.5503
14 50.0 0.6885 0.2439 0.5344
15 50.0 0.7703 0.1121 0.4915
16 50.0 0.8324 0.0766 0.4075
17 50.0 0.6749 0.1437 0.5513
18 50.0 0.6753 0.0682 0.4525
19 50.0 0.5982 0.0263 0.3647
20 50.0 0.4644 0.0103 0.4190
21 65.0 0.8276 0.0786 0.3672
22 65.0 0.6822 0.0603 0.4379
23 65.0 0.8650 0.0405 0.3027
24 65.0 0.8060 0.1113 0.4174
25 65.0 0.8098 0.1288 0.4418
Clear the Table
View plot
1. CLICK View plot to see a graphical representation of the data.
NOTE: See HELP for addition graph commands.
Mole fraction of cyclohexane as function of Mole fraction of cyclohexane
Tools Help
.6
.55
.5
.45
.4
.35
0
.1
.2
.3
.4
X = Var 3
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.


Mole fraction of cyclohexane (Dimensionless) as function of 3 variable(s)
File Edit Action Help
Var 1 Var 2 Var 3 Property
1 35.0 0.5096 0.4257 0.6352
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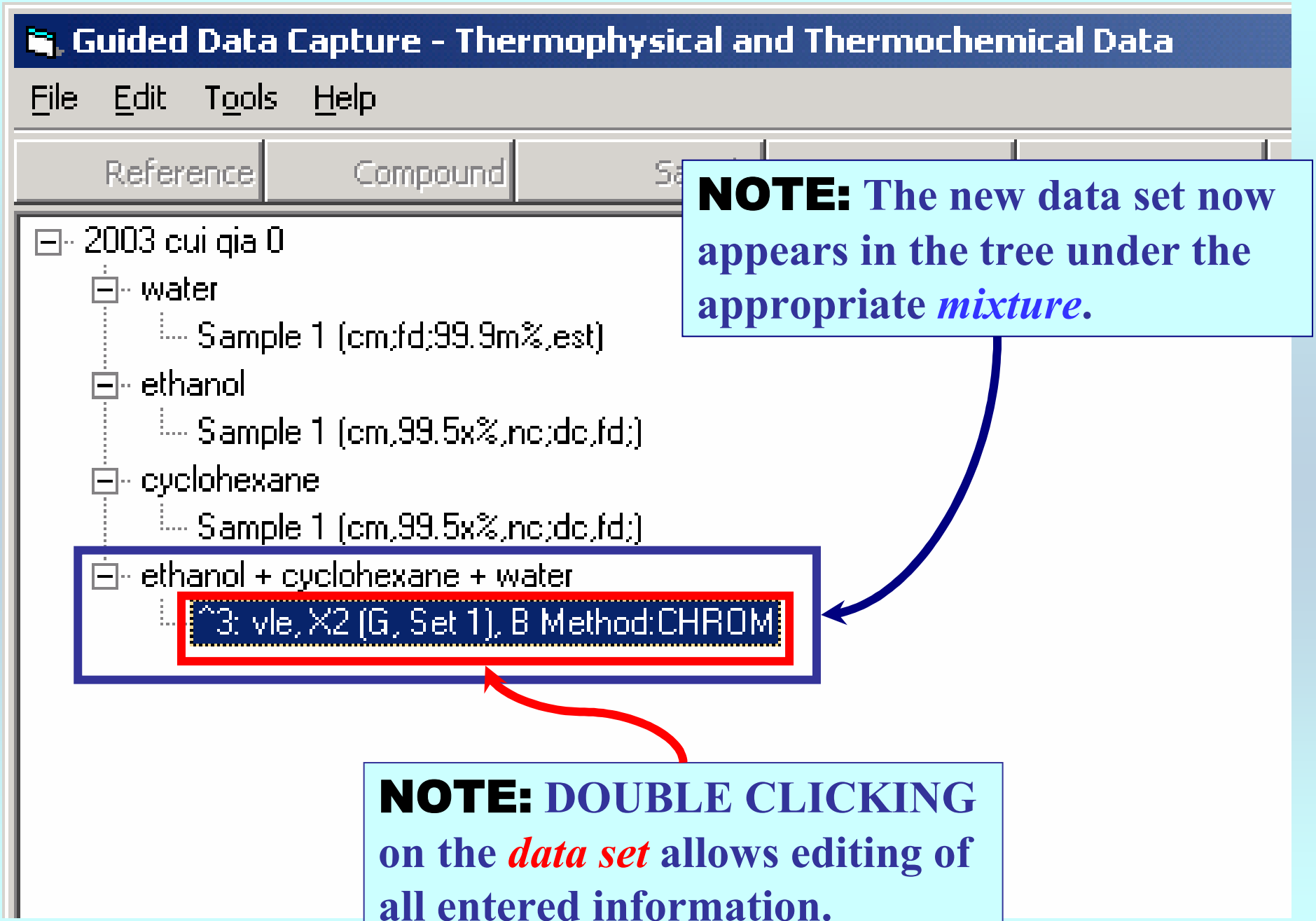
23 65.0 0.8650 0.0405 0.3027
24 65.0 0.8060 0.1113 0.4174
25 65.0 0.8098 0.1288 0.4418
CLICK Accept
Clear the Table
View plot
Accept
Cancel


Guided Data Capture - Thermophysical and Thermochemical Data
File
Edit
Tools
Help
Reference
Compound
2003 cui qia 0
water
Sample 1 (cm;fd;99.9m%,est)
ethanol
Sample 1 (cm,99.5x%,nc;dc,fd;)
cyclohexane
Sample 1 (cm,99.5x%,nc;dc,fd;)
ethanol + cyclohexane + water
^3: vle, X2 (G, Set 1), B Method:CHROM
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.**