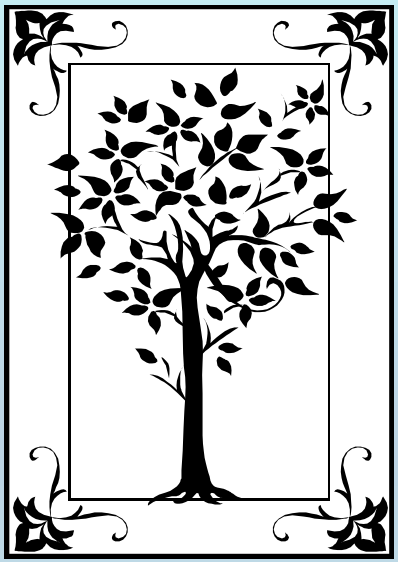
METADATA AND NUMERICAL DATA CAPTURE:
Solid-Liquid Equilibrium Temperatures
(2 components)

Guided Data Capture (GDC)



This tutorial describes
METADATA AND NUMERICAL DATA CAPTURE:
Solid-Liquid Equilibrium Temperatures
(2 components)
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*, 1190−1192

Binary Solid−Liquid Equilibria of *N*,*N*-Dimethylacetamide with 1,2-Dichloroethane, Dichloromethane, and 1-Propanol

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Solid−liquid phase equilibria (SLE) of binary mixtures of *N*,*N*-dimethylacetamide with 1,2-dichloroethane, dichloromethane, and 1-propanol were measured using the visual method at atmospheric pressure. The system *N*,*N*-dimethylacetamide was correlated by the NRTL equation. While the phase diagram $(T, x)_P$ of *N*,*N*-dimethylacetamide with 1-propanol is well represented by modified UNIFAC (Dortmund) assuming eutectic behavior, *N*,*N*-dimethylacetamide with dichloromethane forms a distinct compound with a melting point at equimolar composition.

SLE of a 2-component system
N,N-dimethylacetamide + 1,2-dichloroethane

Table 2. Solid–Liquid Equilibria of *N,N*-Dimethylacetamide + 1,2-Dichloroethane, + Dichloromethane, + 1-Propanol

$H_3CCON(CH_3)_2$ (1) + 1,2-$C_2H_4Cl_2$ (2)		$H_3CCON(CH_3)_2$ (1) + CH_2Cl_2 (2)		$H_3CCON(CH_3)_2$ (1) + 1-C_3H_7OH (2)	
x_1^L	T/K	x_1^L	T/K	x_1^L	T/K
0.0000	237.67				
0.0528	234.73				
0.1207	230.25				
0.1499	227.97				
0.2090	222.80				
0.2557	218.48				
0.3067	212.71				
0.3478	207.64				
0.3986	200.92				
0.4486	202.85				
0.5010	210.64				
0.5462	215.91				
0.5964	221.74				
0.6462	226.62				
0.6980	231.50				
0.7483	235.72				
0.7887	238.80				
0.8451	242.91				
0.8962	246.11				
0.9397	248.44	0.9513	248.92		
1.0000	251.41	1.0000	251.40		

This data set is considered here.
The solid phase is *1,2-dichloroethane.*

NOTE 1: If multiple crystalline phases are present, data for *each phase* are captured separately.

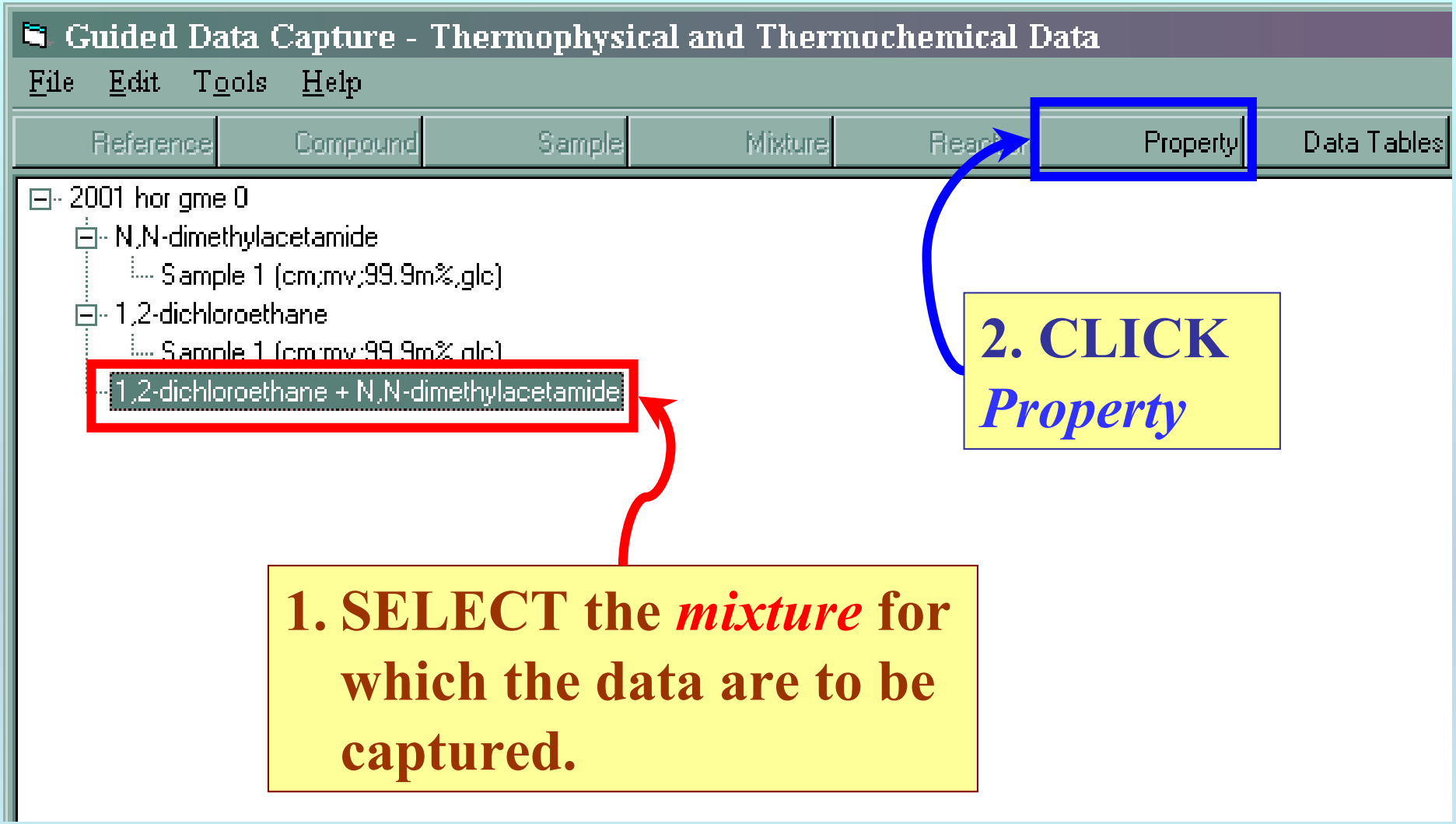
NOTE 2: Stable phases are numbered cr(I), cr(II), etc., with cr(I) nearest the melting temperature.

NOTE: These data are captured as a second data set because the solid phase is *N,N-dimethylacetamide*

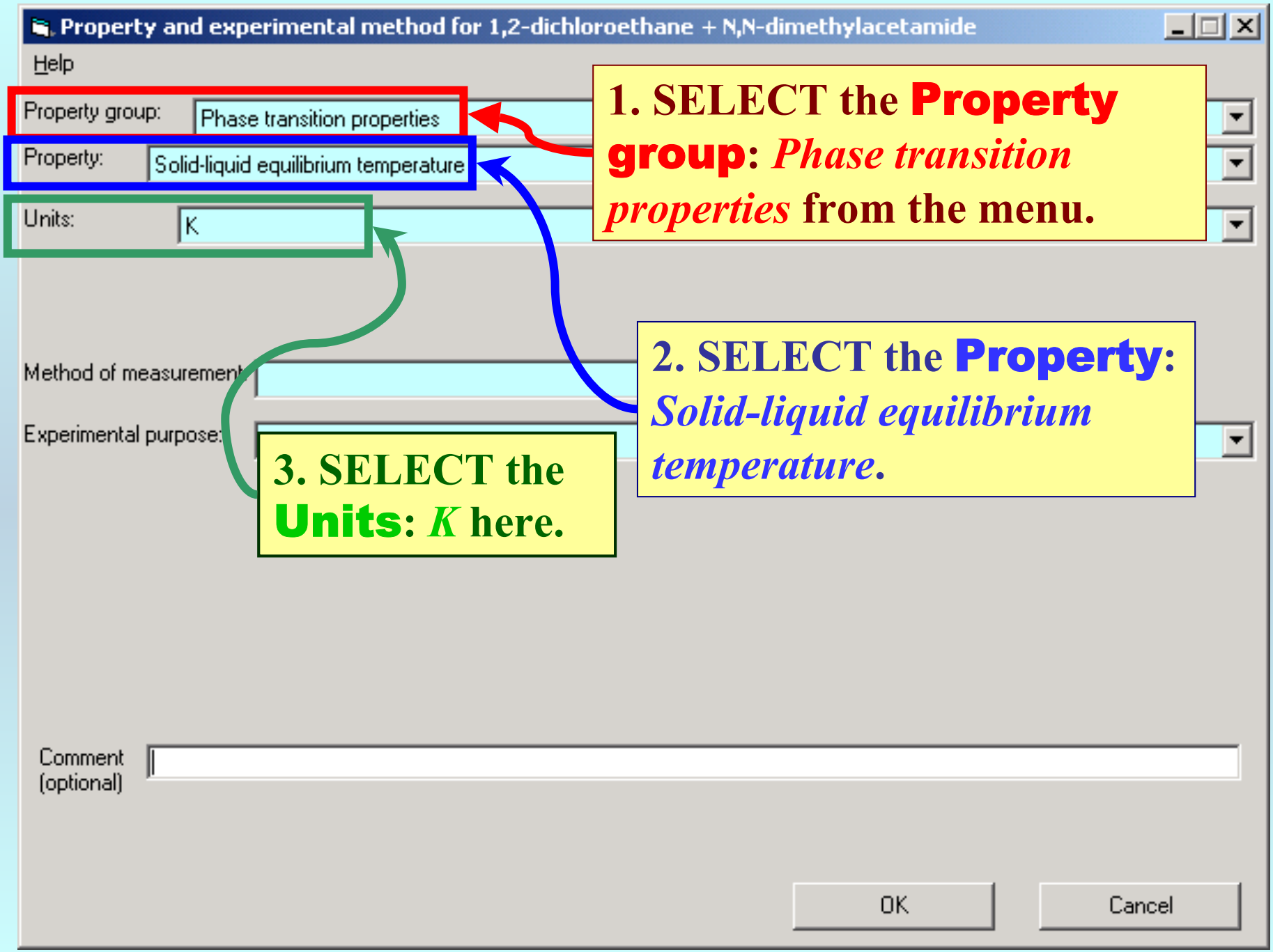
Experimental Method & Uncertainty Estimates:

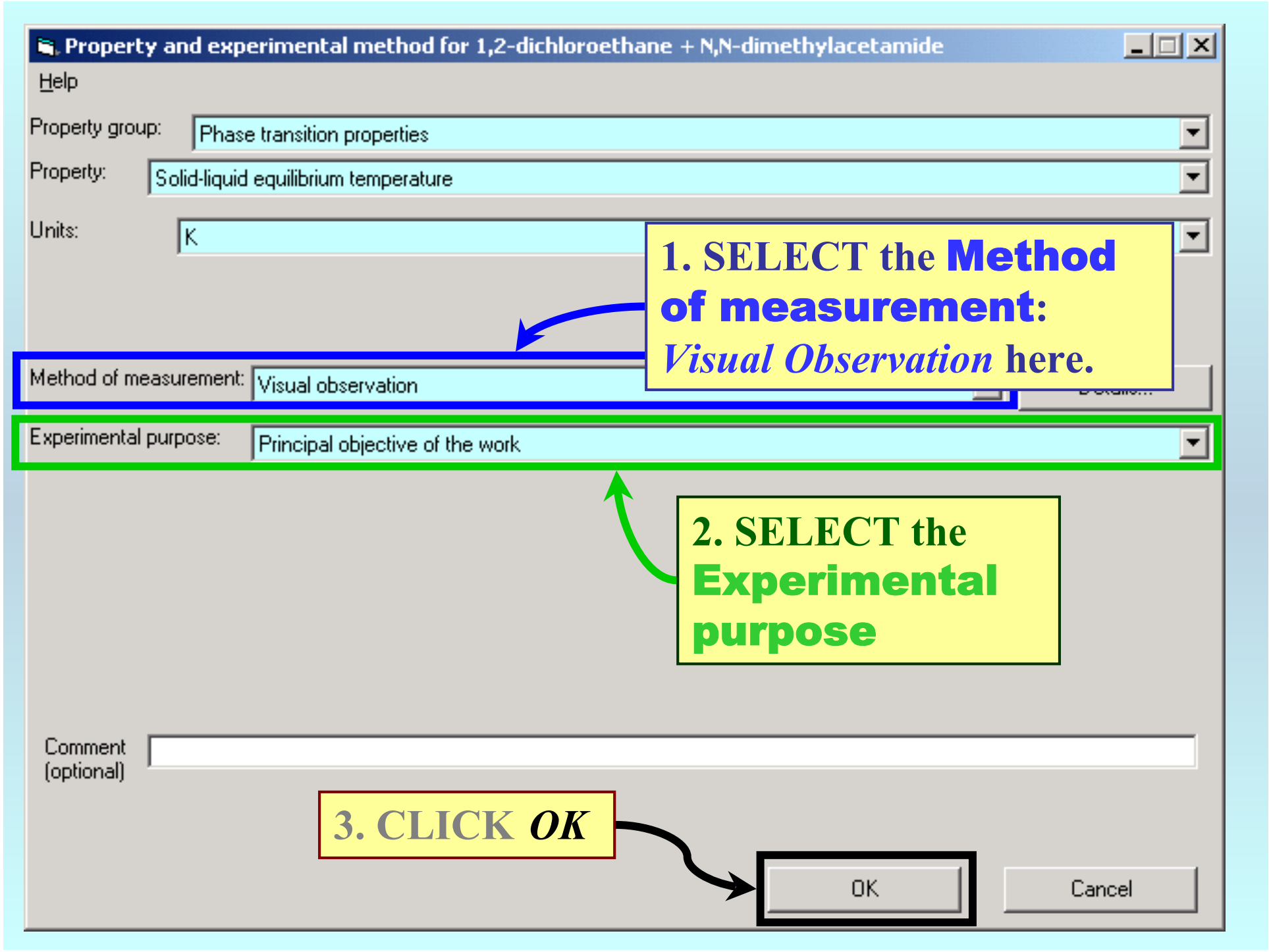
The solid–liquid equilibrium measurements of the pure components and all binary mixtures were performed visually by a static apparatus, which has been described in detail previously.[5,6]

The accuracy of the melting temperature was determined to be ±0.015 K; the accuracy of the composition is ±0.0001.

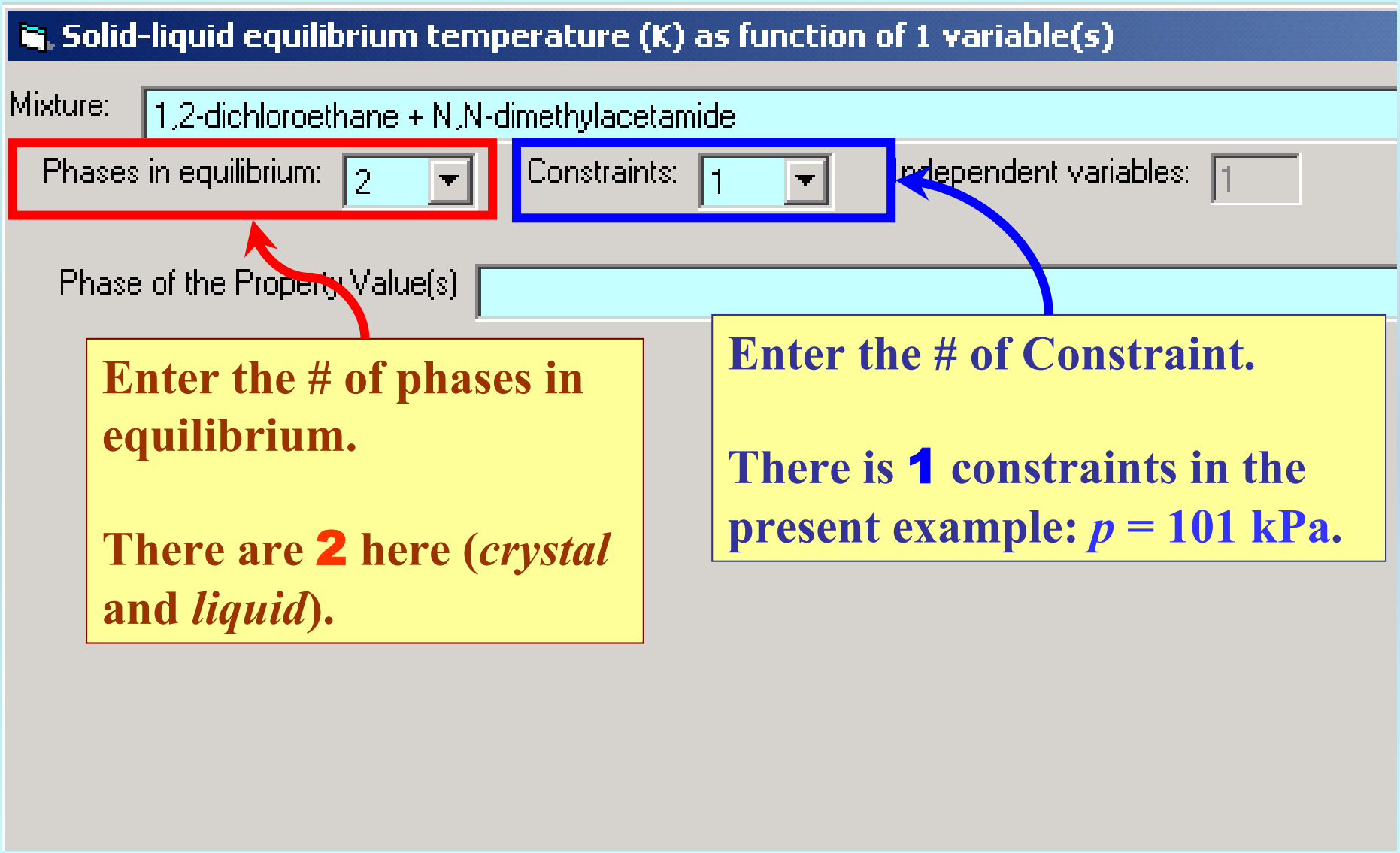


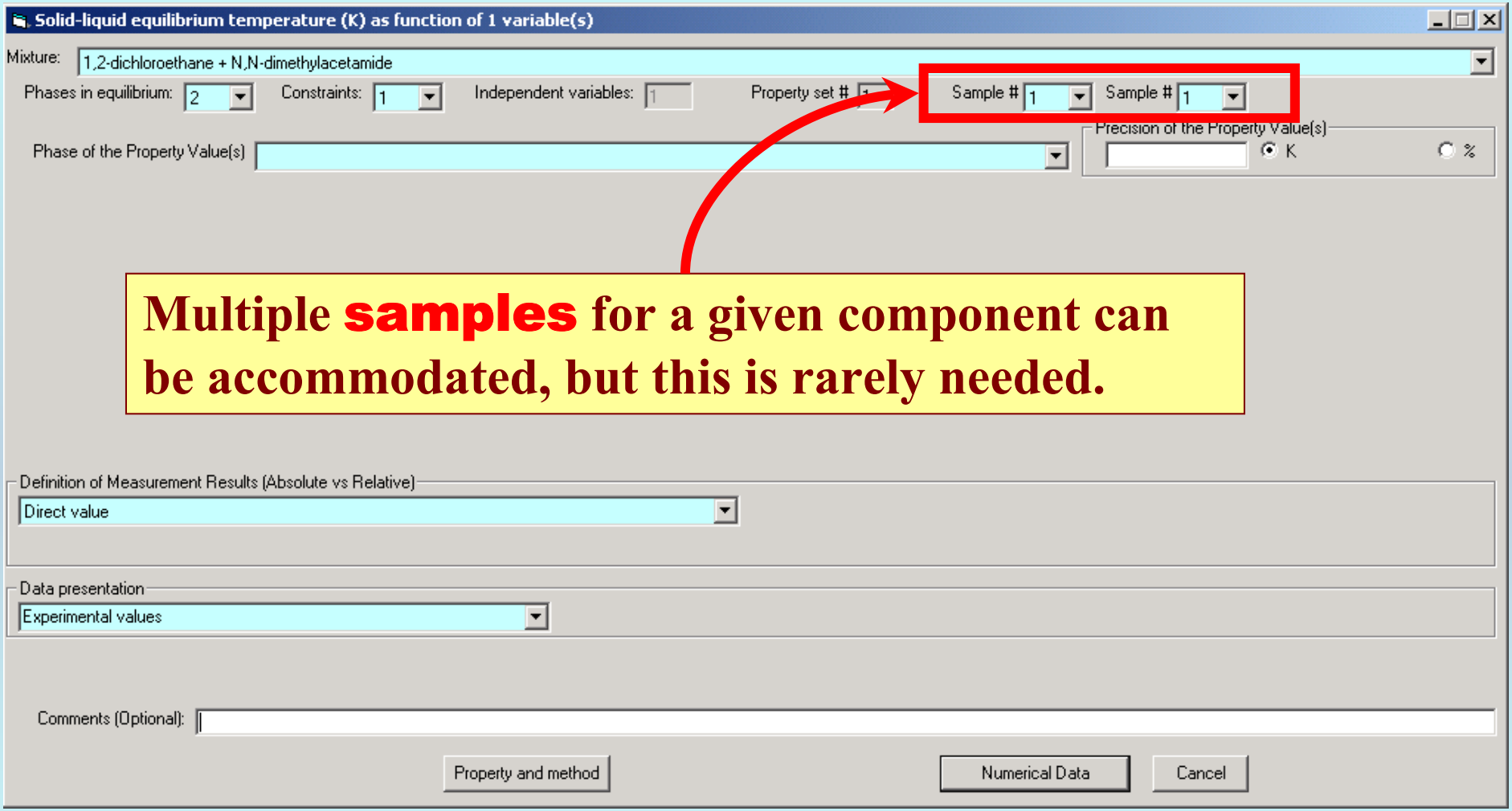
NOTE: The **bibliographic information**, **compound identities**, **sample descriptions**, and **mixture** were entered previously. (There are separate tutorials, which describe capture of this information, if needed.)

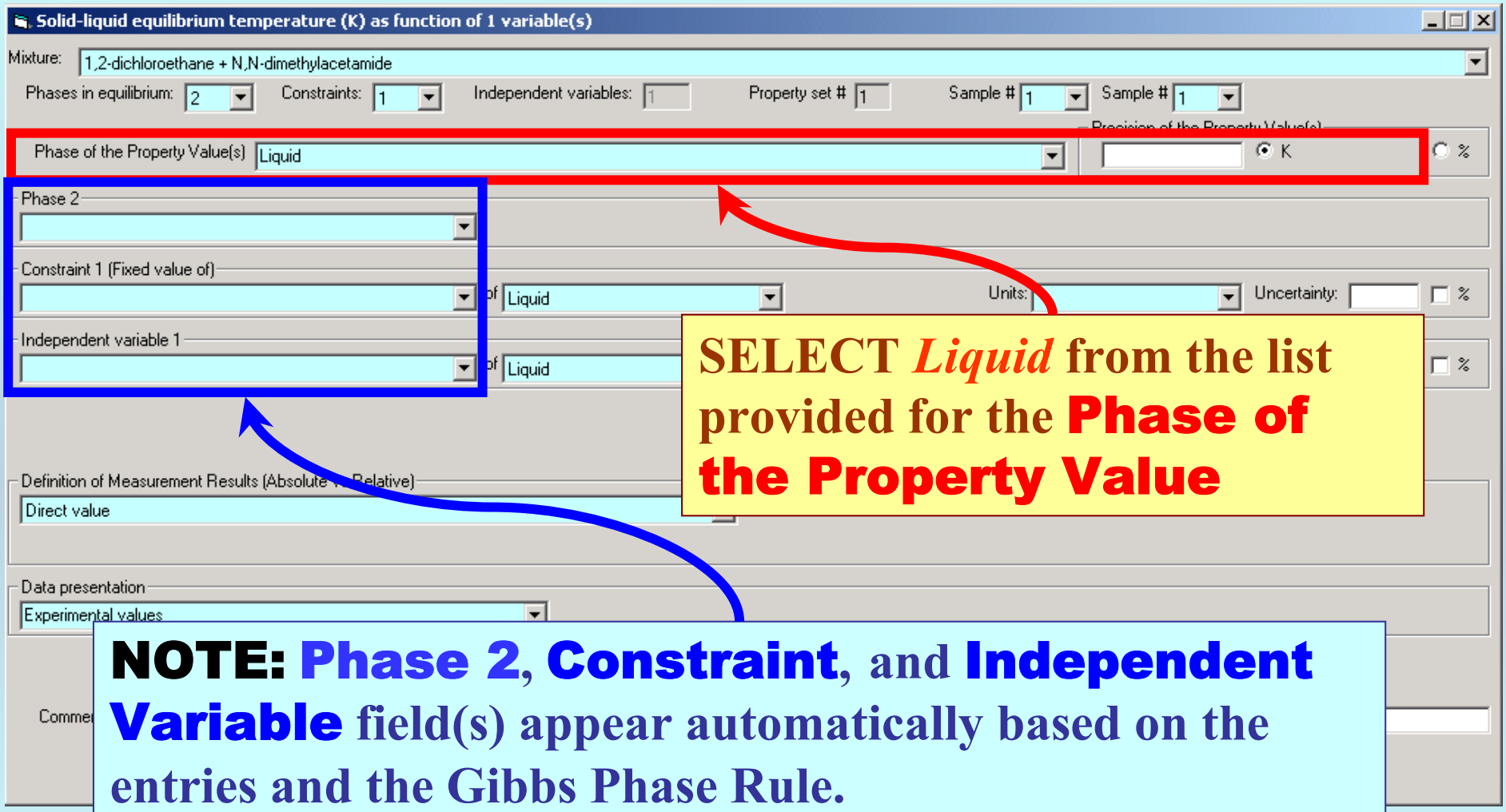

Property and experimental method for 1,2-dichloroethane + N,N-dimethylacetamide
Help
Property group:
Phase transition properties
Property:
Solid-liquid equilibrium temperature
Units:
K
Method of measurement:
Experimental purpose:
Comment (optional)
OK
Cancel
1. SELECT the Property group: Phase transition properties from the menu.
2. SELECT the Property: Solid-liquid equilibrium temperature.
3. SELECT the Units: K here.


Property and experimental method for 1,2-dichloroethane + N,N-dimethylacetamide
Help
Property group:
Phase transition properties
Property:
Solid-liquid equilibrium temperature
Units:
K
1. SELECT the Method of measurement: Visual Observation here.
Method of measurement:
Visual observation
Experimental purpose:
Principal objective of the work
2. SELECT the Experimental purpose
Comment (optional)
3. CLICK OK
OK
Cancel

SELECTION of # of Phases in Equilibrium and # of Constraints

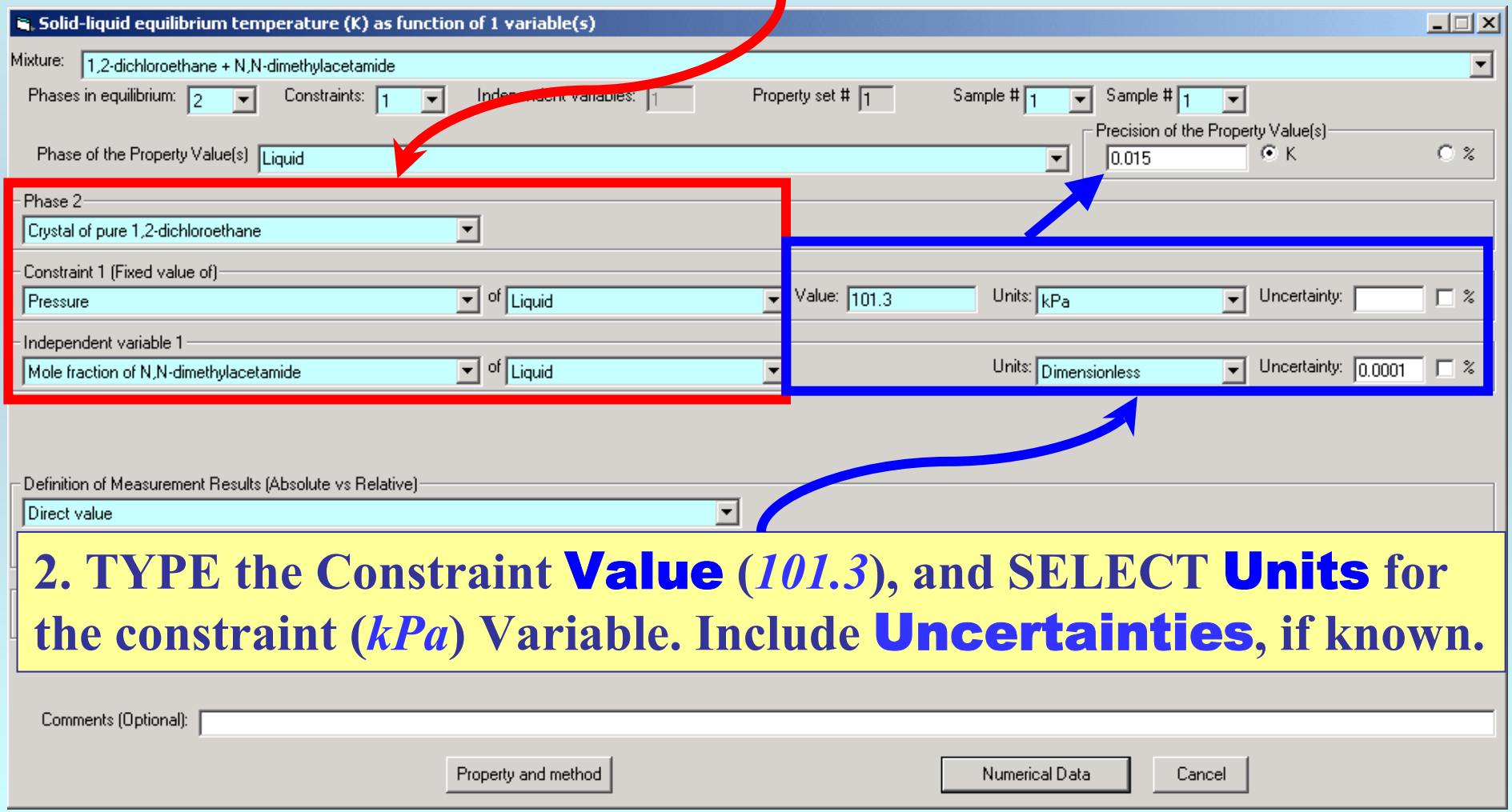



Solid-liquid equilibrium temperature (K) as function of 1 variable(s)
Mixture:
1,2-dichloroethane + N,N-dimethylacetamide
Phases in equilibrium:
2
Constraints:
1
Independent variables:
1
Property set #
1
Sample #
1
Sample #
1
Phase of the Property Value(s)
Precision of the Property Value(s)
K
%
Multiple samples for a given component can be accommodated, but this is rarely needed.
Definition of Measurement Results (Absolute vs Relative)
Direct value
Data presentation
Experimental values
Comments (Optional):
Property and method
Numerical Data
Cancel


Solid-liquid equilibrium temperature (K) as function of 1 variable(s)
Mixture: 1,2-dichloroethane + N,N-dimethylacetamide
Phases in equilibrium: 2
Constraints: 1
Independent variables: 1
Property set # 1
Sample # 1
Sample # 1
Phase of the Property Value(s) Liquid
K
%
Phase 2
Constraint 1 (Fixed value of)
of Liquid
Units:
Uncertainty:
%
Independent variable 1
of Liquid
%
Definition of Measurement Results (Absolute vs. Relative)
Direct value
Data presentation
Experimental values
SELECT Liquid from the list provided for the Phase of the Property Value
NOTE: Phase 2, Constraint, and Independent Variable field(s) appear automatically based on the entries and the Gibbs Phase Rule.

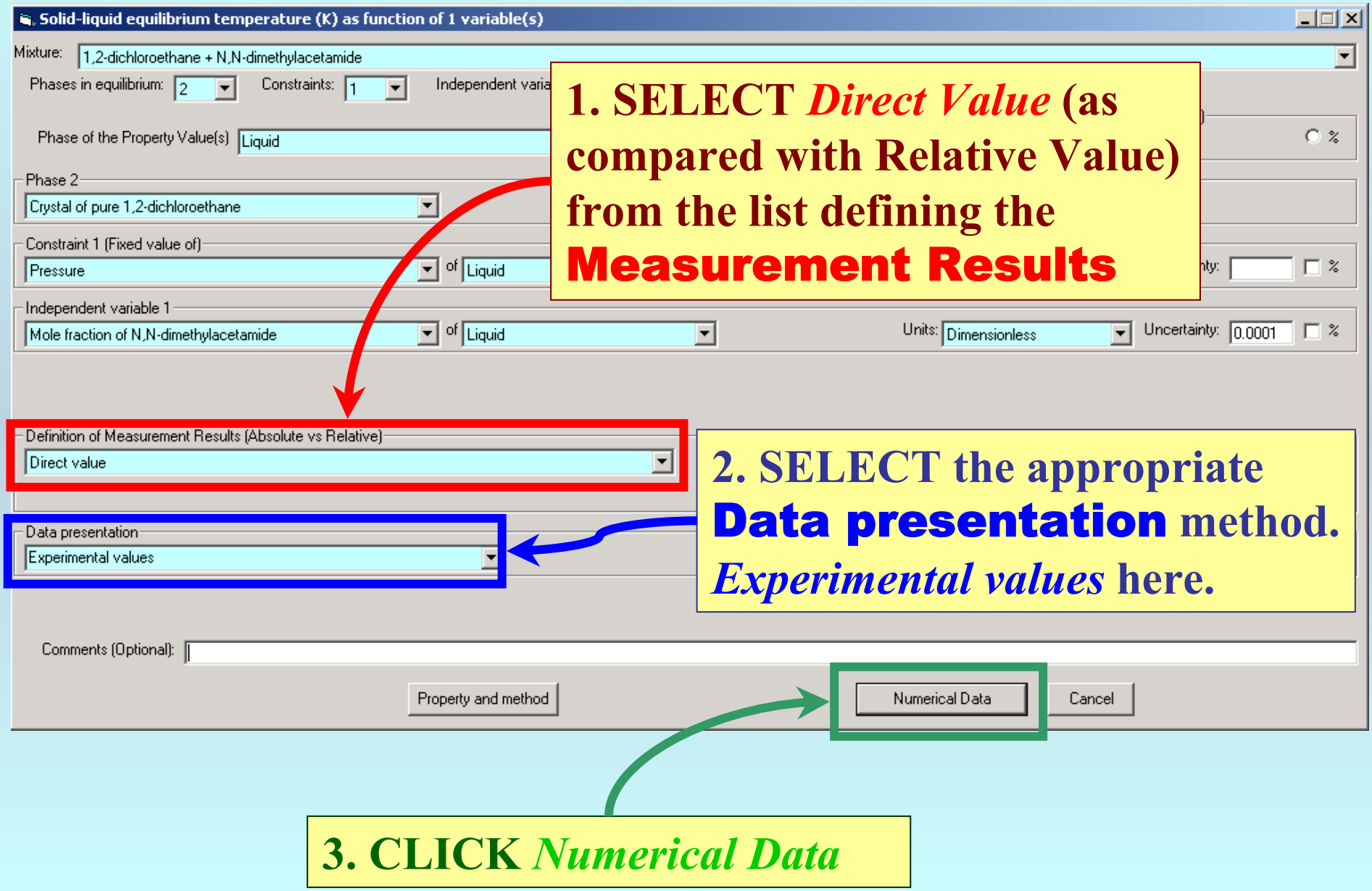
Specification of constraints, constraint values, and constraint units

1. SELECT the Constraint, Phase 2 (*crystal of pure 1,2-dichloroethane*) and the Independent Variable (*Mole fraction of N,N-dimethylacetamide* in the *Liquid*) from the menus.



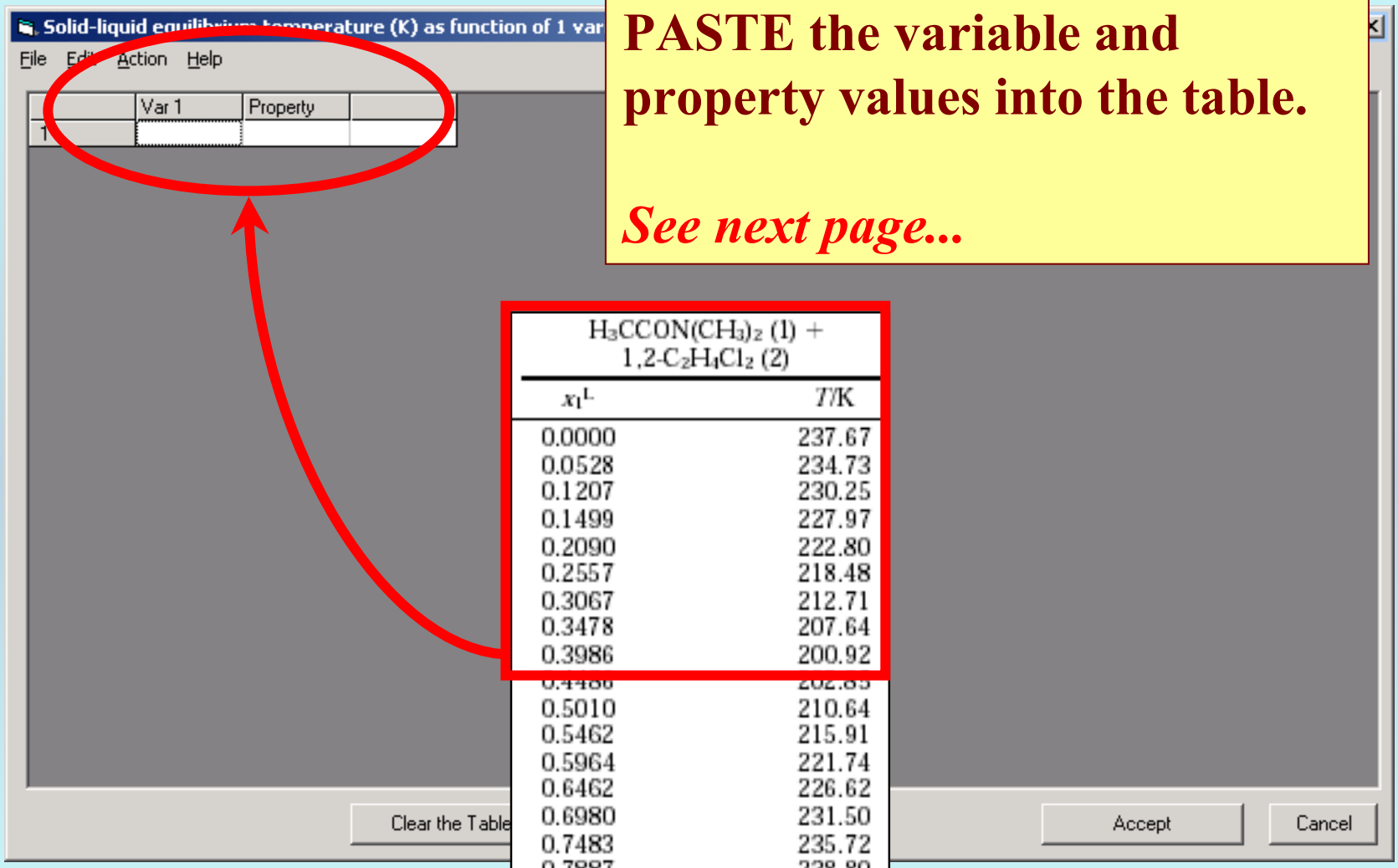
2. TYPE the Constraint Value (*101.3*), and SELECT Units for the constraint (*kPa*) Variable. Include Uncertainties, if known.

Measurement definition and Data presentation



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

See next page...



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x_1^L	T/K
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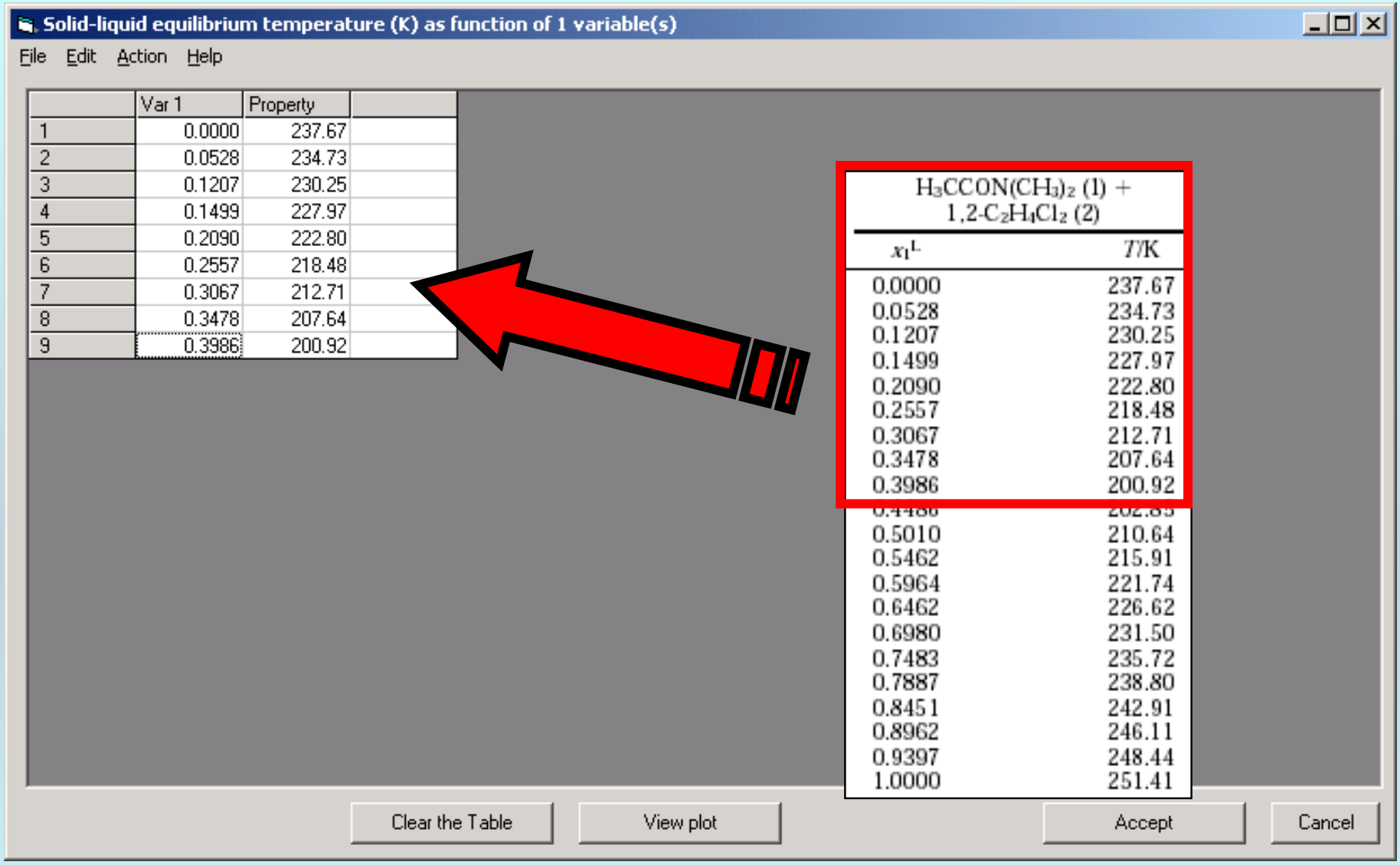
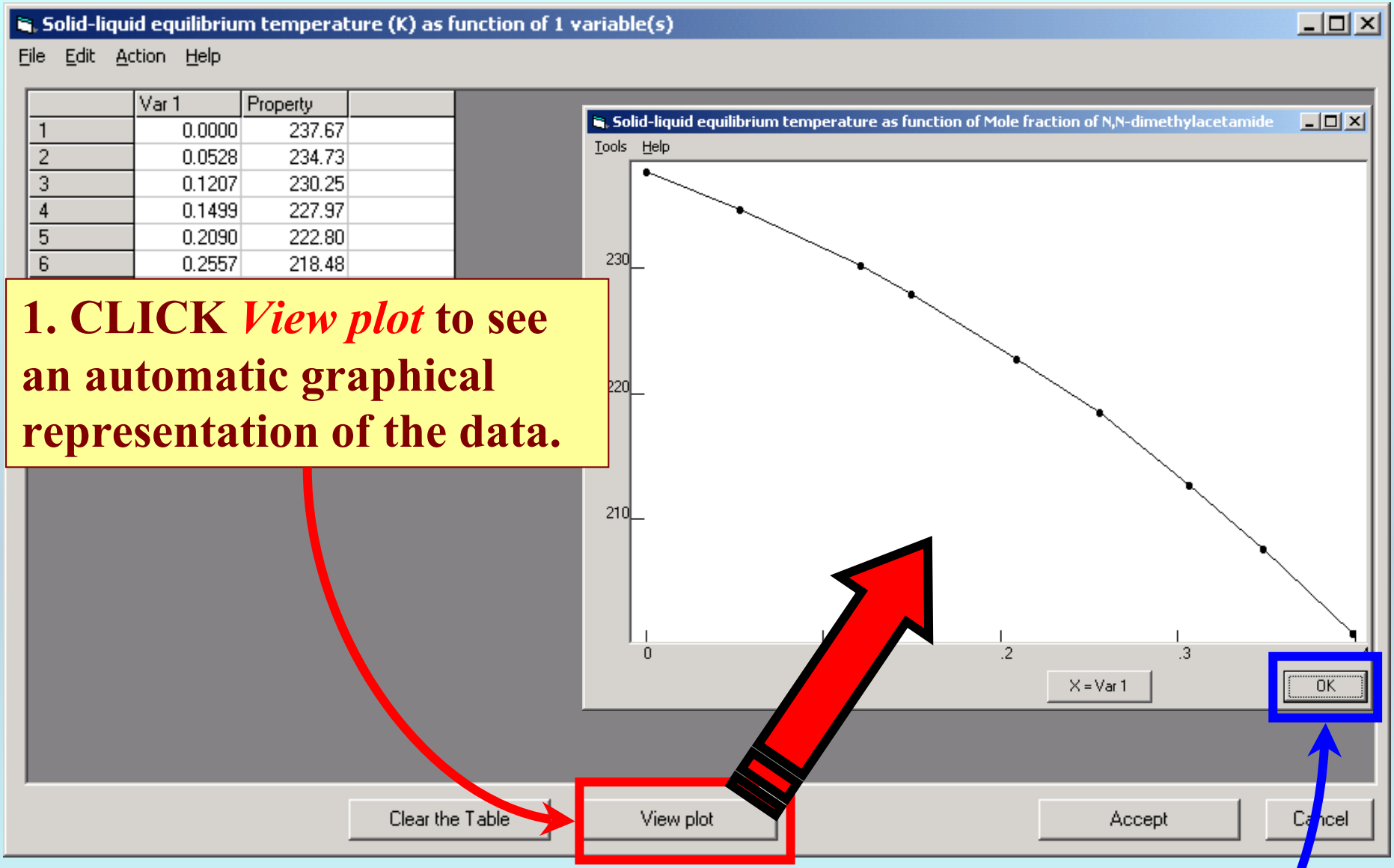
0.5462	215.91
0.5964	221.74
0.6462	226.62
0.6980	231.50
0.7483	235.72
0.7887	238.80
0.8451	242.91
0.8962	246.11
0.9397	248.44
1.0000	251.41

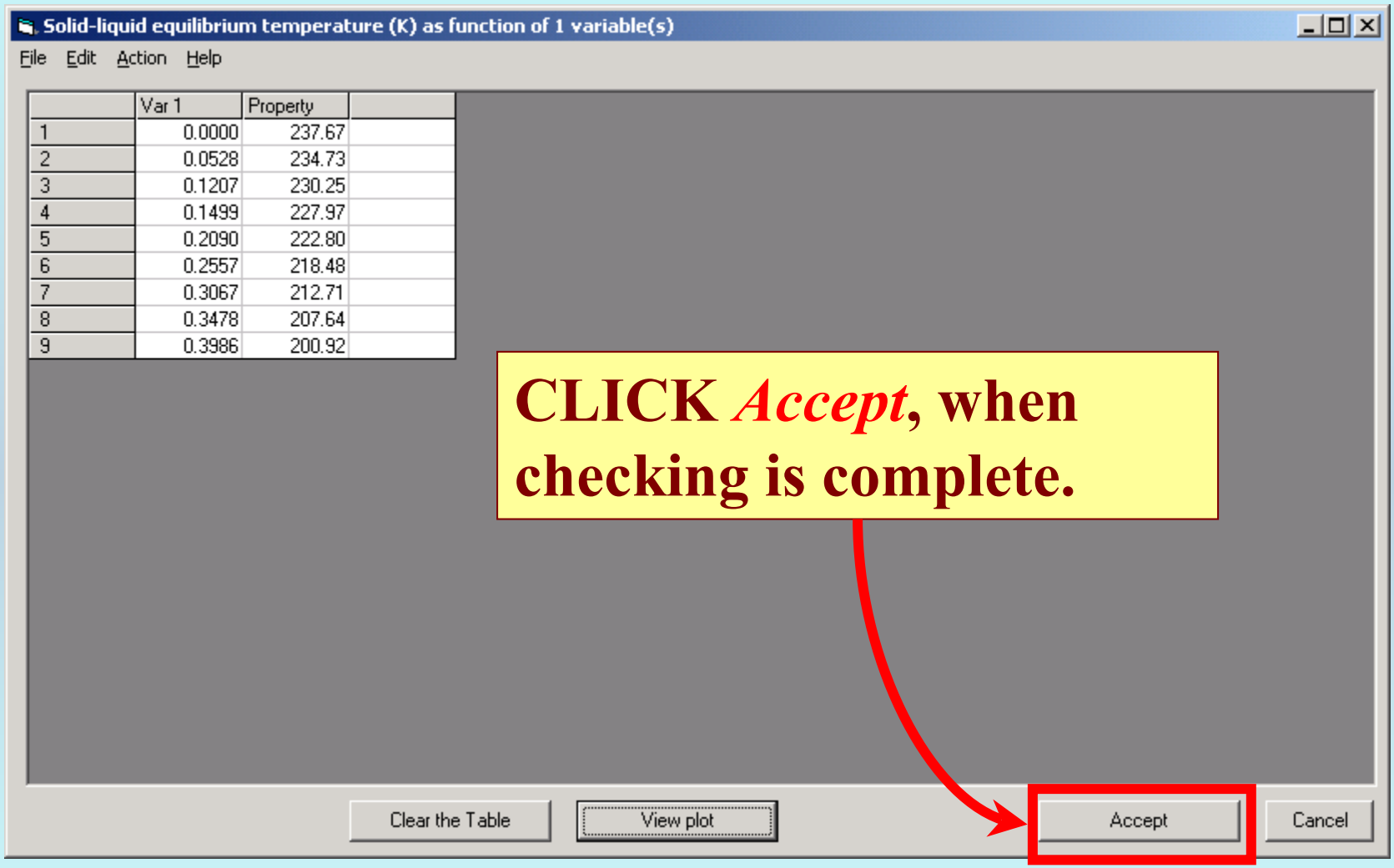


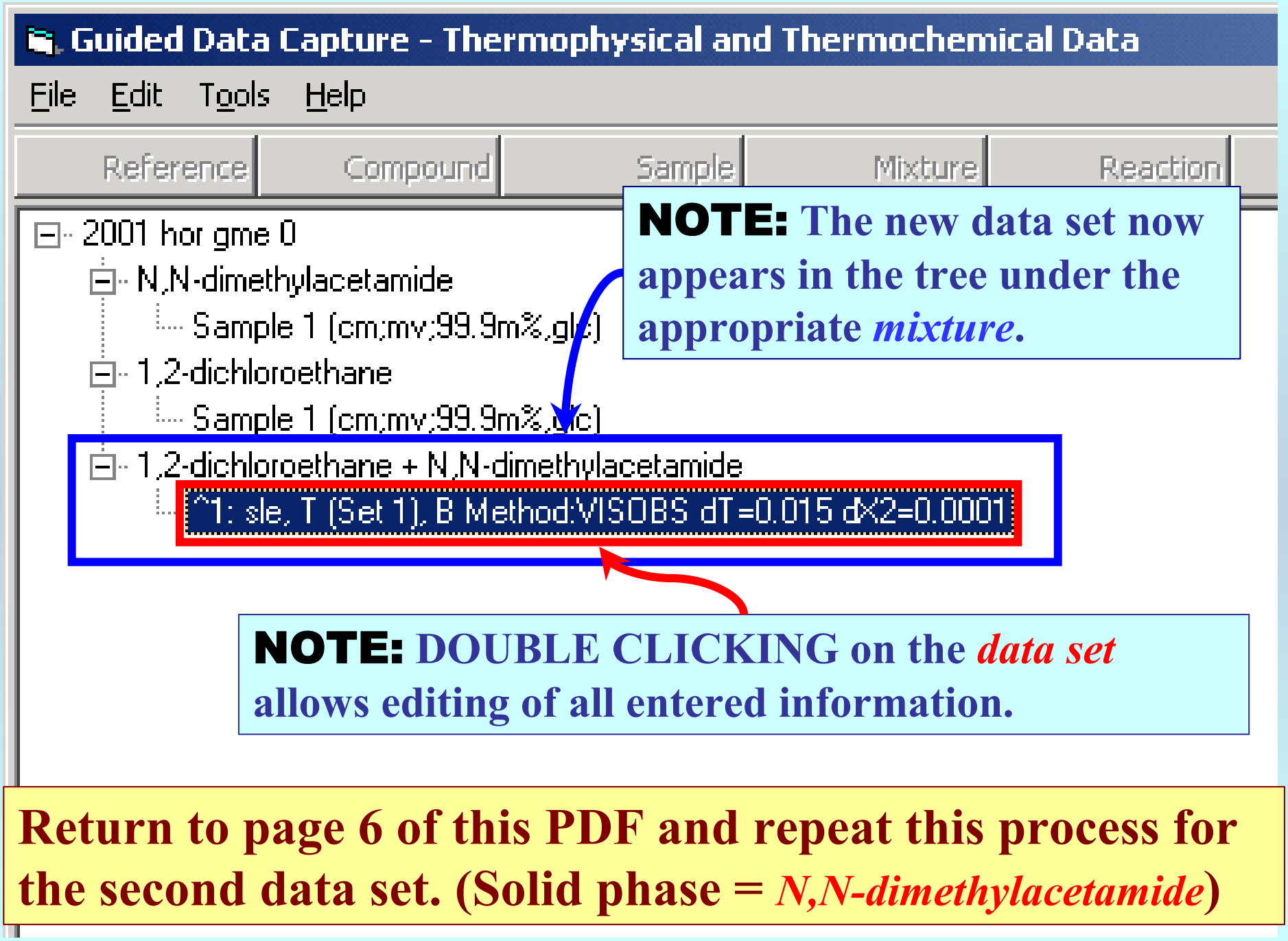
NOTE: Simple CUT/PASTE procedures can be used within the table to convert the original table into the required number of columns. (This can also be done externally in spreadsheet software, e.g., EXCEL.)

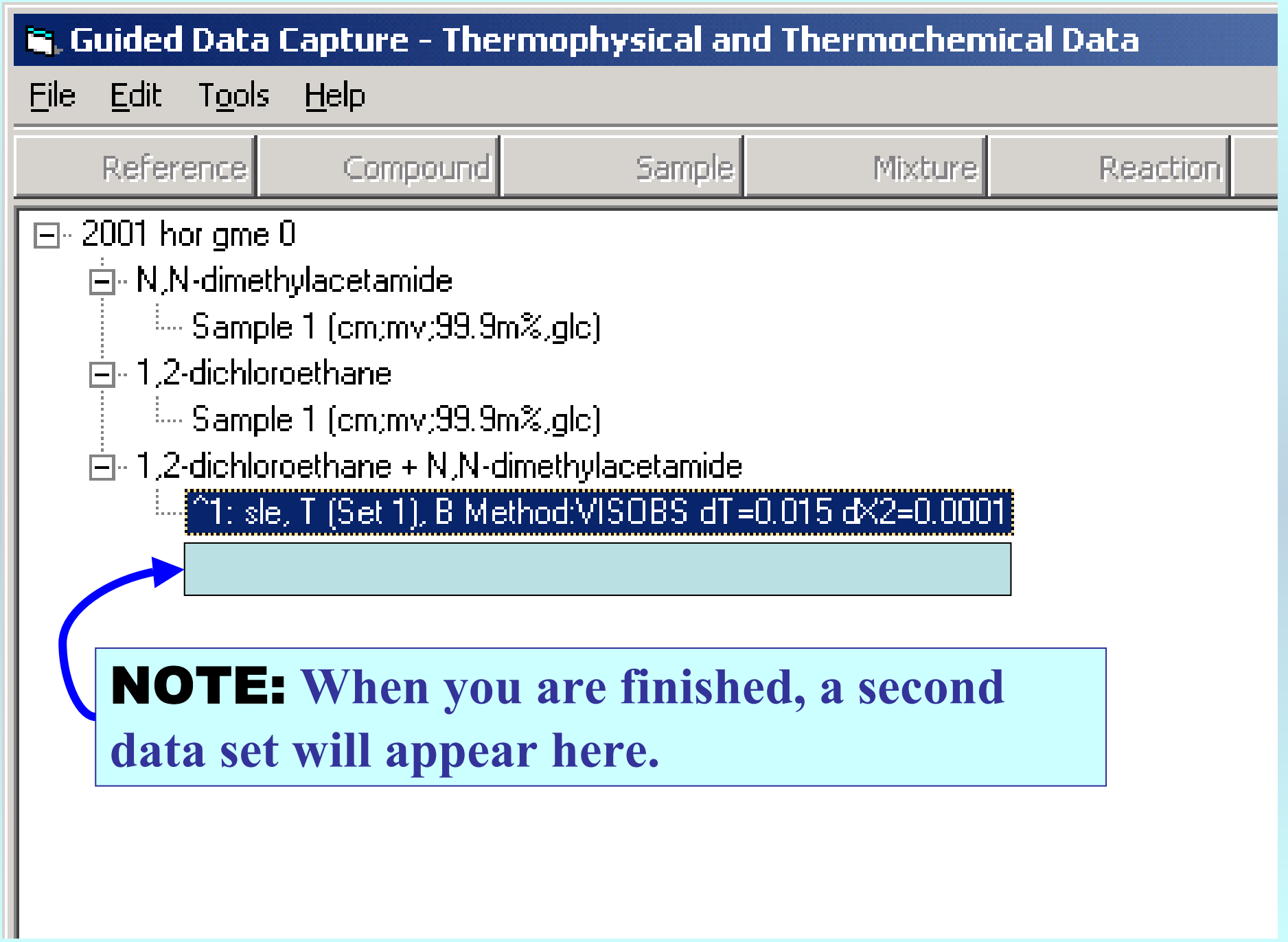


1. CLICK *View plot* to see an automatic graphical representation of the data.

2. Check for typographical errors, and CLICK *OK*, when done.


Solid-liquid equilibrium temperature (K) as function of 1 variable(s)
File Edit Action Help
Var 1 Property
1 0.0000 237.67
2 0.0528 234.73
3 0.1207 230.25
4 0.1499 227.97
5 0.2090 222.80
6 0.2557 218.48
7 0.3067 212.71
8 0.3478 207.64
9 0.3986 200.92
CLICK Accept, when checking is complete.
Clear the Table
View plot
Accept
Cancel


Guided Data Capture - Thermophysical and Thermochemical Data
File Edit Tools Help
Reference Compound Sample Mixture Reaction
2001 hor gme 0
N,N-dimethylacetamide
Sample 1 [cm;mv;99.9m%,glc]
1,2-dichloroethane
Sample 1 [cm;mv;99.9m%,glc]
1,2-dichloroethane + N,N-dimethylacetamide
^1: sle, T (Set 1), B Method:VISOBS dT=0.015 dX2=0.0001
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.
Return to page 6 of this PDF and repeat this process for the second data set. (Solid phase = N,N-dimethylacetamide)


Guided Data Capture - Thermophysical and Thermochemical Data
File Edit Tools Help
Reference Compound Sample Mixture Reaction
2001 hor gme 0
N,N-dimethylacetamide
Sample 1 (cm;mv;99.9m%,glc)
1,2-dichloroethane
Sample 1 (cm;mv;99.9m%,glc)
1,2-dichloroethane + N,N-dimethylacetamide
^1: sle, T (Set 1), B Method:VISOBS dT=0.015 dX2=0.0001
NOTE: When you are finished, a second data set will appear here.

END

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

***or* save your file and exit the program.**