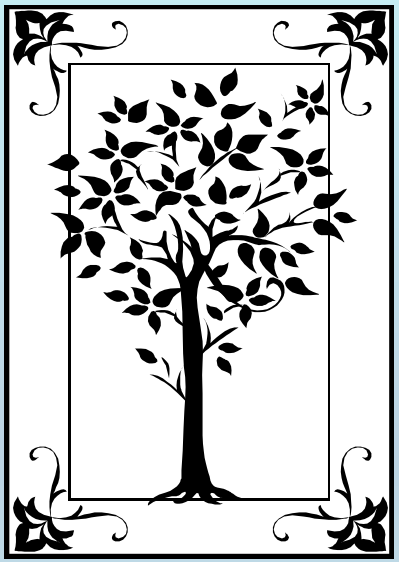
METADATA AND NUMERICAL DATA CAPTURE:
SOLUBILITY
(1 component in 2-component solvent)

Guided Data Capture (GDC)



This tutorial describes
METADATA AND NUMERICAL DATA CAPTURE:
SOLUBILITY
(1 component in 2-component solvent)
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*, 885−887

Solubility of Anthracene in Binary Alcohol + Methyl Acetate Solvent Mixtures at 298.2 K

William E. Acree, Jr.*

Department of Chemistry, University of North Texas, Denton, Texas 76203-5070

Experimental solubilities are reported for anthracene dissolved in eight binary alcohol + methyl acetate solvent mixtures at 25 °C. The alcohol cosolvents studied were 1-propanol, 2-propanol, 1-butanol, 2-butanol, 2-methyl-1-propanol, 1-pentanol, 2-pentanol, and 3-methyl-1-butanol. Results of these measurements are used to test two mathematical representations based upon the combined nearly ideal binary solvent (NIBS)/Redlich−Kister and modified Wilson equations. For the eight systems studied, the combined NIBS/Redlich−Kister equation was found to provide the better mathematical representation of the experimental data, with overall average absolute deviations between measured and calculated values being approximately ±0.5%. Considerably larger deviations were noted in the case of the modified Wilson equation.

SOLUBILITY of 1 component (anthracene) in 1-propanol + methyl acetate

Table 1. Experimental Mole Fraction Solubilities of Anthracene (x_A^{sat}) in Binary Alcohol (B) + Methyl Acetate (C) Solvent Mixtures at 25.0 °C

x_C^o	x_A^{sat}	x_C^o	x_A^{sat}
1-Propanol (B) + Methyl Acetate (C)			
0.0000	0.000 591	0.5952	0.002 74
0.1001	0.000 913	0.7889	0.003 28
0.1904	0.001 230	0.8805	0.003 49
0.3882	0.001 946	1.0000	0.003 64
0.4908	0.002 35		

This data set is considered here.

x_C^o refer to the initial mole fraction composition of the binary solvent calculated as if solute (A) were not present,

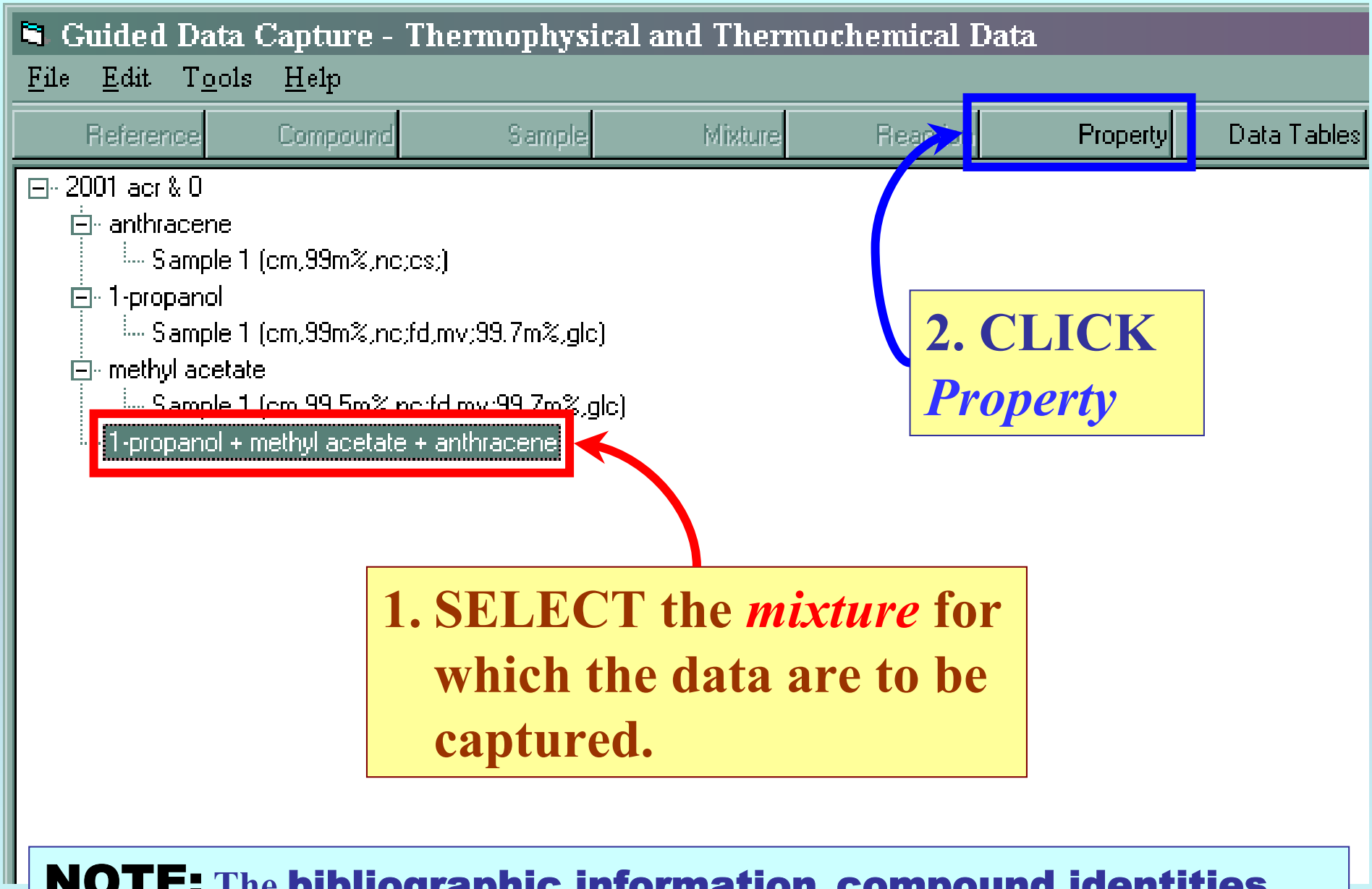
NOTE: This is important in the example.

Experimental Method & Precision Estimates:

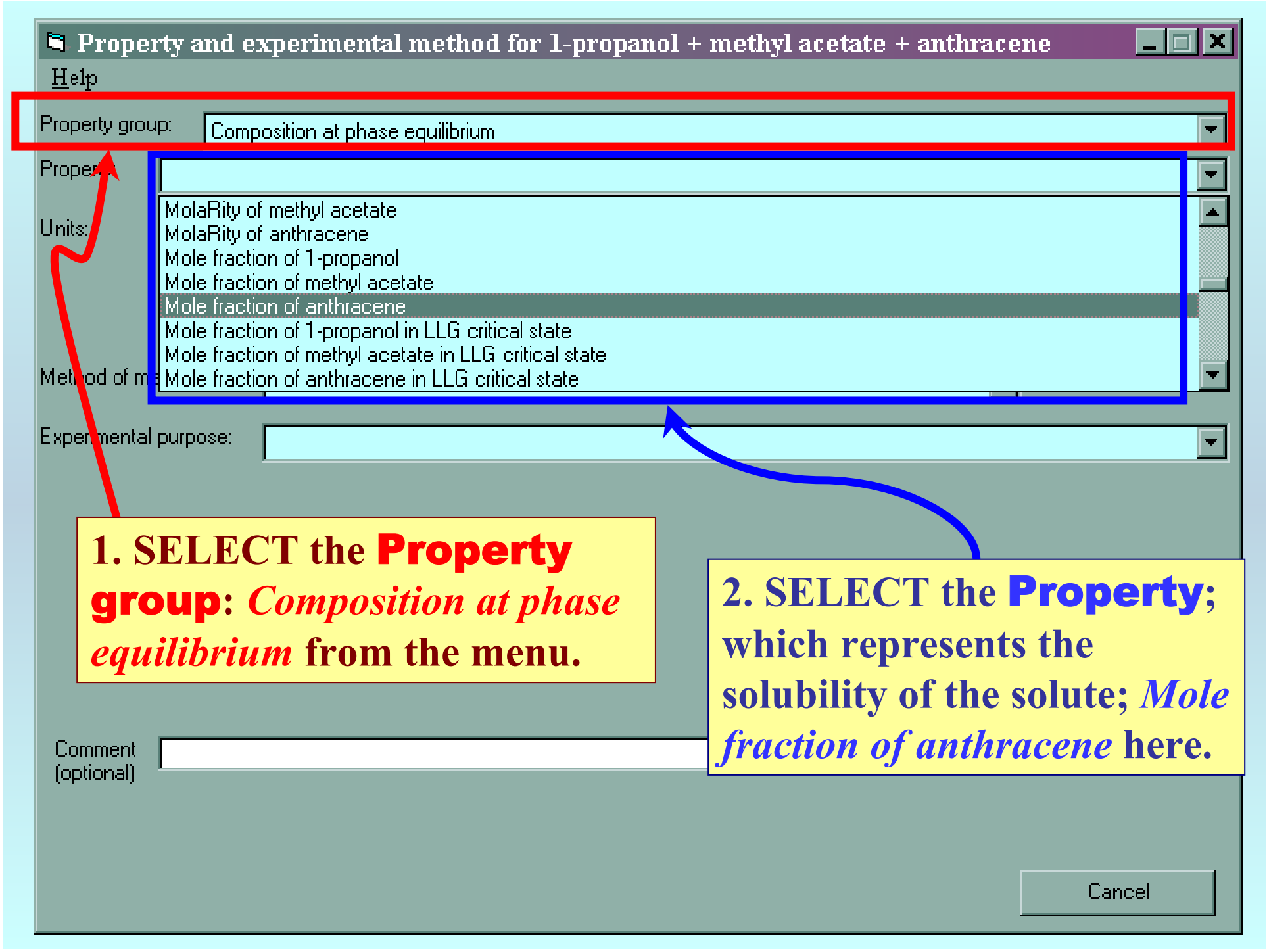
Concentrations of the dilute solutions were determined from a Beer–Lambert law absorbance versus concentration working curve derived from measured absorbances of standard solutions of known molar concentrations.

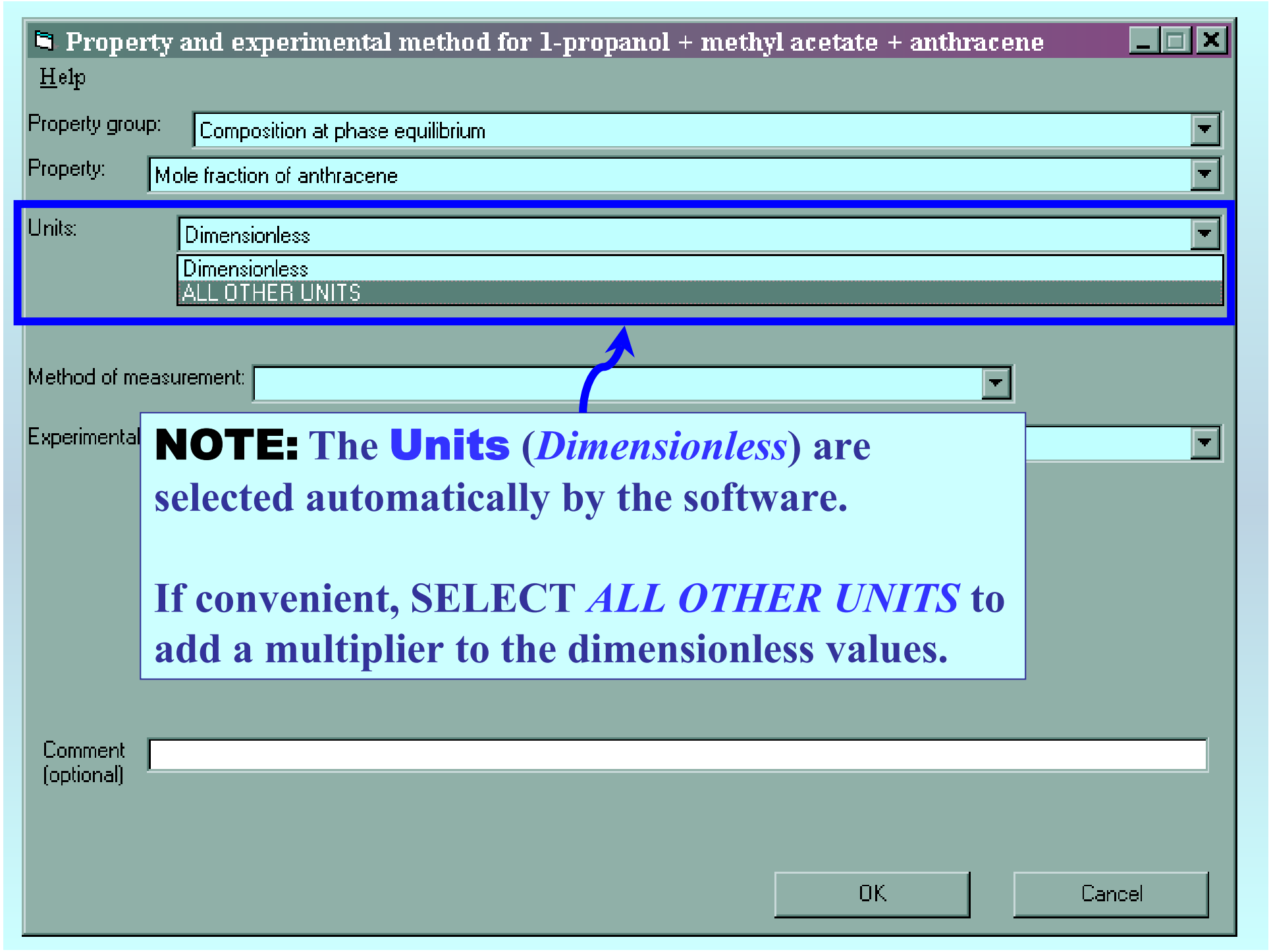
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate in a constant temperature water bath at (25.0 ± 0.1) °C with periodic agitation

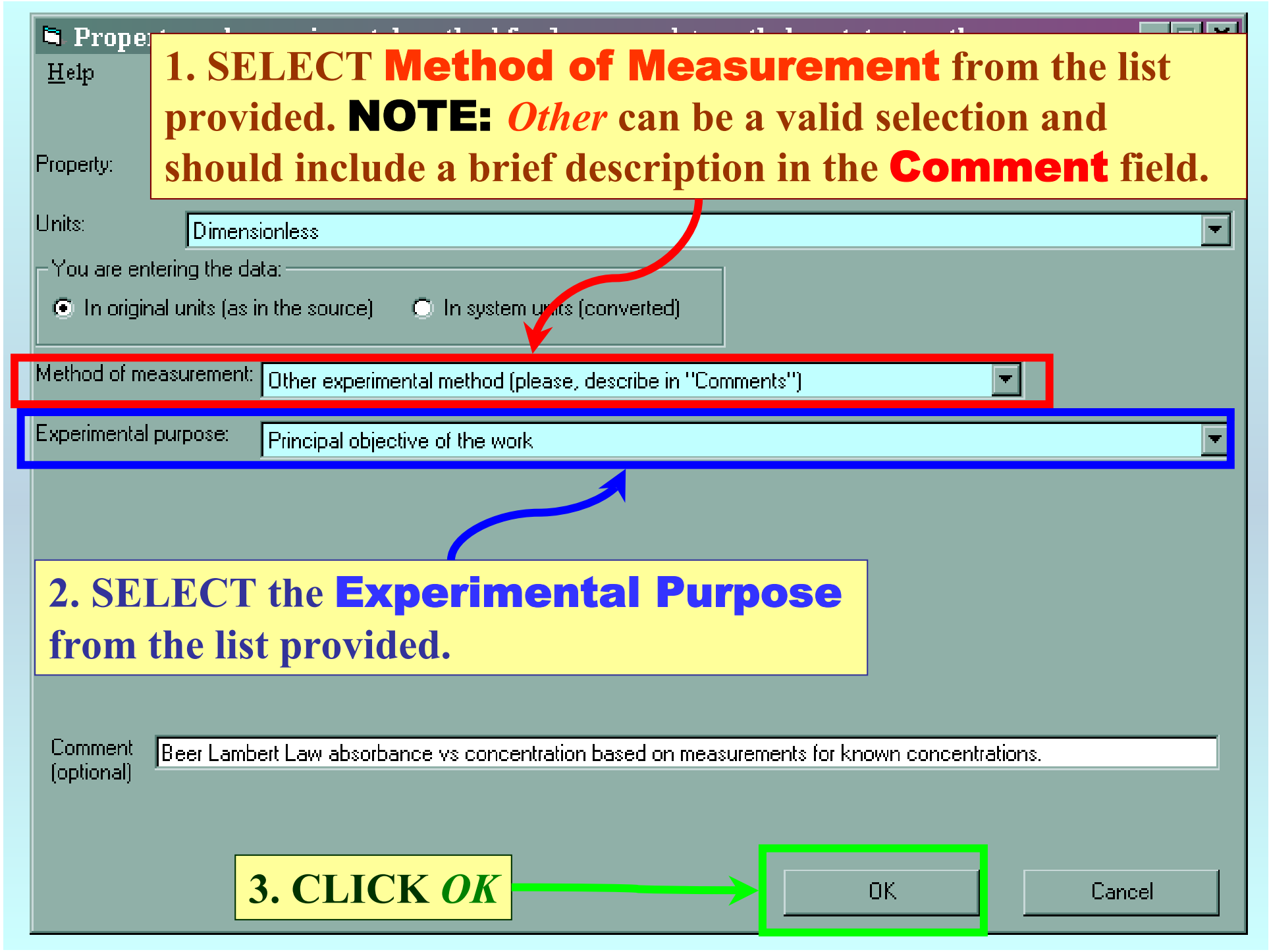
Numerical values represent the average of between four and eight independent determinations, with the measured values being reproducible to within ±1.0%.



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 1-propanol + methyl acetate + anthracene
Help
Property group:
Composition at phase equilibrium
Property:
Units:
MolaRity of methyl acetate
MolaRity of anthracene
Mole fraction of 1-propanol
Mole fraction of methyl acetate
Mole fraction of anthracene
Mole fraction of 1-propanol in LLG critical state
Mole fraction of methyl acetate in LLG critical state
Mole fraction of anthracene in LLG critical state
Method of m
Experimental purpose:
1. SELECT the Property group: Composition at phase equilibrium from the menu.
2. SELECT the Property; which represents the solubility of the solute; Mole fraction of anthracene here.
Comment (optional)
Cancel


Property and experimental method for 1-propanol + methyl acetate + anthracene
Help
Property group:
Composition at phase equilibrium
Property:
Mole fraction of anthracene
Units:
Dimensionless
Dimensionless
ALL OTHER UNITS
Method of measurement:
Experimental
NOTE: The Units (Dimensionless) are selected automatically by the software.
If convenient, SELECT ALL OTHER UNITS to add a multiplier to the dimensionless values.
Comment (optional)
OK
Cancel

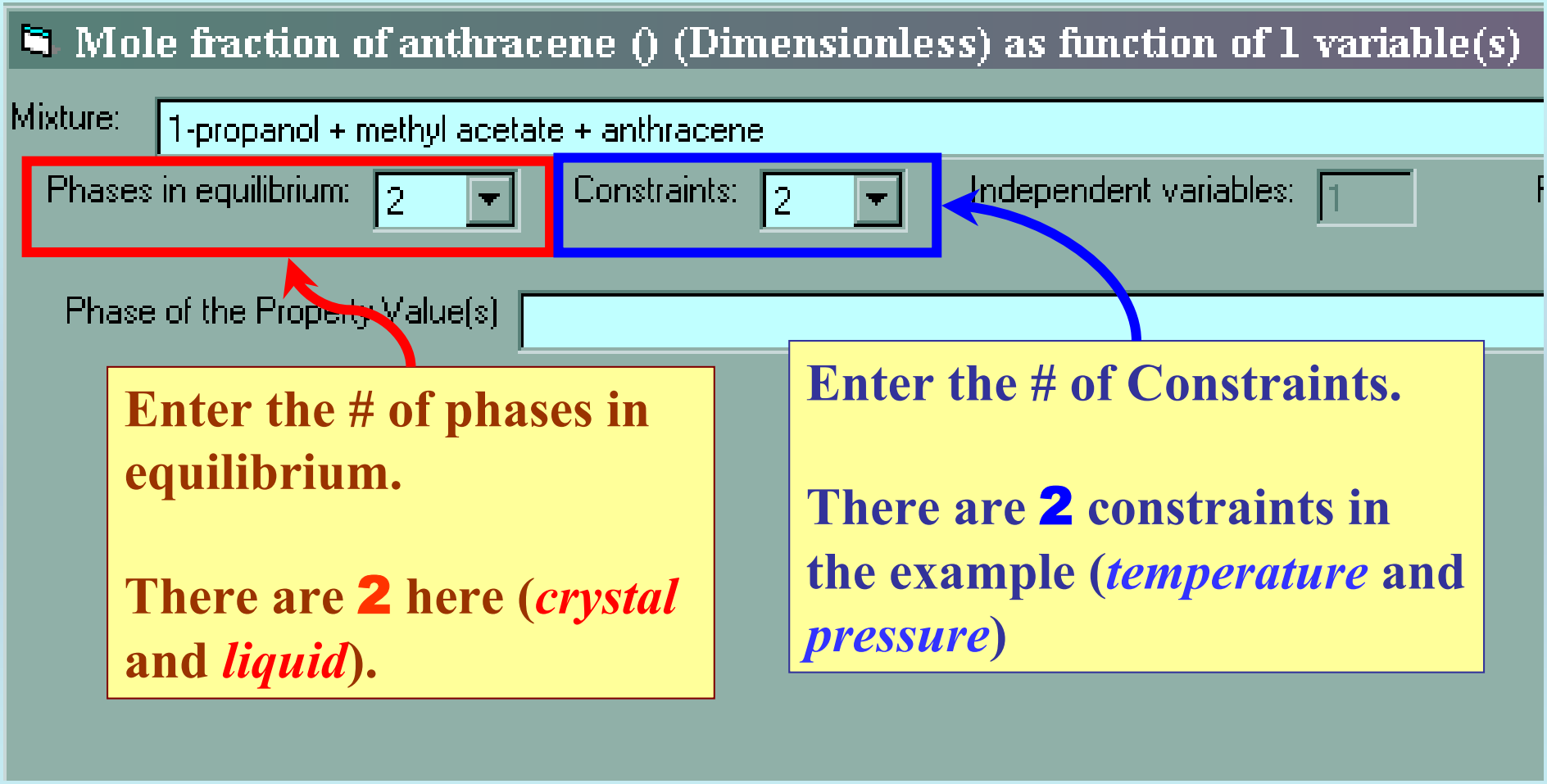


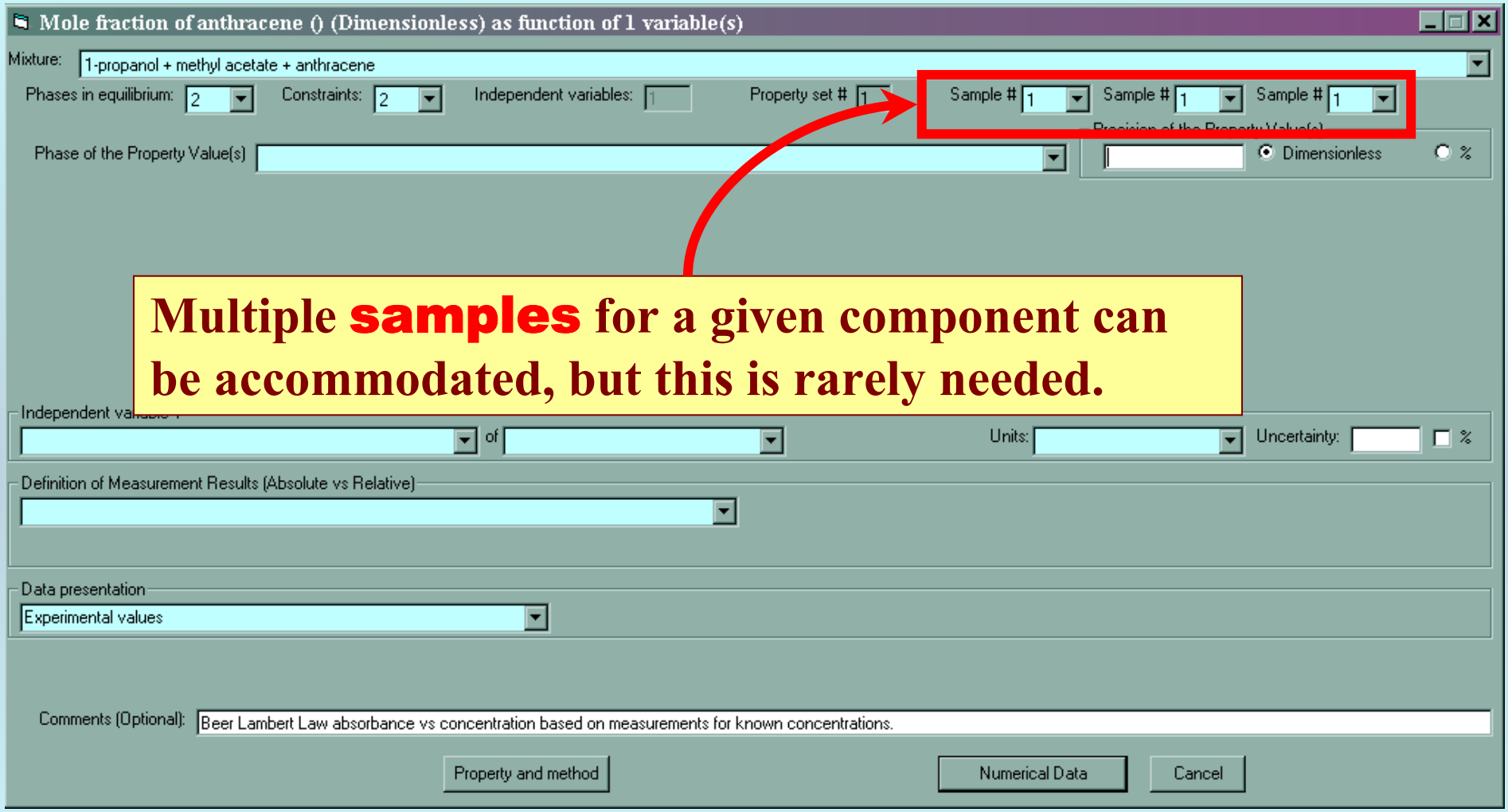
1. SELECT **Method of Measurement** from the list provided. **NOTE:** *Other* can be a valid selection and should include a brief description in the **Comment** field.

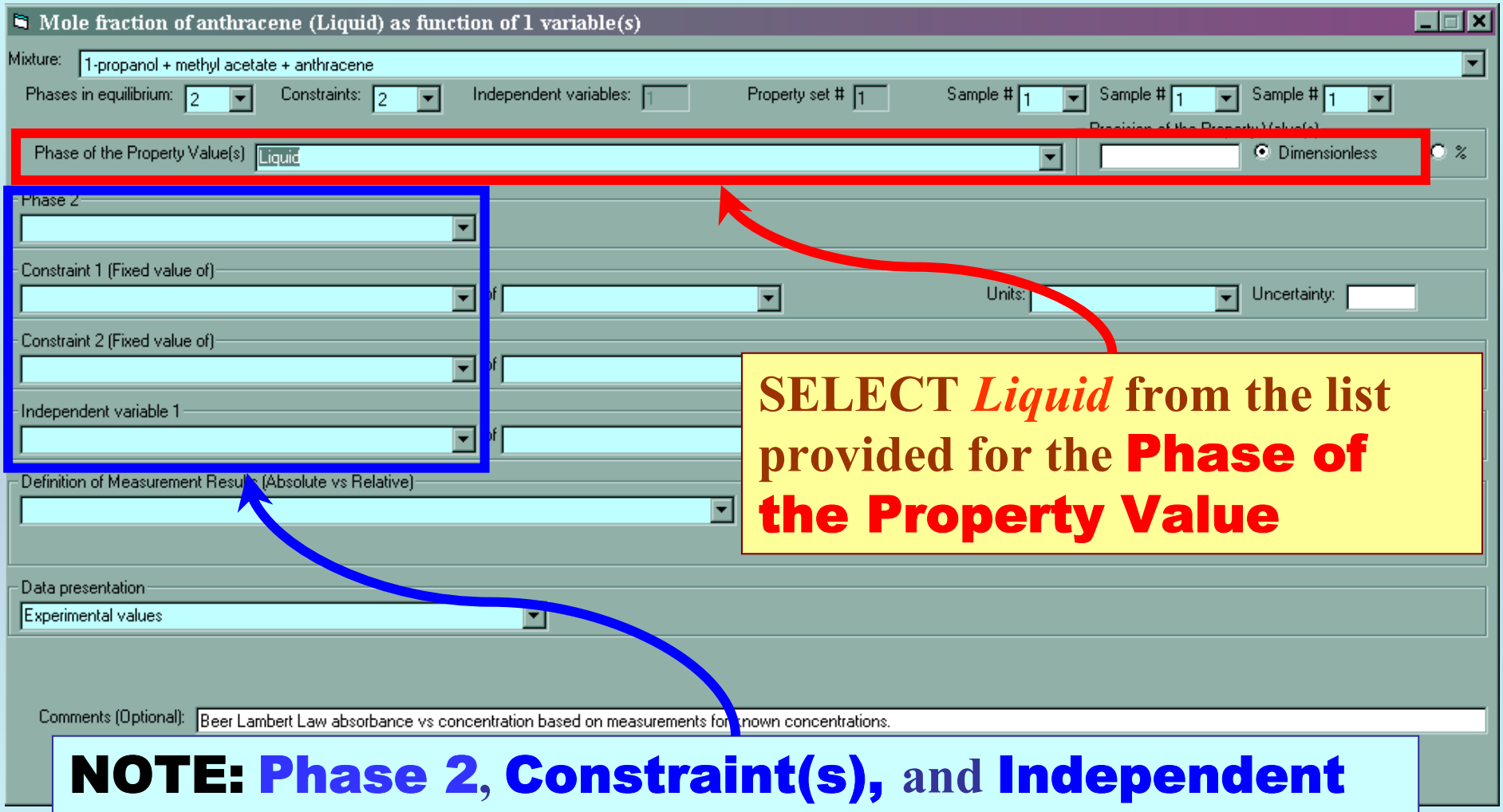
2. SELECT the **Experimental Purpose** from the list provided.

3. CLICK *OK*

SELECTION of # of Phases in Equilibrium and # of Constraints




Mole fraction of anthracene () (Dimensionless) as function of 1 variable(s)
Mixture:
1-propanol + methyl acetate + anthracene
Phases in equilibrium:
2
Constraints:
2
Independent variables:
1
Property set #
1
Sample #
1
Sample #
1
Sample #
1
Phase of the Property Value(s)
Dimensionless
%
Multiple samples for a given component can be accommodated, but this is rarely needed.
of
Units:
Uncertainty:
%
Definition of Measurement Results (Absolute vs Relative)
Data presentation
Experimental values
Comments (Optional):
Beer Lambert Law absorbance vs concentration based on measurements for known concentrations.
Property and method
Numerical Data
Cancel

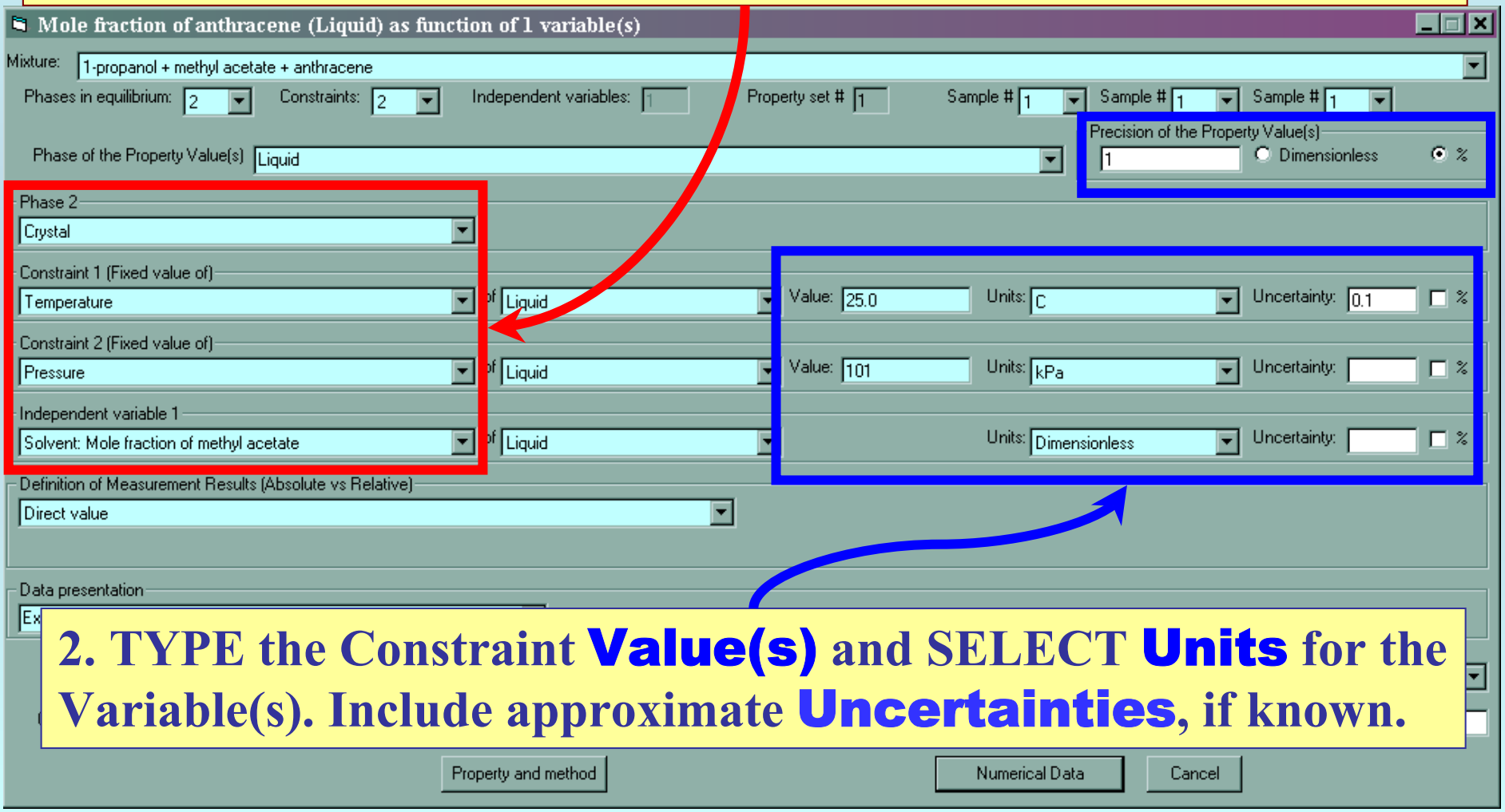


SELECT *Liquid* from the list provided for the Phase of the Property Value

NOTE: Phase 2, Constraint(s), and Independent Variable field(s) appear automatically based on the previous entries and the *Gibbs Phase Rule*.

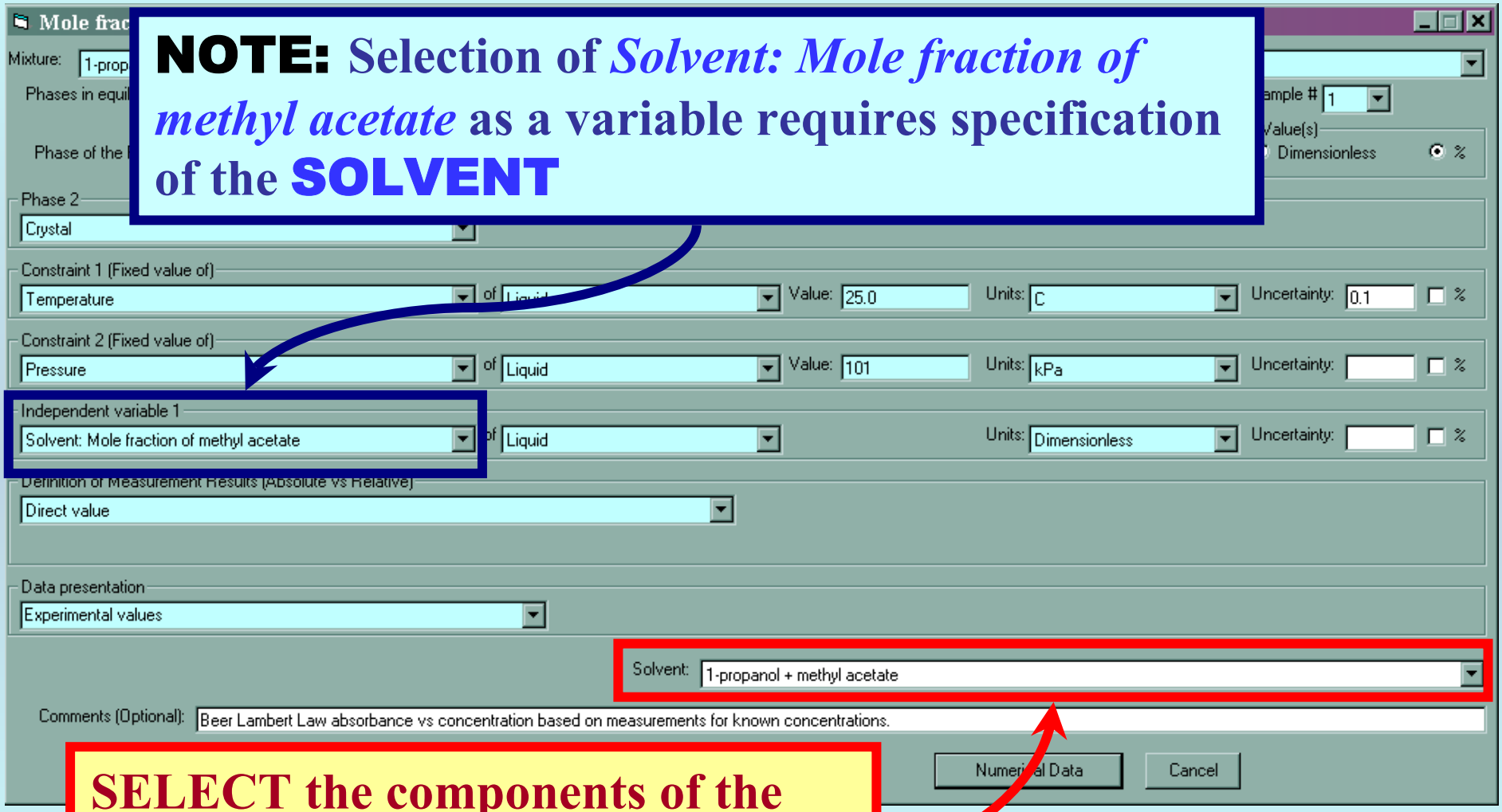
Specification of constraints, constraint values, and constraint units

1. SELECT the Constraints (*T and p here*), Phase 2 (*Crystal* here) and the Independent Variable (*Solvent: Mole fraction of methyl acetate*) from the lists.



2. TYPE the Constraint Value(s) and SELECT Units for the Variable(s). Include approximate Uncertainties, if known.

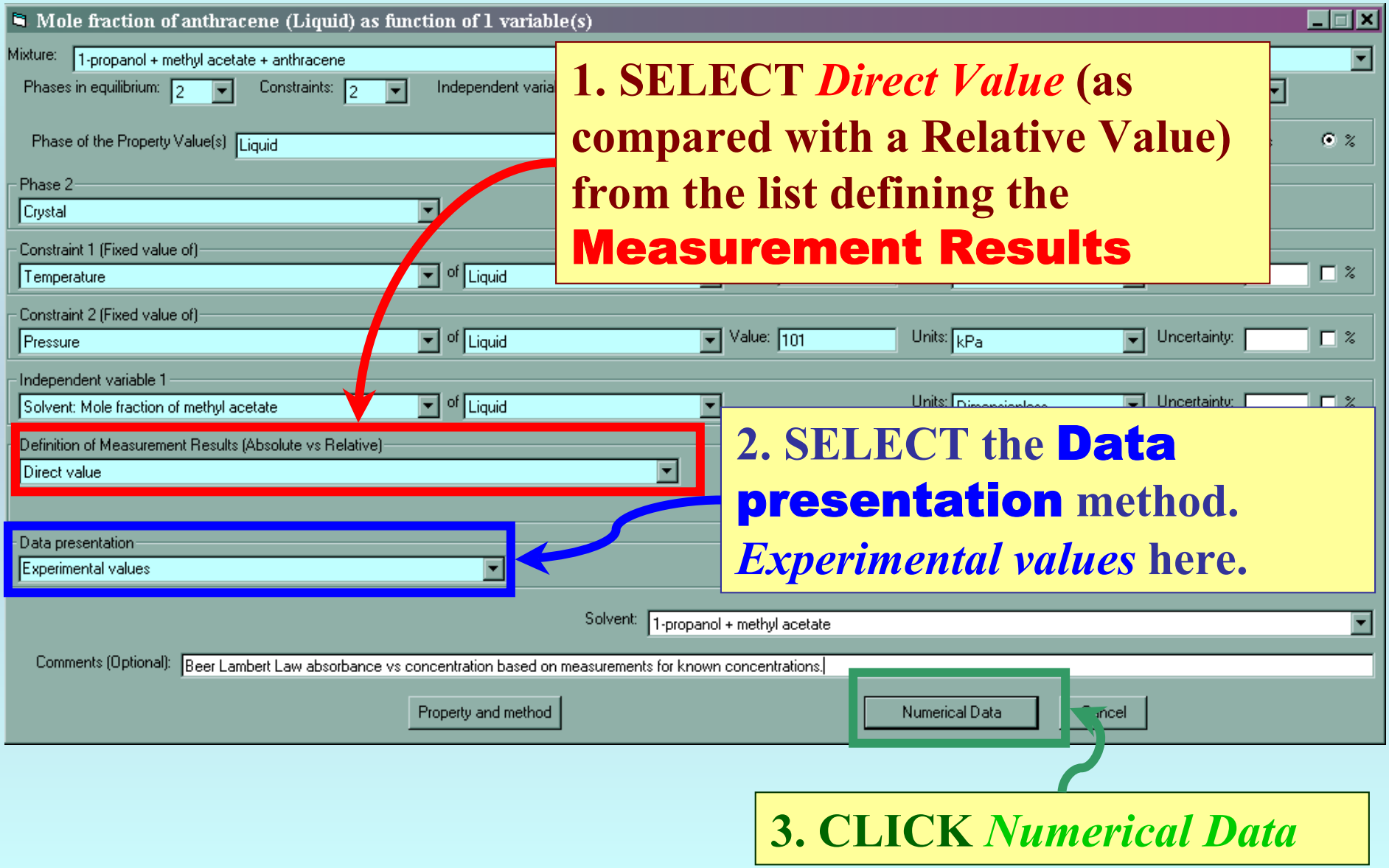
Solvent specification (if needed)

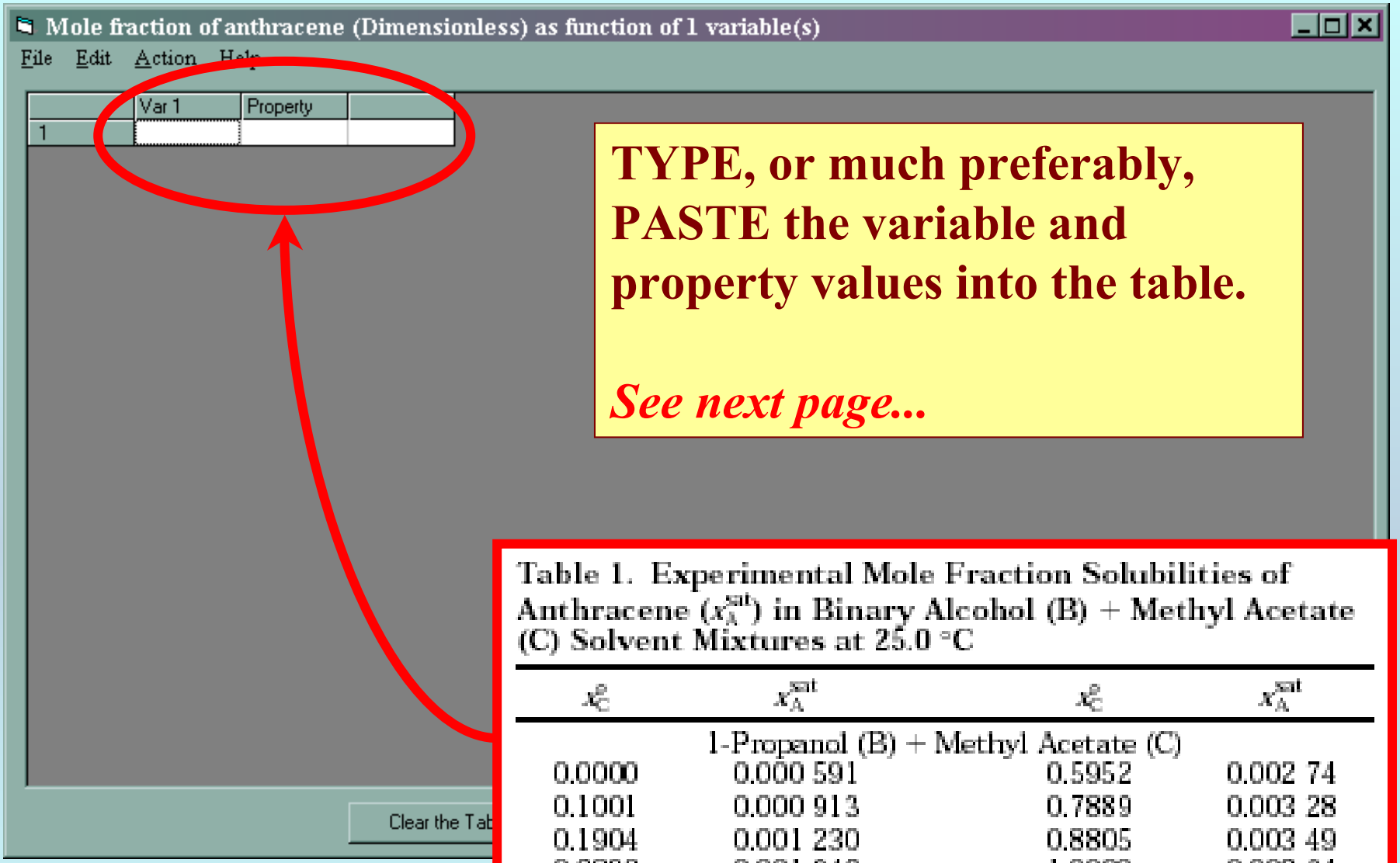


NOTE: Selection of ***Solvent: Mole fraction of methyl acetate*** as a variable requires specification of the **SOLVENT**

SELECT the components of the SOLVENT (*1-propanol + methyl acetate*, here) from the list

Measurement definition and Data presentation





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

See next page...

Table 1. Experimental Mole Fraction Solubilities of Anthracene (x_A^{sat}) in Binary Alcohol (B) + Methyl Acetate (C) Solvent Mixtures at 25.0 °C

x_C^0	x_A^{sat}	x_C^0	x_A^{sat}
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0.1001	0.000 913	0.7889	0.003 28
0.1904	0.001 230	0.8805	0.003 49
0.3882	0.001 946	1.0000	0.003 64
0.4908	0.002 35		

Mole fraction of anthracene (Dimensionless) as function of 1 variable(s)

File Edit Action Help

	Var 1	Property
1	0.0000	0.000591
2	0.1001	0.000913
3	0.1904	0.001230
4	0.3882	0.001946
5	0.4908	0.00235
6	0.5952	0.00274
7	0.7889	0.00328
8	0.8805	0.00349
9	1.0000	0.00364

Clear the Table

Table 1. Experimental Mole Fraction Solubilities of Anthracene (x_A^{sat}) in Binary Alcohol (B) + Methyl Acetate (C) Solvent Mixtures at 25.0 °C

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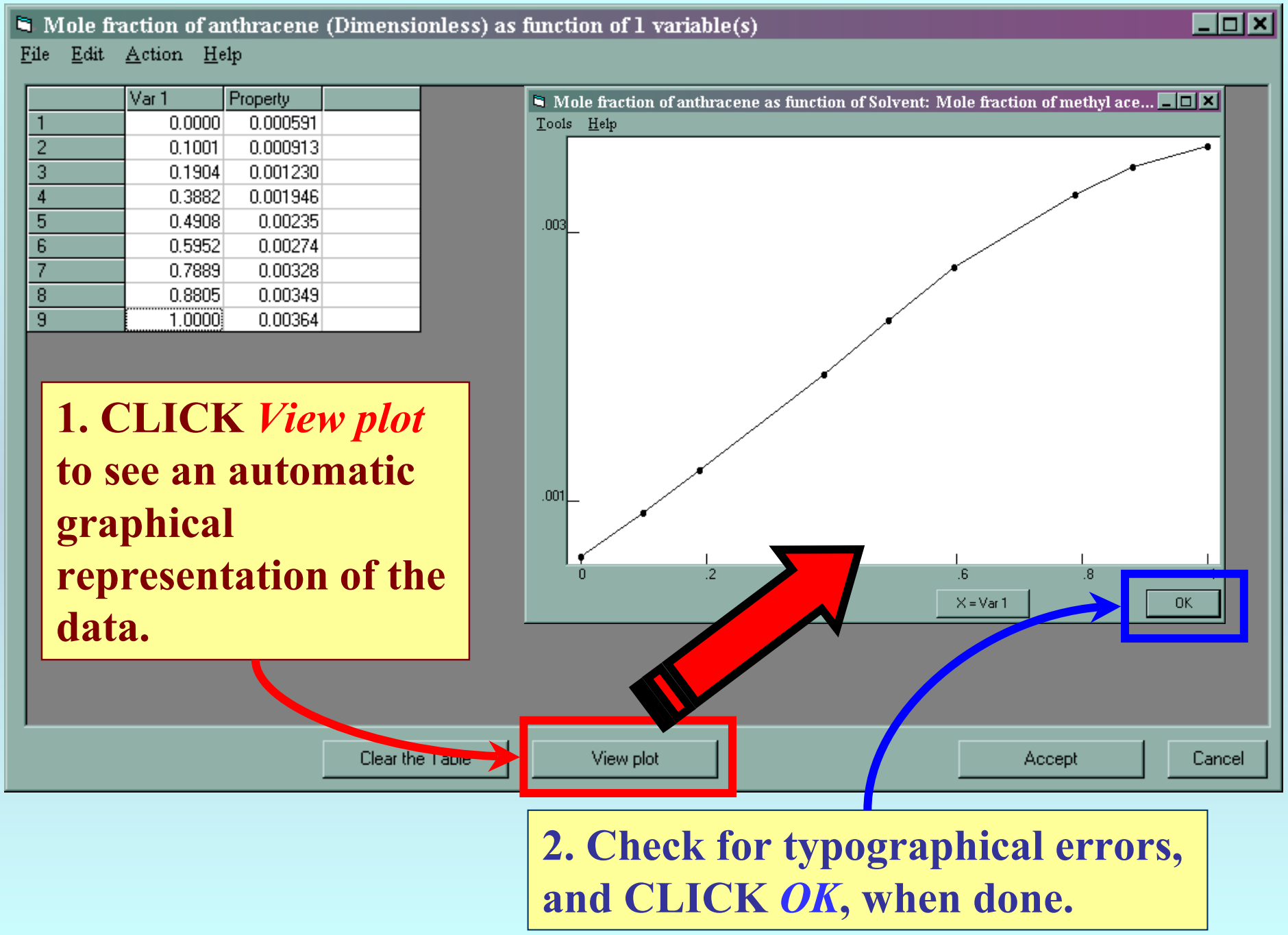
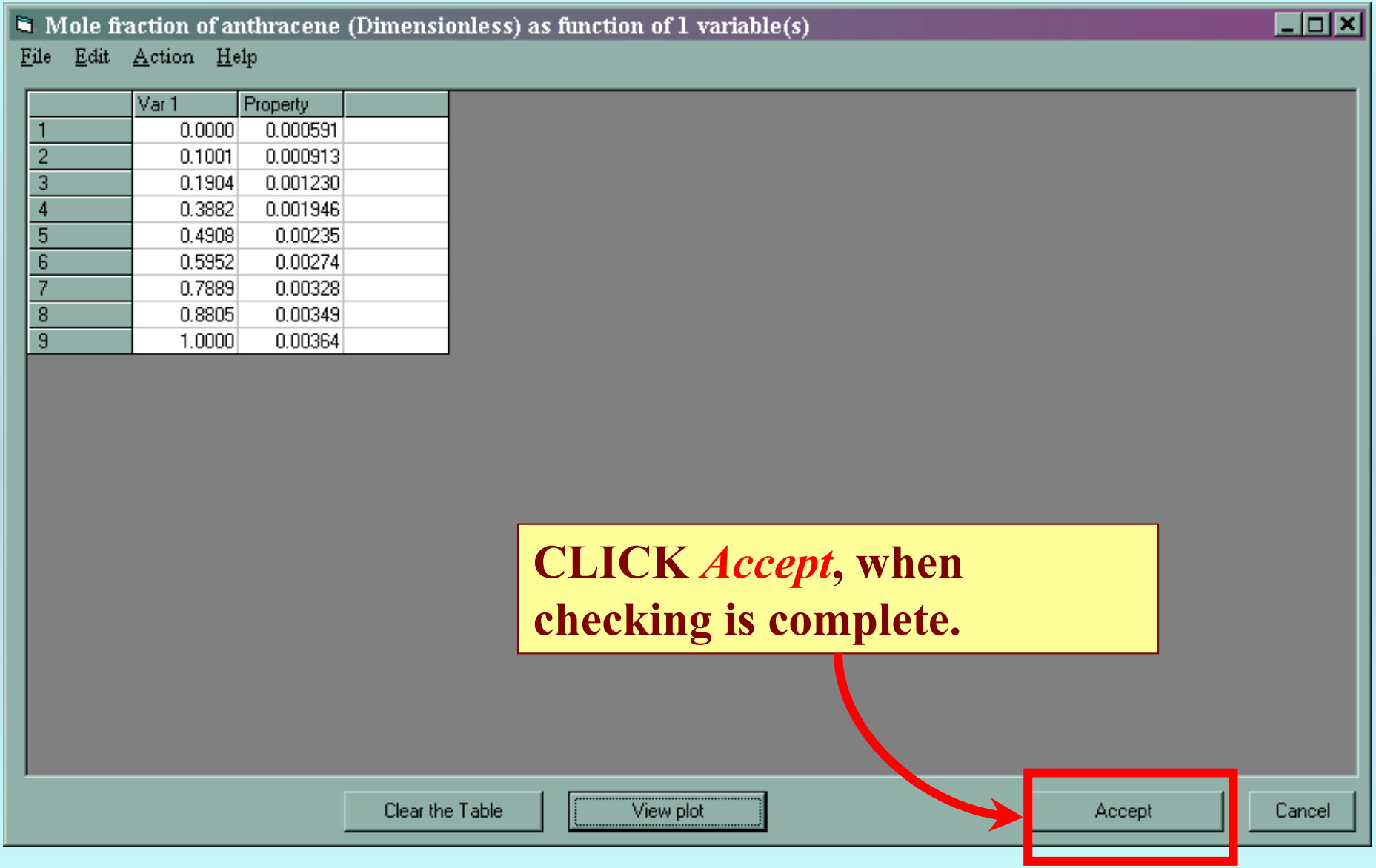
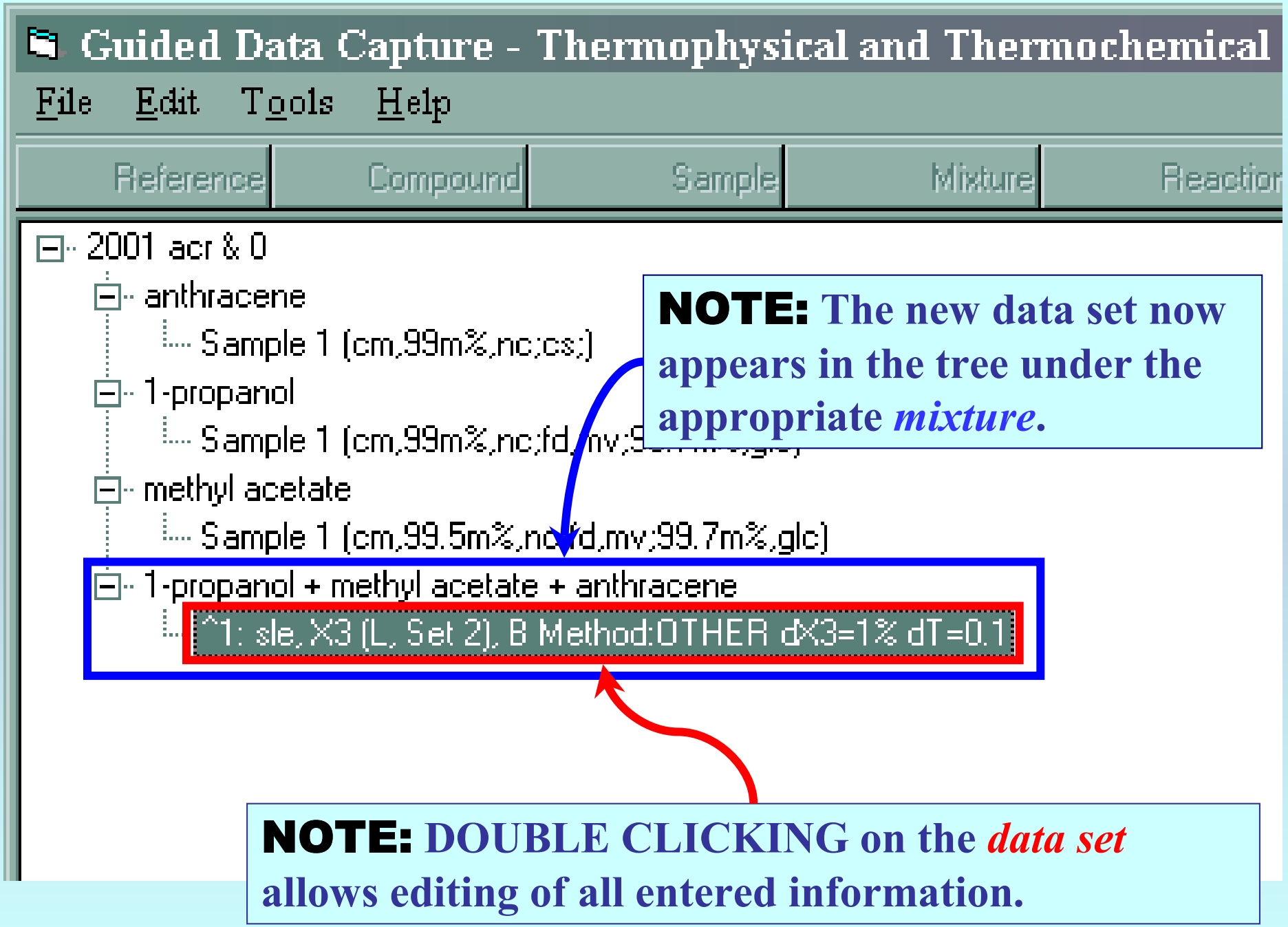
0.3882	0.001 946	1.0000	0.003 64
0.4908	0.002 35		

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 anthracene (Dimensionless) as function of 1 variable(s)
File Edit Action Help
Var 1 Property
1 0.0000 0.000591
2 0.1001 0.000913
3 0.1904 0.001230
4 0.3882 0.001946
5 0.4908 0.00235
6 0.5952 0.00274
7 0.7889 0.00328
8 0.8805 0.00349
9 1.0000 0.00364
Mole fraction of anthracene as function of Solvent: Mole fraction of methyl ace...
Tools Help
.003
.001
0
.2
.6
.8
X = Var 1
OK
1. CLICK View plot to see an automatic graphical representation of the data.
Clear the Table
View plot
Accept
Cancel
2. Check for typographical errors, and CLICK OK, when done.


Mole fraction of anthracene (Dimensionless) as function of 1 variable(s)
File Edit Action Help
Var 1 Property
1 0.0000 0.000591
2 0.1001 0.000913
3 0.1904 0.001230
4 0.3882 0.001946
5 0.4908 0.00235
6 0.5952 0.00274
7 0.7889 0.00328
8 0.8805 0.00349
9 1.0000 0.00364
CLICK Accept, when checking is complete.
Clear the Table
View plot
Accept
Cancel


Guided Data Capture - Thermophysical and Thermochemical
File Edit Tools Help
Reference Compound Sample Mixture Reaction
2001 acr & 0
anthracene
Sample 1 (cm,99m%,nc;cs;)
1-propanol
Sample 1 (cm,99m%,nc;fd,mv;
methyl acetate
Sample 1 (cm,99.5m%,nc;fd,mv;99.7m%,glc)
1-propanol + methyl acetate + anthracene
^1: sle, X3 (L, Set 2), B Method:OTHER dX3=1% dT=0.1
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.**