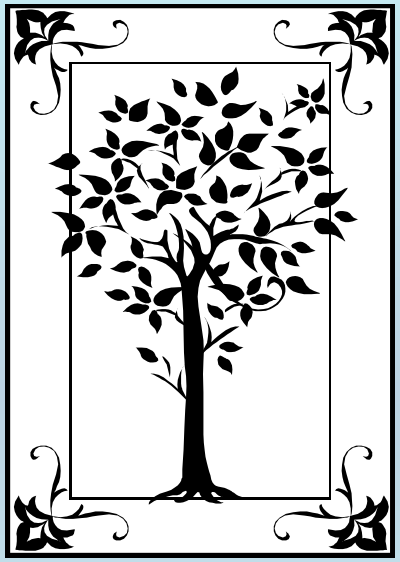
METADATA AND NUMERICAL DATA CAPTURE:
Vapor-Liquid Equilibria: *PTx*
(DEW POINT PRESSURES)

Guided Data Capture (GDC)



This tutorial describes
METADATA AND NUMERICAL DATA CAPTURE:
for **Vapor-Liquid Equilibria (2 components):**
***PTx* data (Dew Point pressures)**
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:

64 *J. Chem. Eng. Data* 1997, *42*, 64−68

High-Pressure Phase Equilibria in the Binary System (Methane + 5-α-Cholestane)

Eckhard Flöter, Christof Brumm, Theodoor W. de Loos,* and Jakob de Swaan Arons

Delft University of Technology, Faculty of Chemical Engineering and Materials Science, Laboratory of Applied Thermodynamics and Phase Equilibria, Julianalaan 136, 2628 BL Delft, The Netherlands

In this paper, experimental data on the phase behavior of the binary system (methane + 5-α-cholestane) are presented. Experiments were carried out according to the synthetic method. The temperature range investigated was from 320 K to 450 K. The pressures applied did not exceed 250 MPa. Vapor−liquid equilibria have been measured for 18 different mixtures. Additionally, the melting curve of pure 5-α-cholestane and the course of the three-phase curve (solid 5-α-cholestane + liquid + vapor) was determined. The second critical end point was located at a temperature $T = (342.2 \pm 0.5)$ K, a pressure $p = (193.3 \pm 0.4)$ MPa, and a mole fraction of 5-α-cholestane in the critical fluid phase $x = 0.049 \pm 0.004$.

PTx dew-point data for methane + 5-α-cholestane

Table 2. Vapor−Liquid Equilibrium Data for (Methane (A) + 5-α-Cholestane (B))[a]

T/K	p/MPa	T/K	p/MPa	T/K	p/MPa	T/K	p/MPa	T/K	p/MPa
				$x_B = 0.005$ (d.p.)					
330.45	139.28	360.72	136.28	400.67	97.06	433.82	84.85		
341.47	130.08	376.40	108.26	408.78	93.86	445.35	81.05		
353.34	121.47	385.47	103.86	420.63	89.45	458.23	77.05		
				$x_B = 0.010$ (d.p.)					
335.72	168.70	368.13	139.28	404.15	117.47	439.28	101.86	470.74	90.45
346.67	157.29	379.11	131.68	415.52	111.87	451.70	97.06		
358.12	147.09	391.13	124.47	427.14	106.66	463.02	93.05		
				$x_B = 0.021$ (d.p.)					
325.47	207.52	354.12	171.90	383.38	147.09	417.53	126.67	451.78	111.27
335.80	192.71	361.43	164.70	395.00	139.28	429.25	120.87	462.67	107.06
347.17	179.51	373.17	154.69	406.15	132.68	441.19	115.67		
				$x_B = 0.030$ (d.p.)					
325.53	214.53	359.25	172.90	385.11	151.49	418.30	131.28	453.25	115.47
336.47	198.92	370.69	162.70	396.28	143.88	431.15	124.87	464.31	111.07
348.31	184.31	377.38	157.09	407.35	136.68	441.51	120.27		
				$x_B = 0.041$ (d.p.)					
325.45	215.33	358.17	174.70	395.29	145.89	429.49	127.27	462.89	113.07
336.29	200.12	370.57	163.90	407.42	138.28	440.57	122.07		
347.35	186.71	381.13	155.49	419.23	132.18	451.60	117.67		
				$x_B = 0.046$ (d.p.)					
339.41	196.45	393.72	146.95	435.12	124.75				
357.18	176.25	432.58	125.95	458.63	115.15				

This data set is considered here.

Experimental Method:

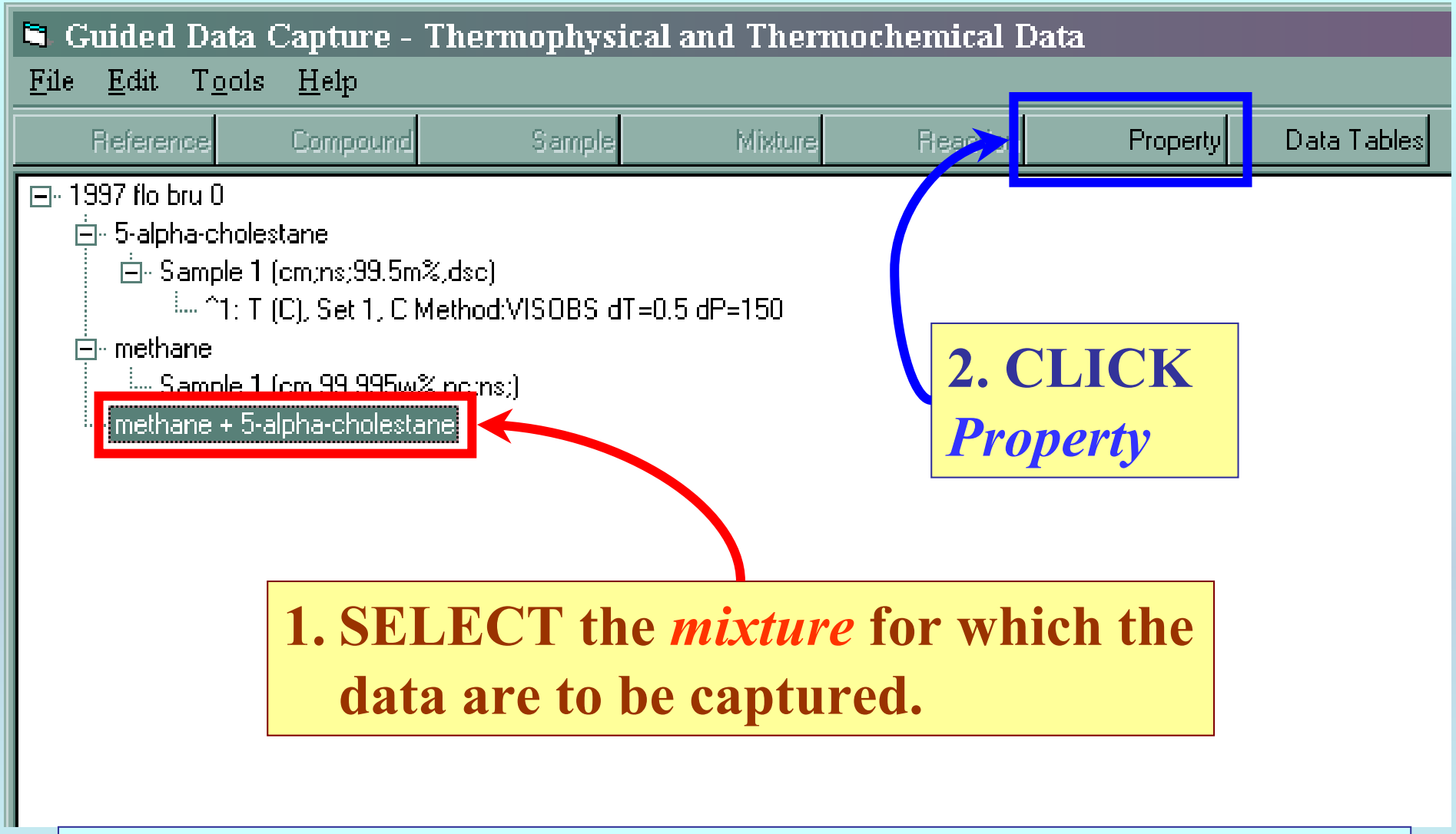
The high-pressure experiments were carried out using a sapphire windowed autoclave (de Loos et al., 1980)

Precision/Uncertainty Information:

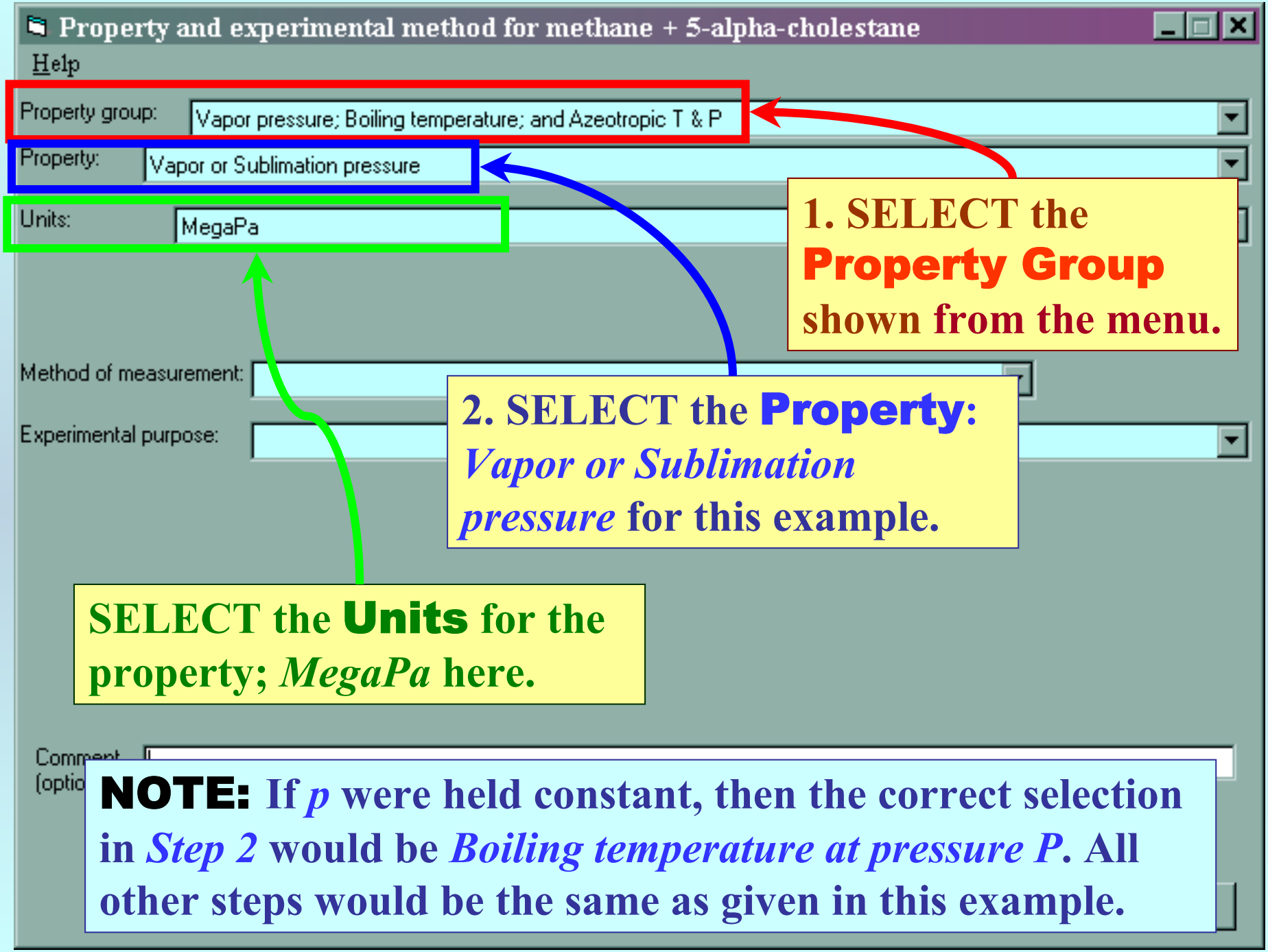
This allows the determination of transition temperatures with an accuracy better than ±0.04 K. The pressures are measured and kept constant with dead weight gauges. The uncertainty of the pressure reading was at most ±0.08 MPa.

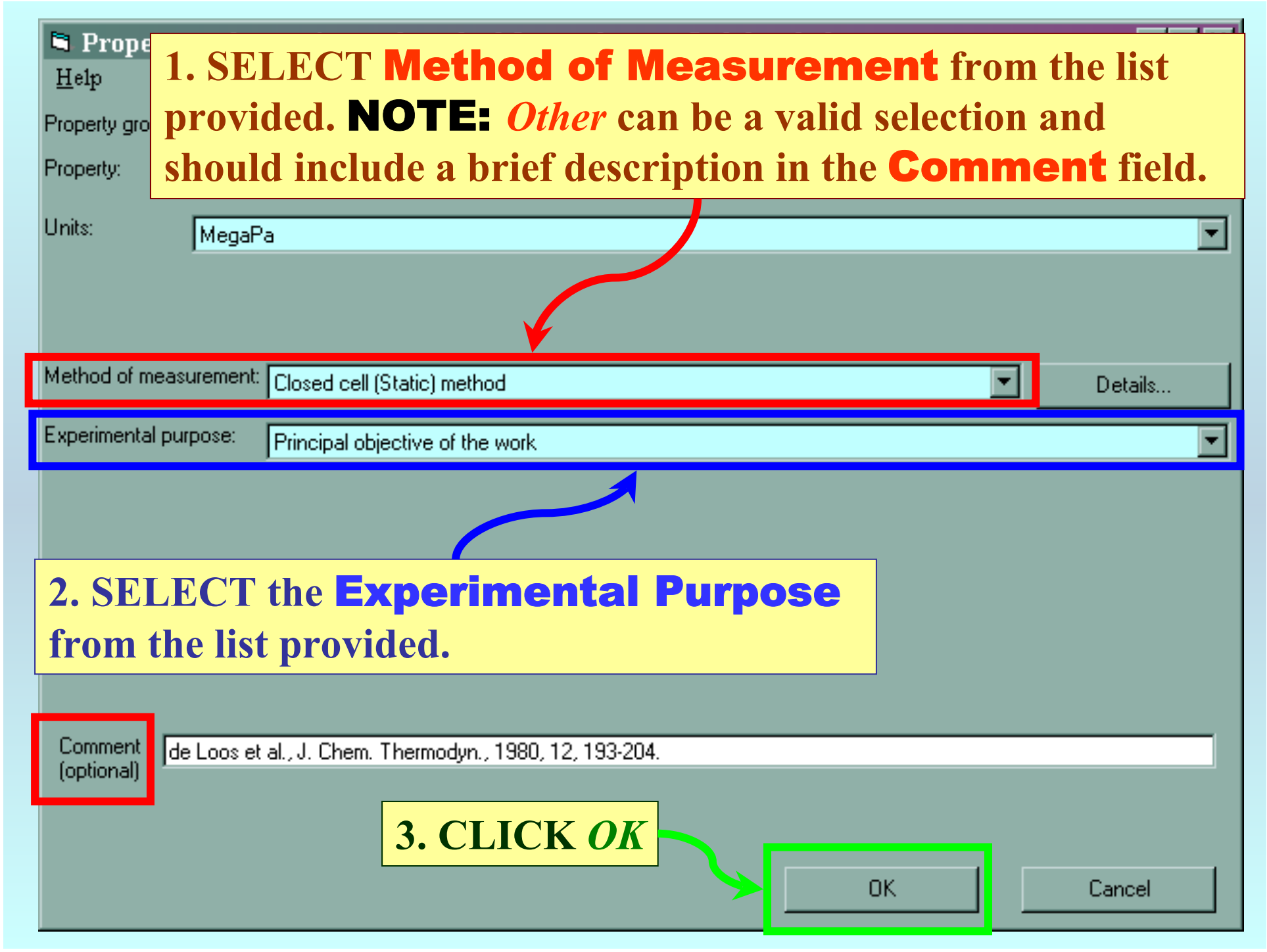
Since the measurements on top of the above given hardware accuracies also depend on the visibility of the transition under consideration, the vapor−liquid equilibrium measurements justify an accuracy better than ±0.15 MPa.

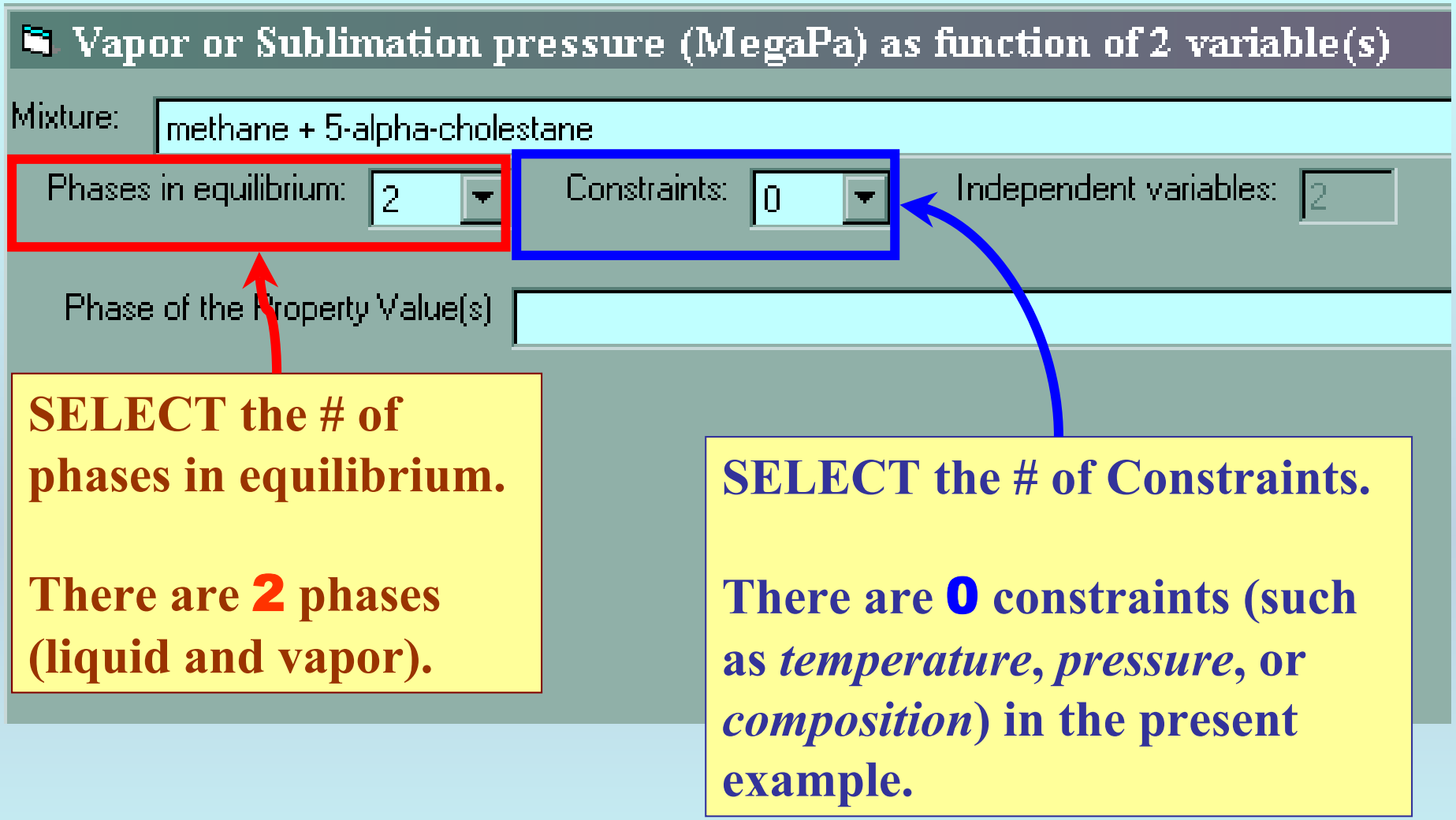
The accuracy of the given compositions is better than ±0.004 for the mole fraction of cholestane with a tendency to decrease with decreasing cholestane mole fraction.

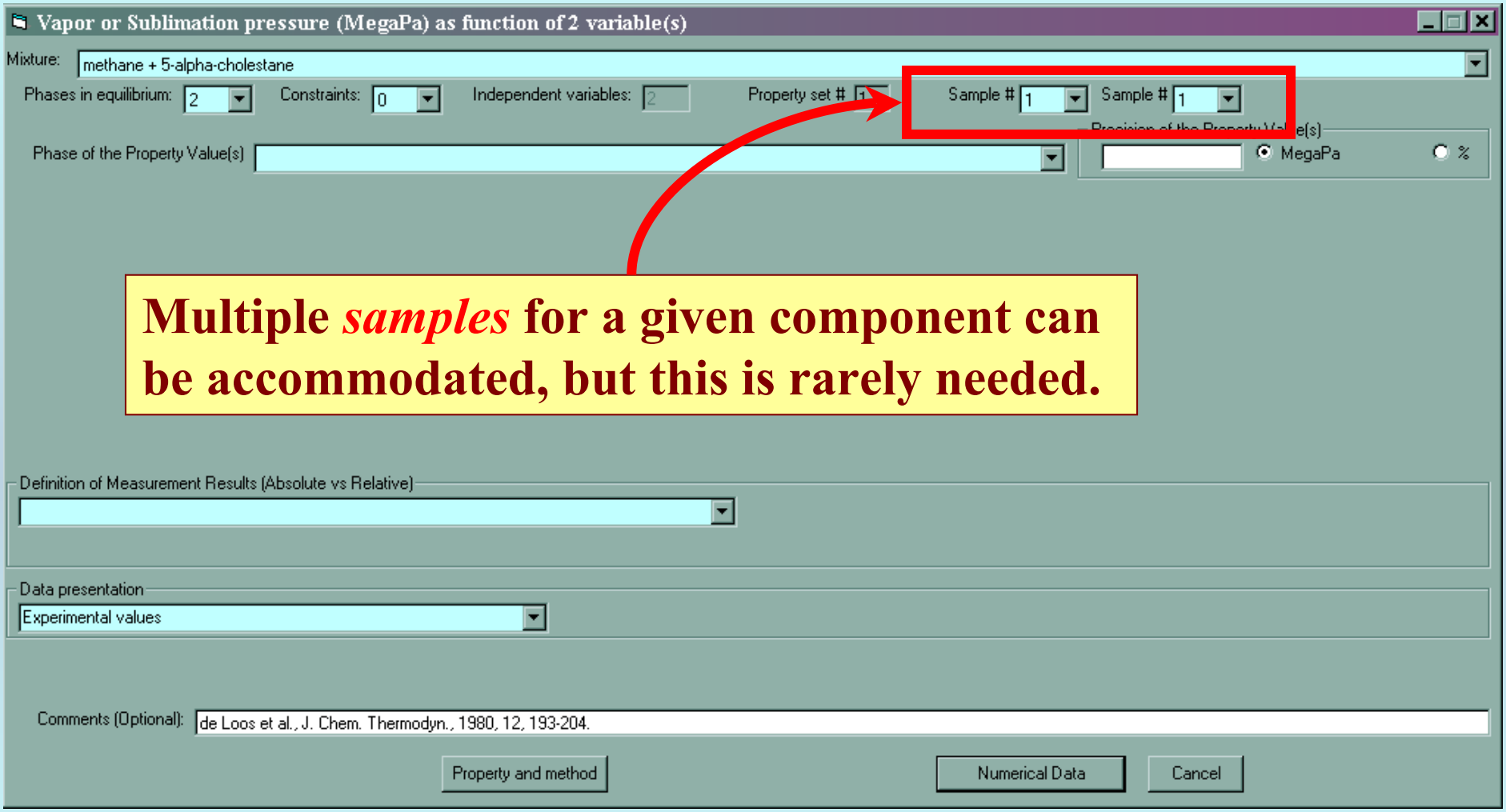


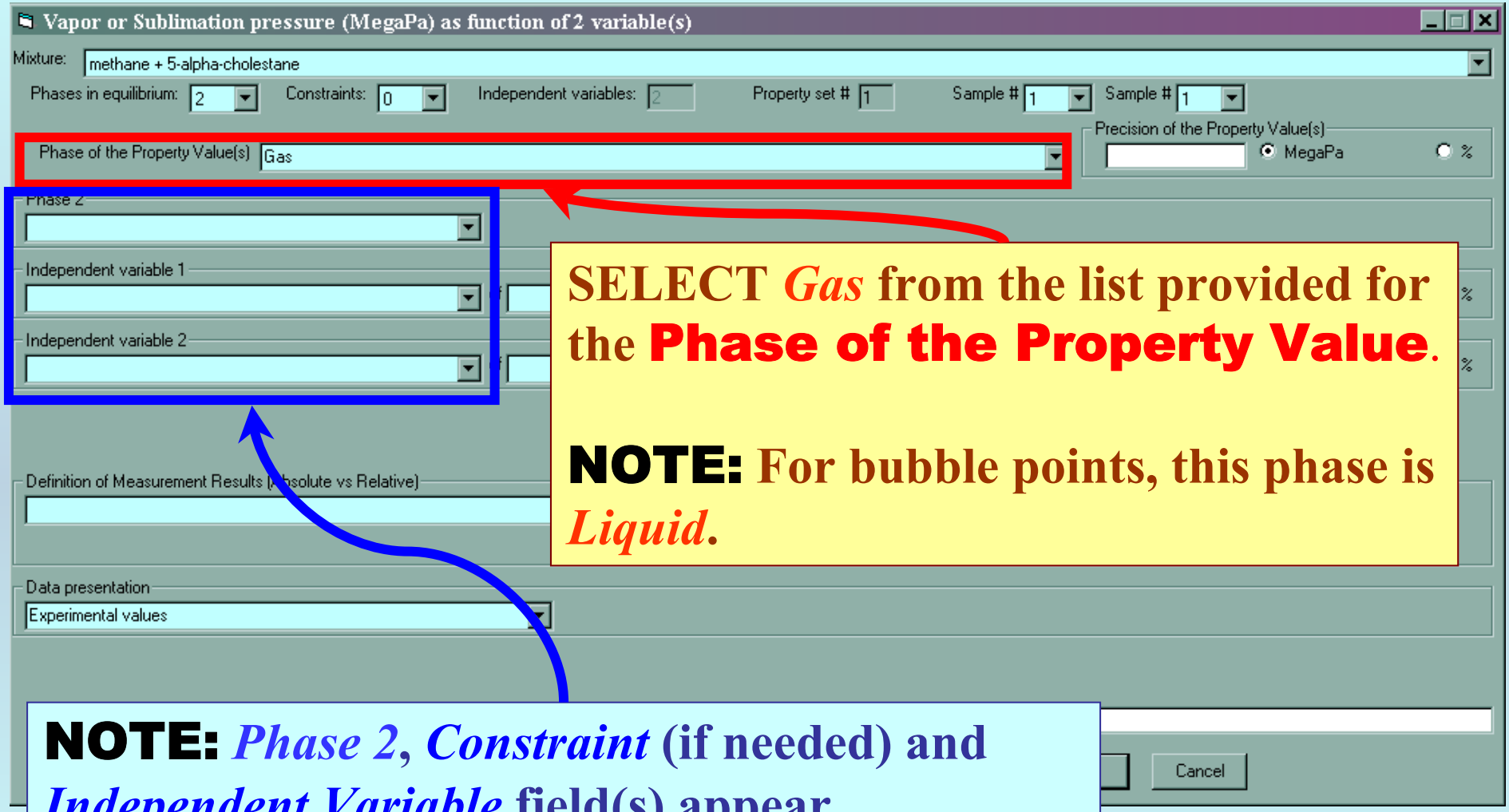
NOTE: The **bibliographic information**, **compound identities**, **sample descriptions**, and **mixture** were entered previously. (There are separate tutorials related to capture of this information, if needed.)


Property and experimental method for methane + 5-alpha-cholestane
Help
Property group:
Vapor pressure; Boiling temperature; and Azeotropic T & P
Property:
Vapor or Sublimation pressure
Units:
MegaPa
Method of measurement:
Experimental purpose:
1. SELECT the Property Group shown from the menu.
2. SELECT the Property: Vapor or Sublimation pressure for this example.
SELECT the Units for the property; MegaPa here.
NOTE: If p were held constant, then the correct selection in Step 2 would be Boiling temperature at pressure P. All other steps would be the same as given in this example.


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.
Help
Property gro
Property:
Units:
MegaPa
Method of measurement:
Closed cell (Static) method
Details...
Experimental purpose:
Principal objective of the work
2. SELECT the Experimental Purpose from the list provided.
Comment (optional)
de Loos et al., J. Chem. Thermodyn., 1980, 12, 193-204.
3. CLICK OK
OK
Cancel


Vapor or Sublimation pressure (MegaPa) as function of 2 variable(s)
Mixture:
methane + 5-alpha-cholestane
Phases in equilibrium:
2
Constraints:
0
Independent variables:
2
Phase of the Property Value(s)
SELECT the # of phases in equilibrium.
There are 2 phases (liquid and vapor).
SELECT the # of Constraints.
There are 0 constraints (such as temperature, pressure, or composition) in the present example.


Vapor or Sublimation pressure (MegaPa) as function of 2 variable(s)
Mixture:
methane + 5-alpha-cholestane
Phases in equilibrium:
2
Constraints:
0
Independent variables:
2
Property set #
1
Sample #
1
Sample #
1
Phase of the Property Value(s)
MegaPa
%
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):
de Loos et al., J. Chem. Thermodyn., 1980, 12, 193-204.
Property and method
Numerical Data
Cancel

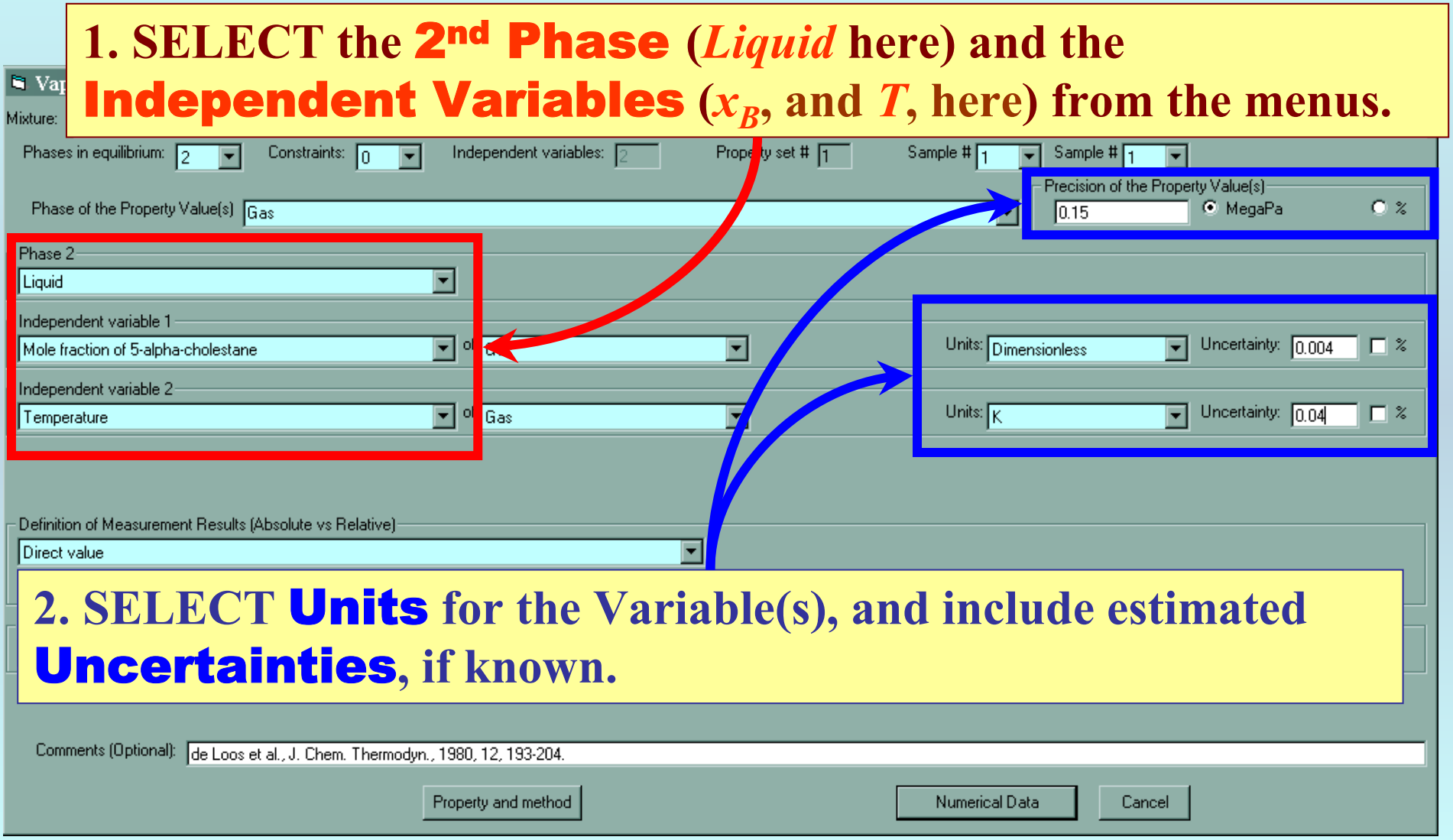


SELECT *Gas* from the list provided for the Phase of the Property Value.

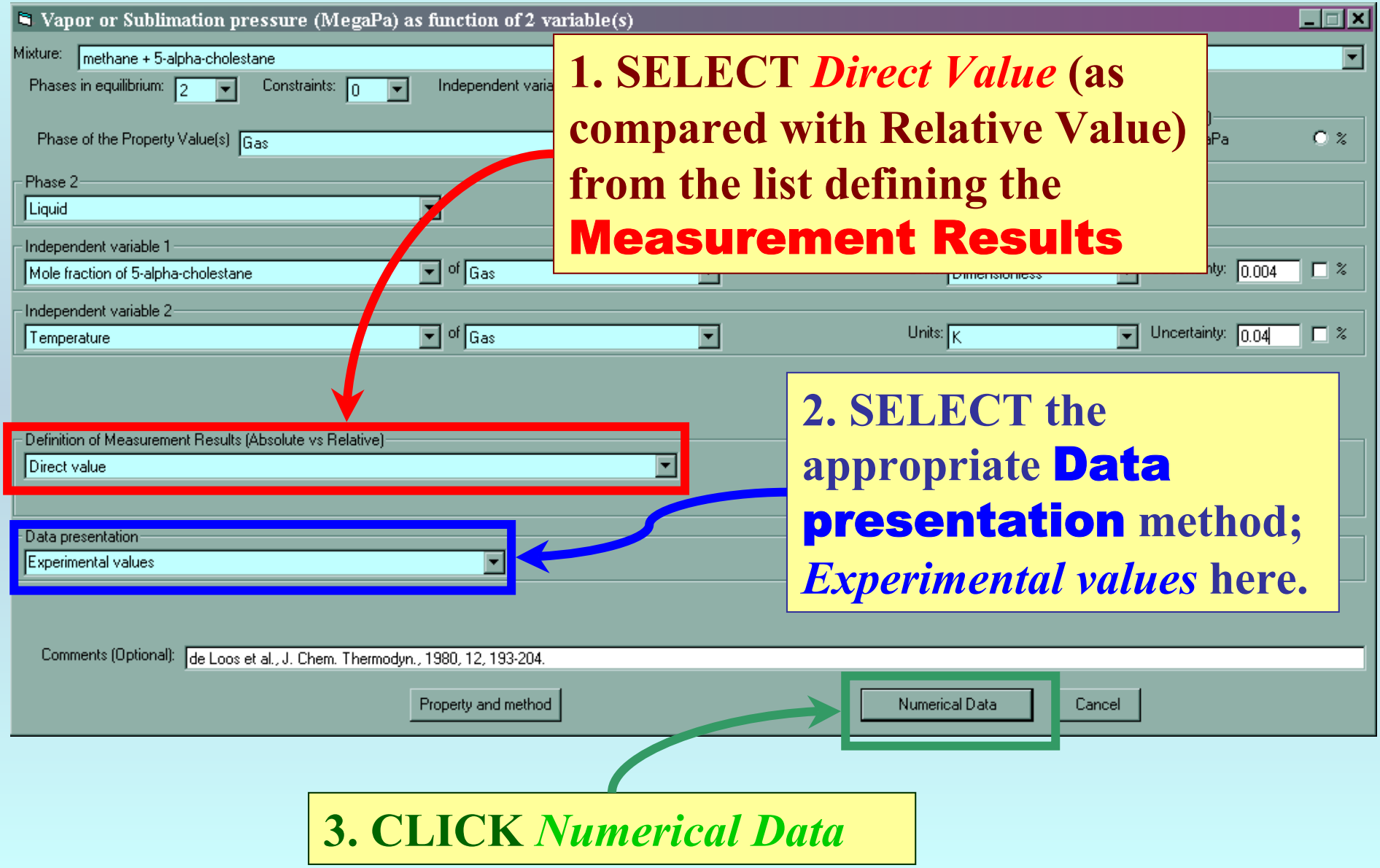
NOTE: For bubble points, this phase is *Liquid*.

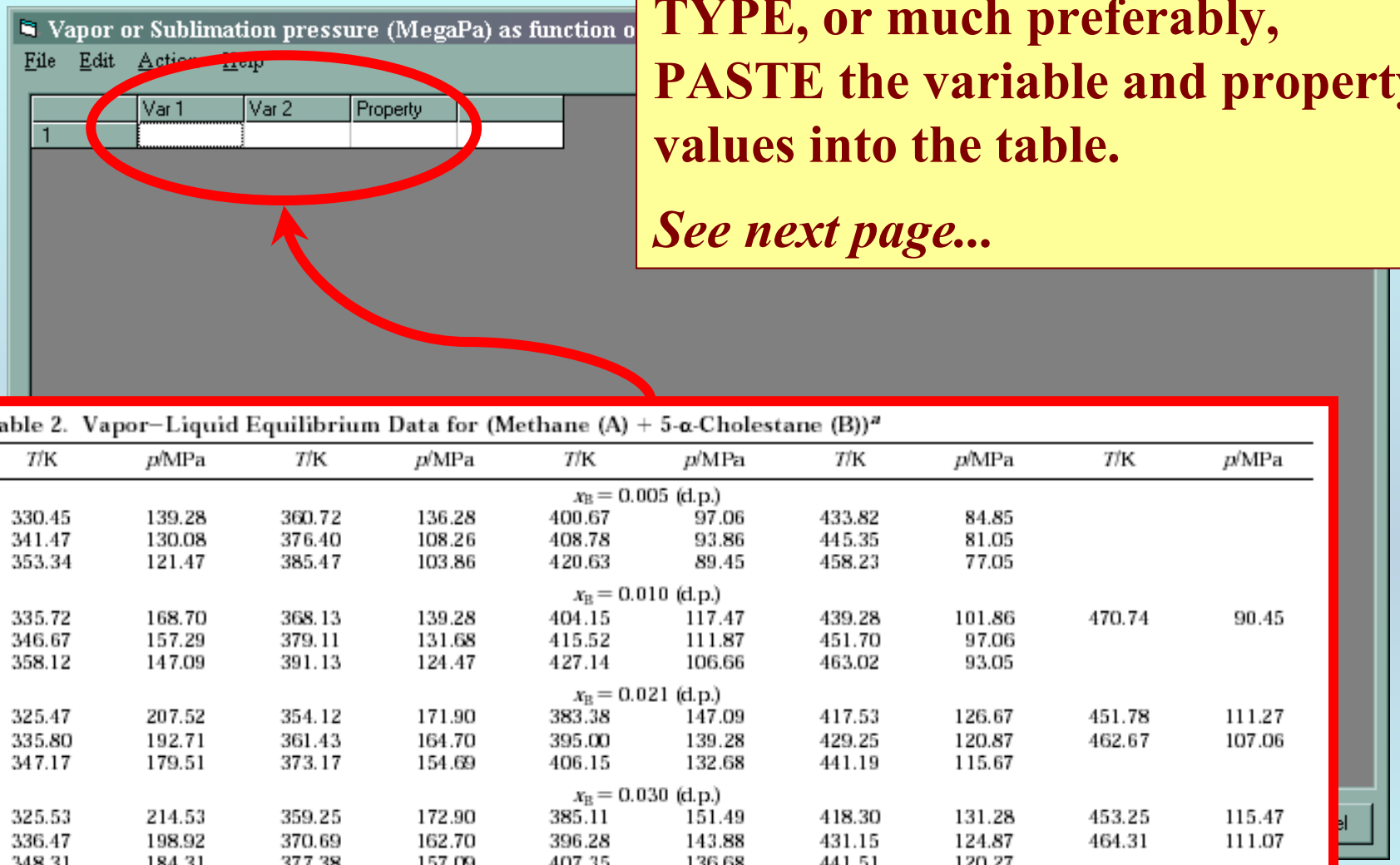
NOTE: *Phase 2*, *Constraint* (if needed) and *Independent Variable* field(s) appear automatically based on the Gibbs Phase Rule.

Specification of 2nd phase, constraint(s) if needed, and independent variable(s)



Measurement definition and Data presentation





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

See next page...

Table 2. Vapor–Liquid Equilibrium Data for (Methane (A) + 5-α-Cholestane (B))[a]

T/K	p/MPa	T/K	p/MPa	T/K	p/MPa	T/K	p/MPa	T/K	p/MPa
				$x_B = 0.005$ (d.p.)					
330.45	139.28	360.72	136.28	400.67	97.06	433.82	84.85		
341.47	130.08	376.40	108.26	408.78	93.86	445.35	81.05		
353.34	121.47	385.47	103.86	420.63	89.45	458.23	77.05		
				$x_B = 0.010$ (d.p.)					
335.72	168.70	368.13	139.28	404.15	117.47	439.28	101.86	470.74	90.45
346.67	157.29	379.11	131.68	415.52	111.87	451.70	97.06		
358.12	147.09	391.13	124.47	427.14	106.66	463.02	93.05		
				$x_B = 0.021$ (d.p.)					
325.47	207.52	354.12	171.90	383.38	147.09	417.53	126.67	451.78	111.27
335.80	192.71	361.43	164.70	395.00	139.28	429.25	120.87	462.67	107.06
347.17	179.51	373.17	154.69	406.15	132.68	441.19	115.67		
				$x_B = 0.030$ (d.p.)					
325.53	214.53	359.25	172.90	385.11	151.49	418.30	131.28	453.25	115.47
336.47	198.92	370.69	162.70	396.28	143.88	431.15	124.87	464.31	111.07
348.31	184.31	377.38	157.09	407.35	136.68	441.51	120.27		
				$x_B = 0.041$ (d.p.)					
325.45	215.33	358.17	174.70	395.29	145.89	429.49	127.27	462.89	113.07
336.29	200.12	370.57	163.90	407.42	138.28	440.57	122.07		
347.35	186.71	381.13	155.49	419.23	132.18	451.60	117.67		
				$x_B = 0.046$ (d.p.)					
339.41	196.45	393.72	146.95	435.12	124.75				
357.18	176.25	432.58	125.95	458.63	115.15				

Vapor or Sublimation pressure (MegaPa) as function of 2 variable(s)

File Edit Action Help

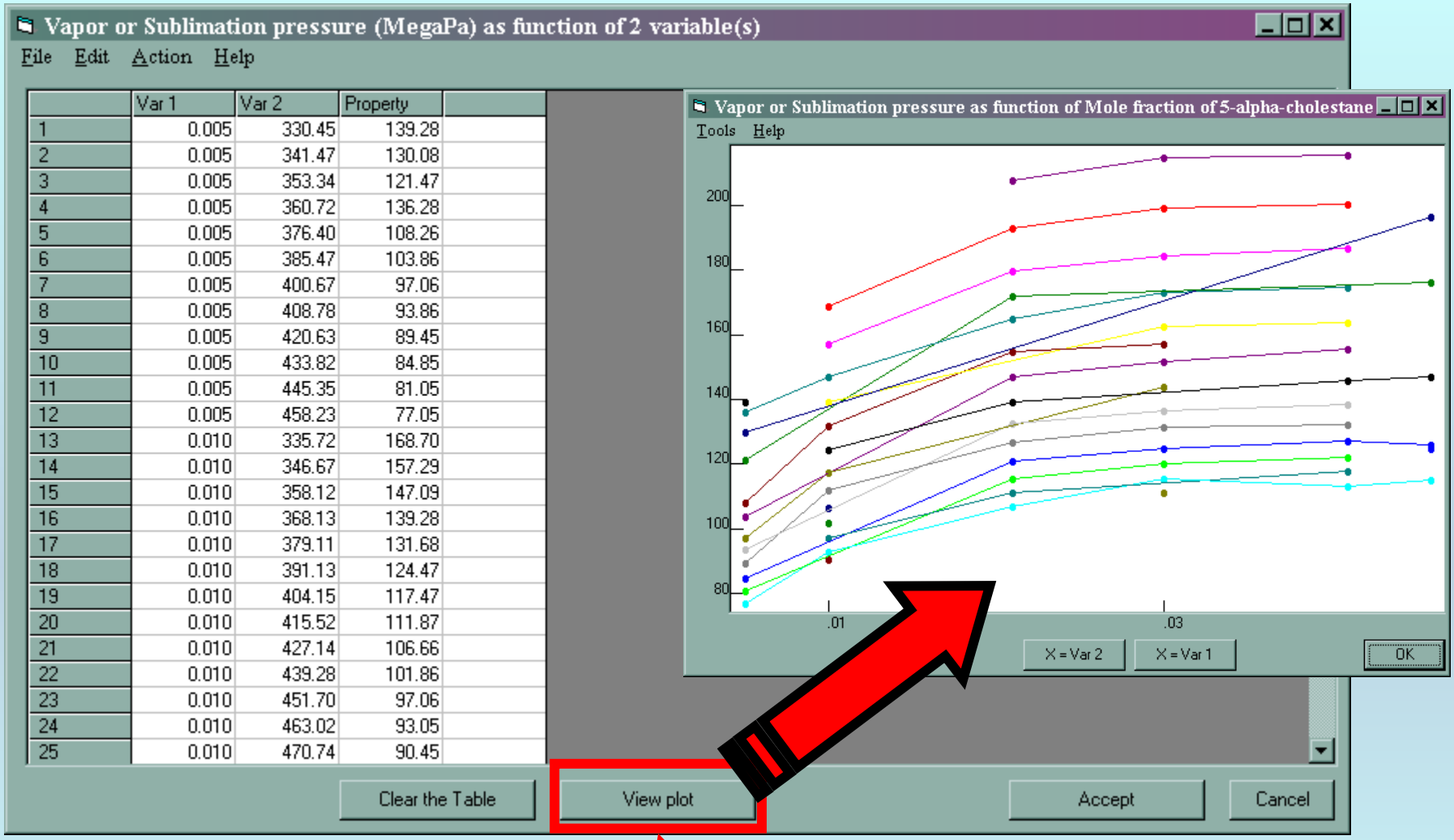
	Var 1	Var 2	Property
1	0.005	330.45	139.28
2	0.005	341.47	130.08
3	0.005	353.34	121.47
4	0.005	360.72	136.28
5	0.005	376.40	108.26
6	0.005	385.47	103.86
7	0.005	400.67	97.06
8	0.005	408.78	93.86
9	0.005	420.63	89.45
10	0.005	433.82	84.85
11	0.005	445.35	81.05
12	0.005	458.23	77.05
13	0.010	335.72	168.70
14	0.010	346.67	157.29
15	0.010	358.12	147.
16	0.010	368.13	
17	0.010	379.11	13
18	0.010	391.13	124.47
19	0.010	404.15	117.47
20	0.010	415.52	111.87
21	0.010	427.14	106.66
22	0.010	439.28	101.86
23	0.010	451.70	97.06
24	0.010	463.02	93.05
25	0.010	470.74	90.45

Clear the Table | View plot | Accept | Cancel

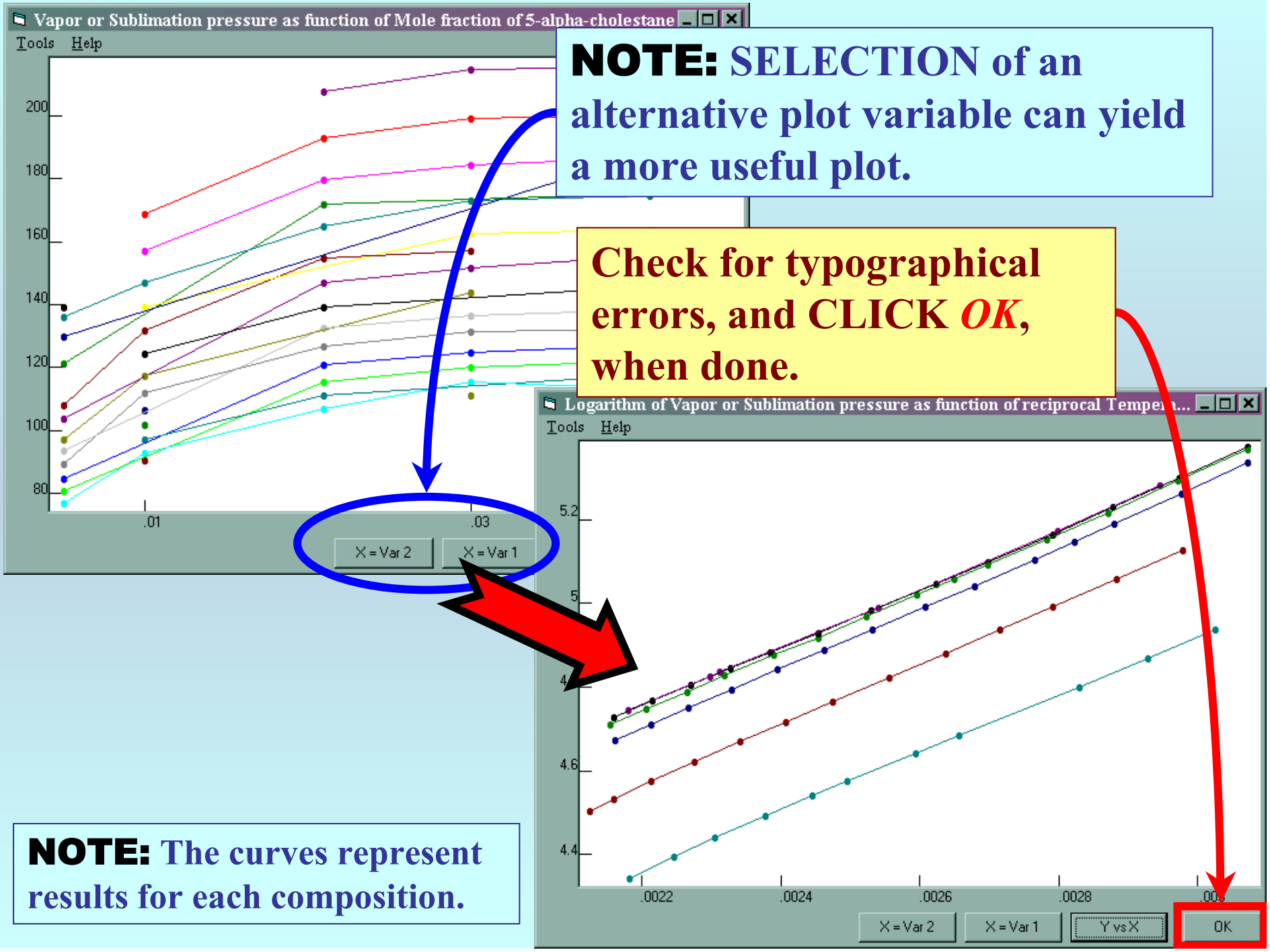
Table 2. Vapor–Liquid Equilibrium Data for (Methane (A) + 5-α-Cholestane (B))[a]

T/K	p/MPa	T/K	p/MPa	T/K	p/MPa	T/K	p/MPa	T/K	p/MPa
				$x_B = 0.005$ (d.p.)					
330.45	139.28	360.72	136.28	400.67	97.06	433.82	84.85		
341.47	130.08	376.40	108.26	408.78	93.86	445.35	81.05		
353.34	121.47	385.47	103.86	420.63	89.45	458.23	77.05		
				$x_B = 0.010$ (d.p.)					
335.72	168.70	368.13	139.28	404.15	117.47	439.28	101.86	470.74	90.45
346.67	157.29	379.11	131.68	415.52	111.87	451.70	97.06		
358.12	147.09	391.13	124.47	427.14	106.66	463.02	93.05		
				$x_B = 0.021$ (d.p.)					
325.47	207.52	354.12	171.90	383.38	147.09	417.53	126.67	451.78	111.27
335.80	192.71	361.43	164.70	395.00	139.28	429.25	120.87	462.67	107.06
347.17	179.51	373.17	154.69	406.15	132.68	441.19	115.67		
				$x_B = 0.030$ (d.p.)					
325.53	214.53	359.25	172.90	385.11	151.49	418.30	131.28	453.25	115.47
336.47	198.92	370.69	162.70	396.28	143.88	431.15	124.87	464.31	111.07
348.31	184.31	377.38	157.09	407.35	136.68	441.51	120.27		
				$x_B = 0.041$ (d.p.)					
325.45	215.33	358.17	174.70	395.29	145.89	429.49	127.27	462.89	113.07
336.29	200.12	370.57	163.90	407.42	138.28	440.57	122.07		
347.35	186.71	381.13	155.49	419.23	132.18	451.60	117.67		
				$x_B = 0.046$ (d.p.)					
339.41	196.45	393.72	146.95	435.12	124.75				
357.18	176.25	432.58	125.95	458.63	115.15				

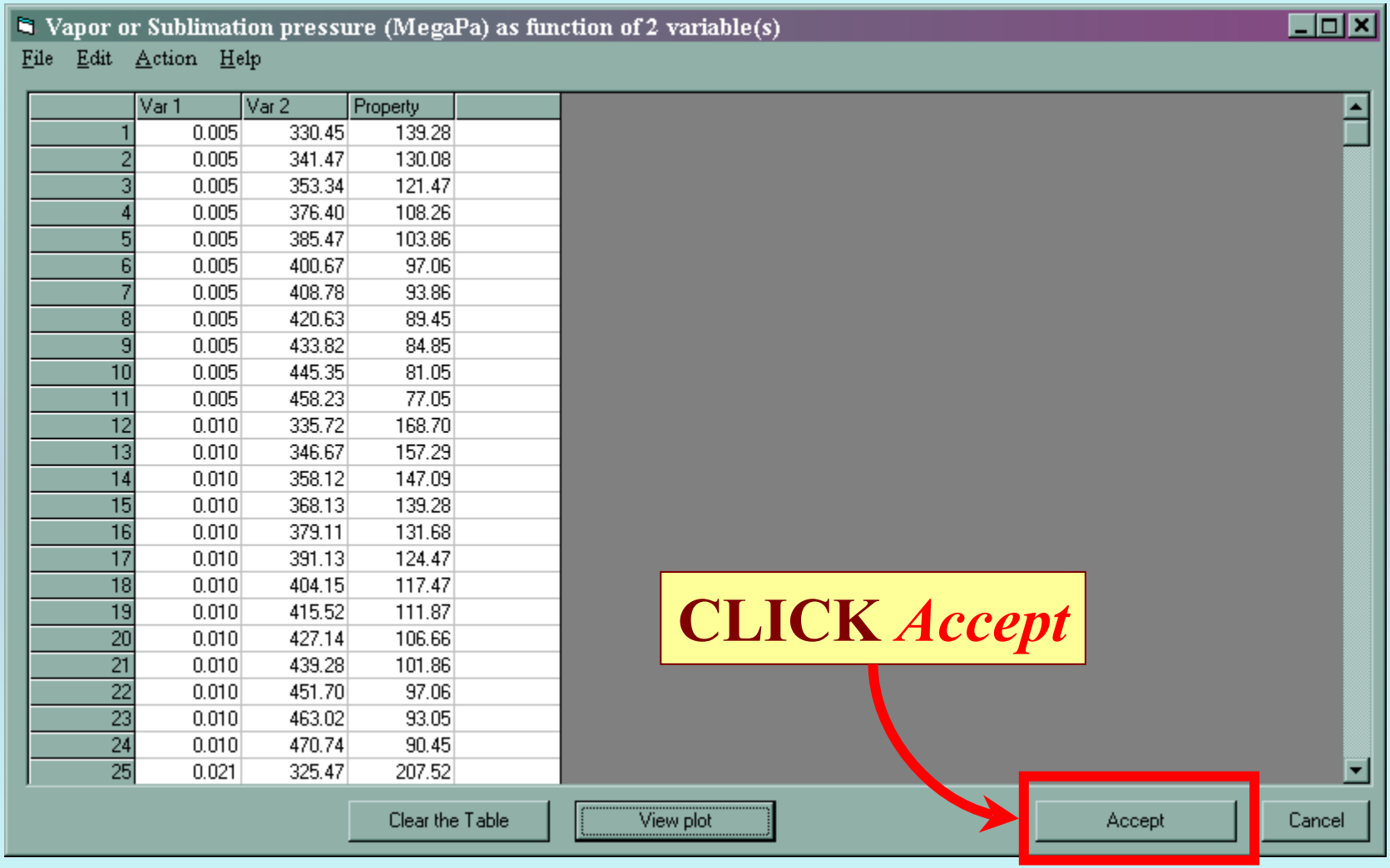
NOTE: Simple CUT/PASTE procedures can be used within the table to convert the original table into the required number of columns. (This can also be done externally in spreadsheet software; e.g., EXCEL.)

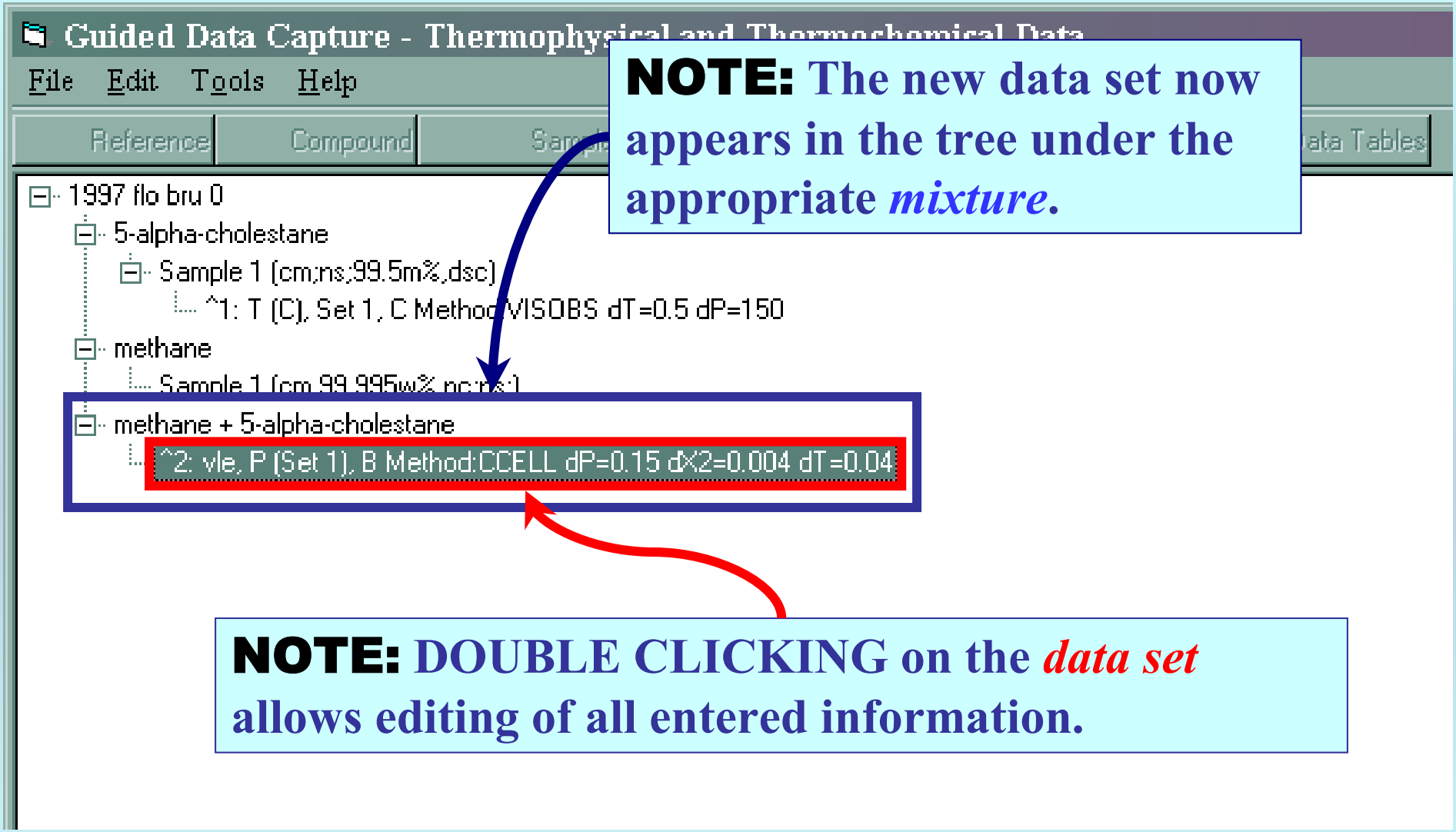


CLICK *View plot* to see an automatic graphical representation of the data. *NOT very helpful in this case!* See next page...


Vapor or Sublimation pressure as function of Mole fraction of 5-alpha-cholestane
Tools Help
200
180
160
140
120
100
80
.01
.03
X = Var 2
X = Var 1
NOTE: SELECTION of an alternative plot variable can yield a more useful plot.
Check for typographical errors, and CLICK OK, when done.
Logarithm of Vapor or Sublimation pressure as function of reciprocal Tempe...
Tools Help
5.2
5
4.6
4.4
.0022
.0024
.0026
.0028
X = Var 2
X = Var 1
Y vs X
OK
NOTE: The curves represent results for each composition.

You are returned to the previous screen...




Guided Data Capture - Thermophysical and Thermochemical Data
File Edit Tools Help
Reference
Compound
Data Tables
1997 flo bru 0
5-alpha-cholestane
Sample 1 (cm;ns;99.5m%,dsc)
^1: T (C), Set 1, C Method:VISOBS dT=0.5 dP=150
methane
methane + 5-alpha-cholestane
^2: vle, P (Set 1), B Method:CCELL dP=0.15 d^2=0.004 dT=0.04
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.**