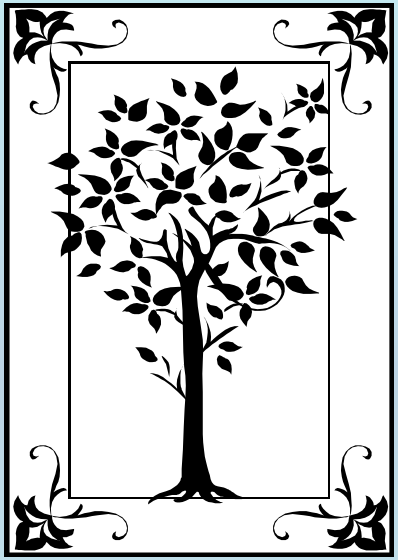
METADATA AND NUMERICAL DATA CAPTURE:
Thermal Expansivity
$\alpha = (1/V_m)(\partial V_m/\partial T)_p$

Guided Data Capture (GDC)



This tutorial describes
METADATA AND NUMERICAL DATA CAPTURE:
THERMAL EXPANSIVITIES
for 1 component
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:

Determination of isobaric thermal expansivity of organic compounds from 0.1 to 30 MPa at 30 °C with an isothermal pressure scanning microcalorimeter

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Thermal expansivities for 1 component
n-hexane

Table 4. Thermal expansivities of n-hexane as a function of pressure at 30°C

P / bar	$10^3\,\alpha$ /K^{-1}	Absolute deviation * / %	$10^3\,\alpha_{literature}$ [2,10] / K^{-1}	Difference ** / %
5	1.353	0.21	1.365 [2]	0.87
10	1.347	0.22		
20	1.338	0.17		
27	1.319	0.18	1.289 [2]	-2.32
40	1.299	0.13		
49	1.287	0.13	1.304 [2]	1.29
60	1.262	0.96		
70	1.250	0.85		
80	1.237	0.78		
90	1.221	0.91		
100	1.210	0.85		
110	1.198	0.81		
120	1.187	0.77		
130	1.176	0.65		
141	1.164	0.65	1.216 [10]	4.24
145	1.161	[illegible]	1.181 [2]	1.68
160	1.147	0.54		
170	1.137	0.47		
180	1.127	0.45		
190	1.118	0.45		
200	1.110	0.40		
210	1.100	0.35		
220	1.092	0.2		
230	1.083	0.2		
245	1.071	0.2		
250	1.069	0.2		
260	1.060	0.2		
270	1.053	0.3		
280	1.045	0.28		
290	1.039	0.34		
300	1.033	0.45		

This data set is considered here.

* : absolute deviation = (average of the absolute deviation of data points from their mean)/arithmetic mean

** : Difference = (literature – results) / literature

In [2], T = 301.5 K and in [10], T = 303.15 K

Experimental Method Info :

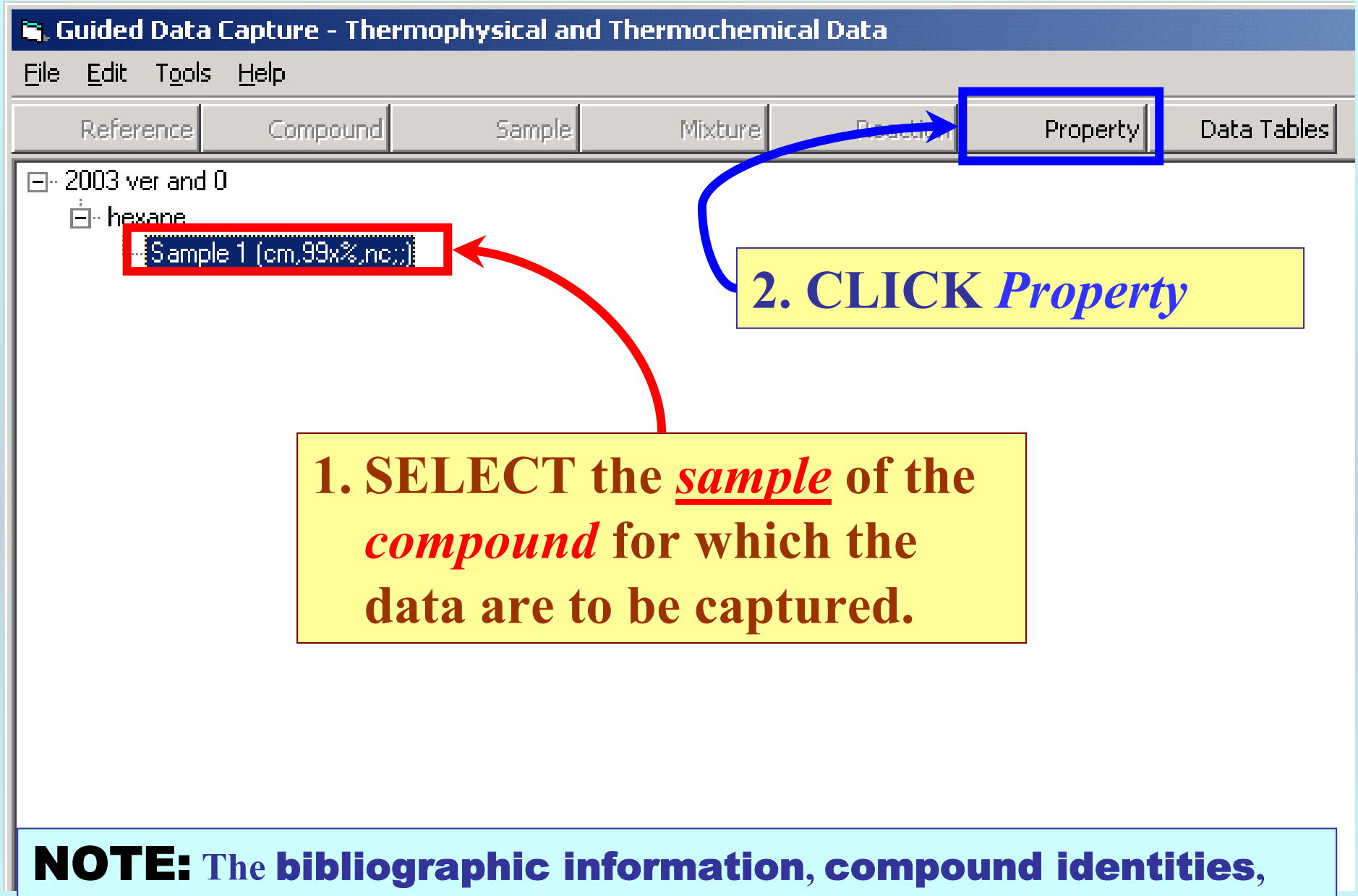
Scanning transitiometry

Uncertainty estimates:

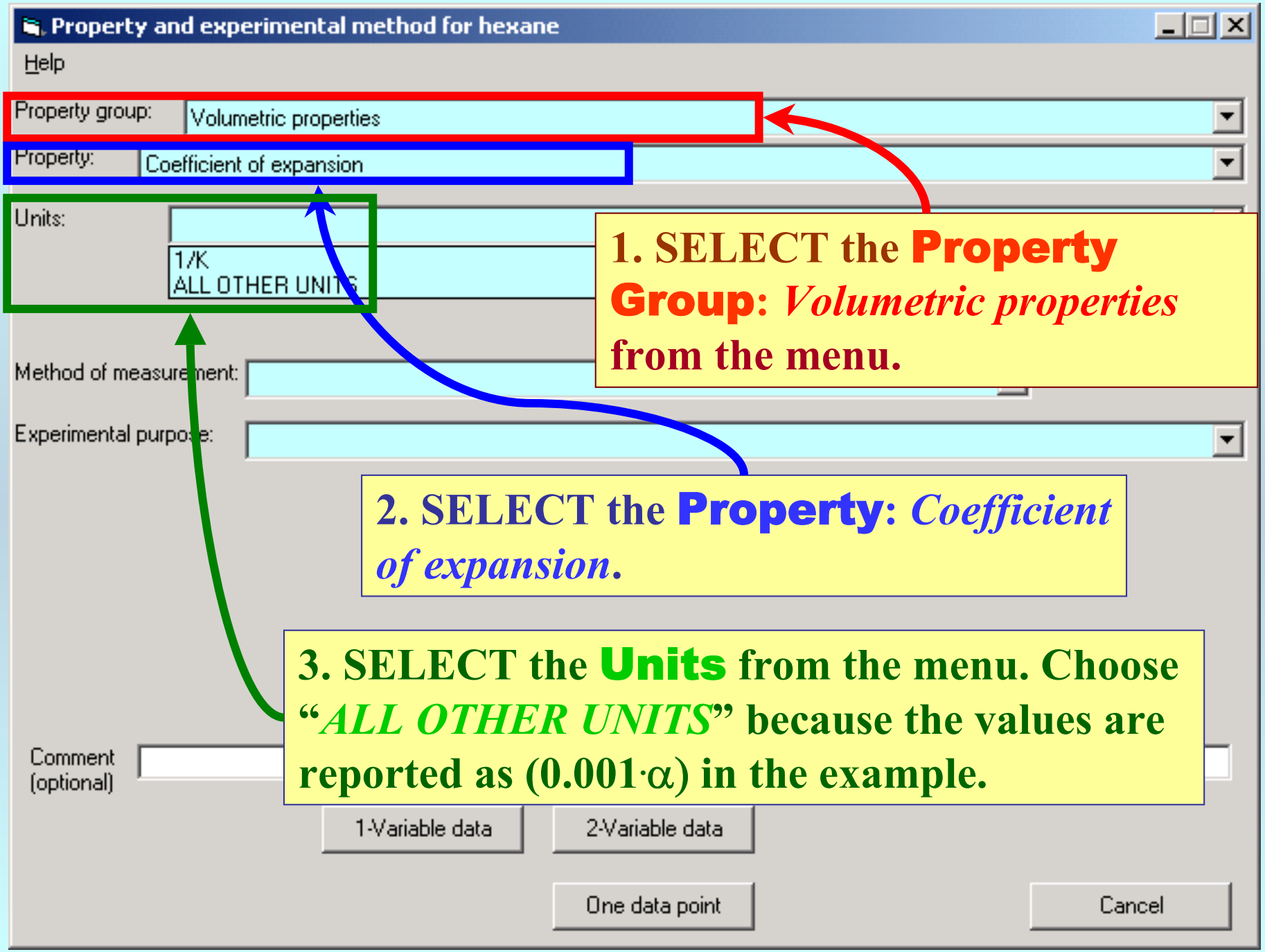
Table 2. Uncertainty of the different sensors

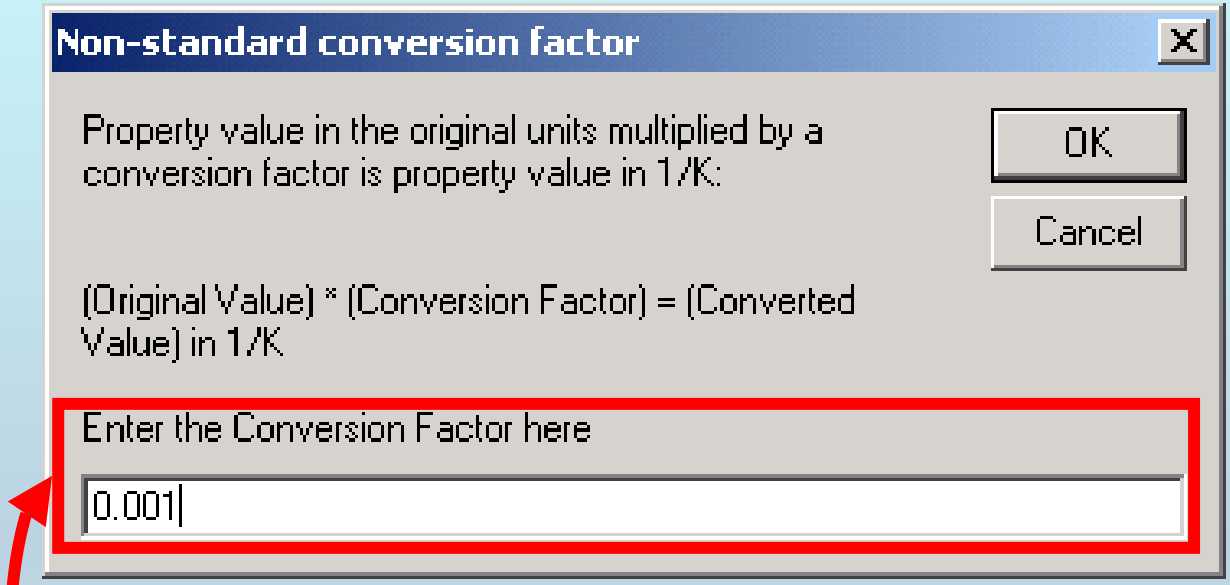
Signals	Sensors	Range	Uncertainty
Pressure	ISCO Pump	0.7 to 514 bar	± 0.5 % of full scale
Temperature	Microcalorimeter	20 to 80 °C	0.03 °C
Time	Computer	-	0.01 s
Voltage (heat signal)	Microcalorimeter	0.15 µW to 3000 µW	0.1 %

the uncertainty has been evaluated at 2 %.

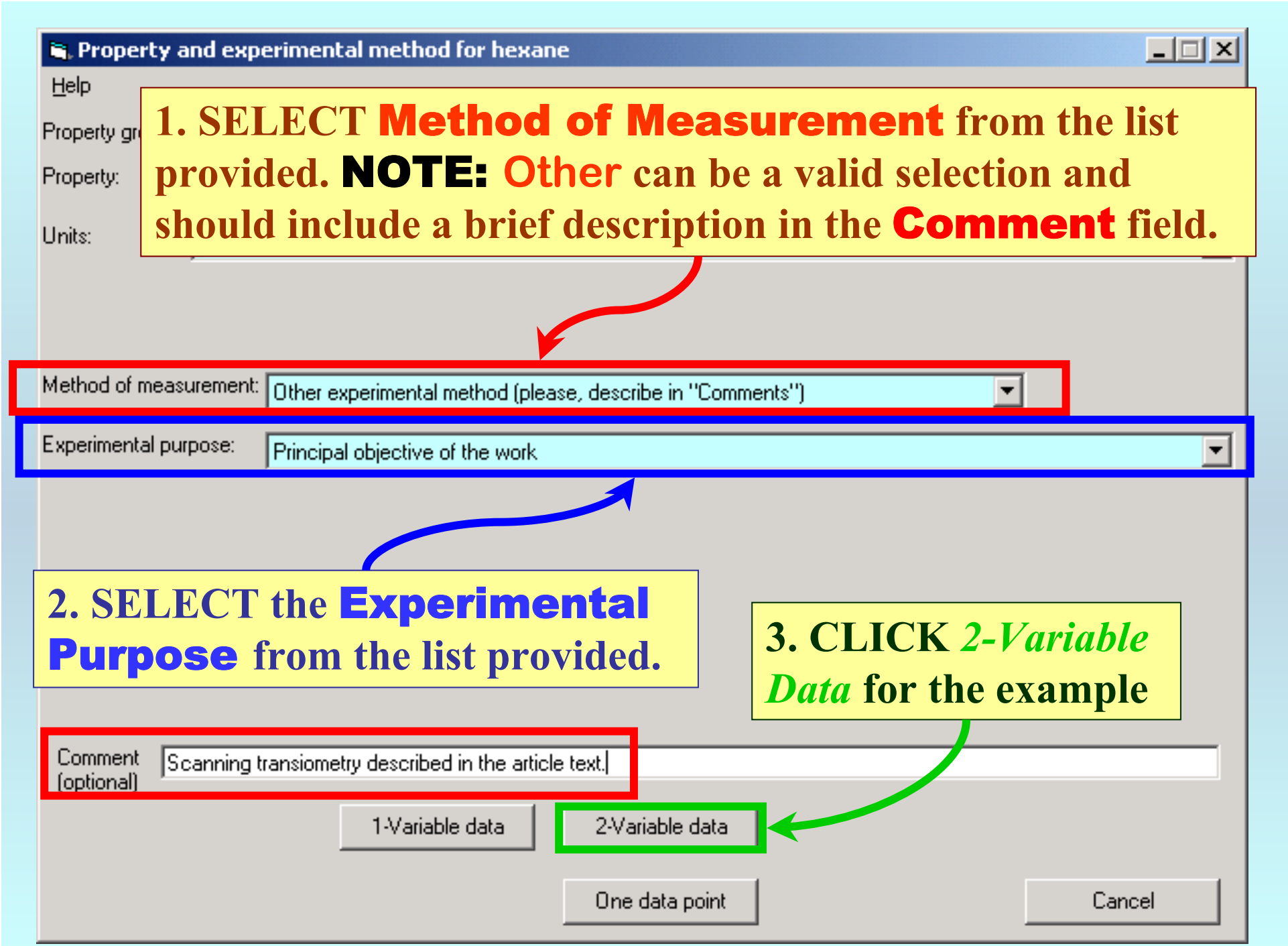


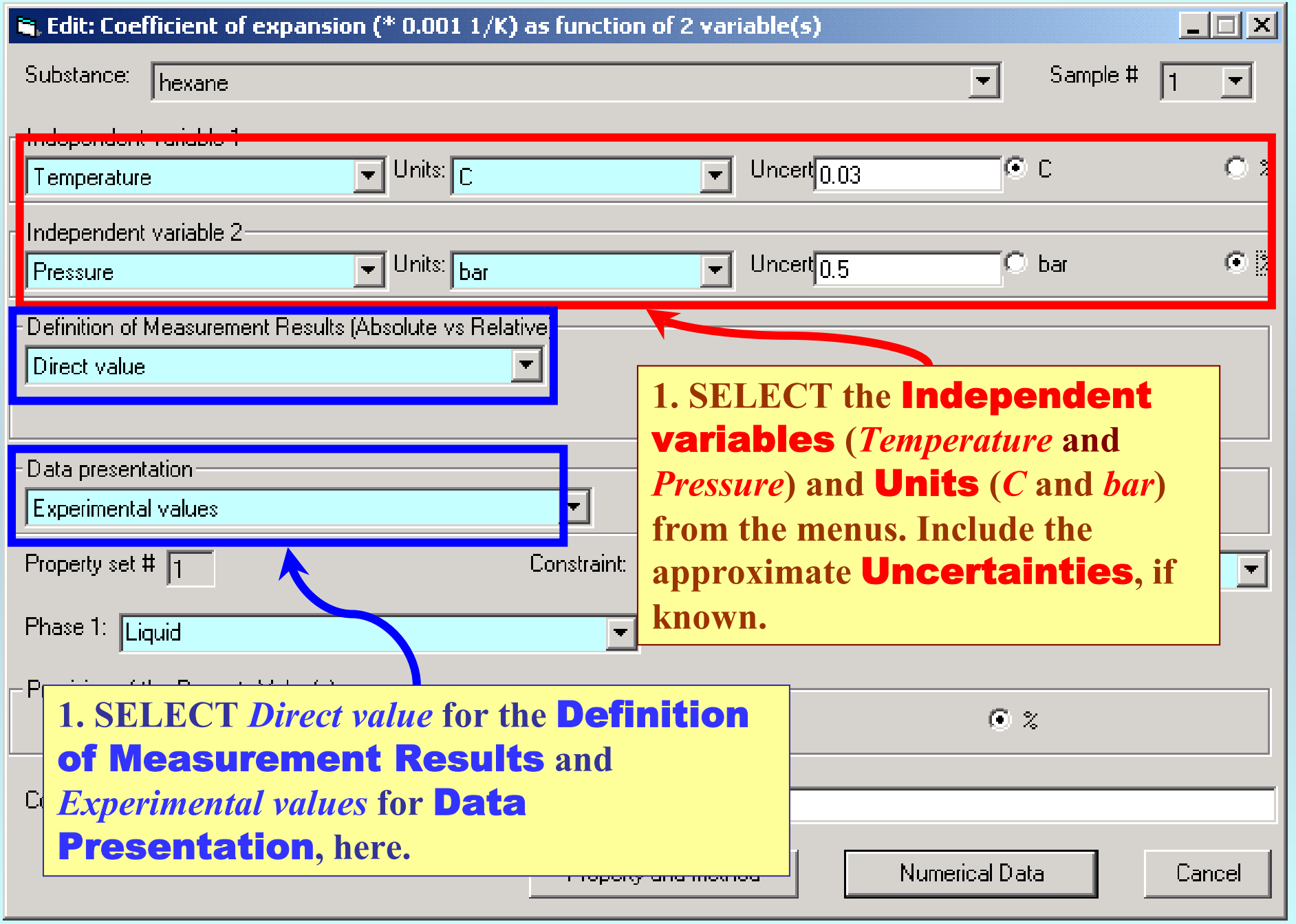
NOTE: The **bibliographic information**, **compound identities**, **sample descriptions**, and **mixture** were entered previously. (There are separate tutorials, which describe capture of this information, if needed.)

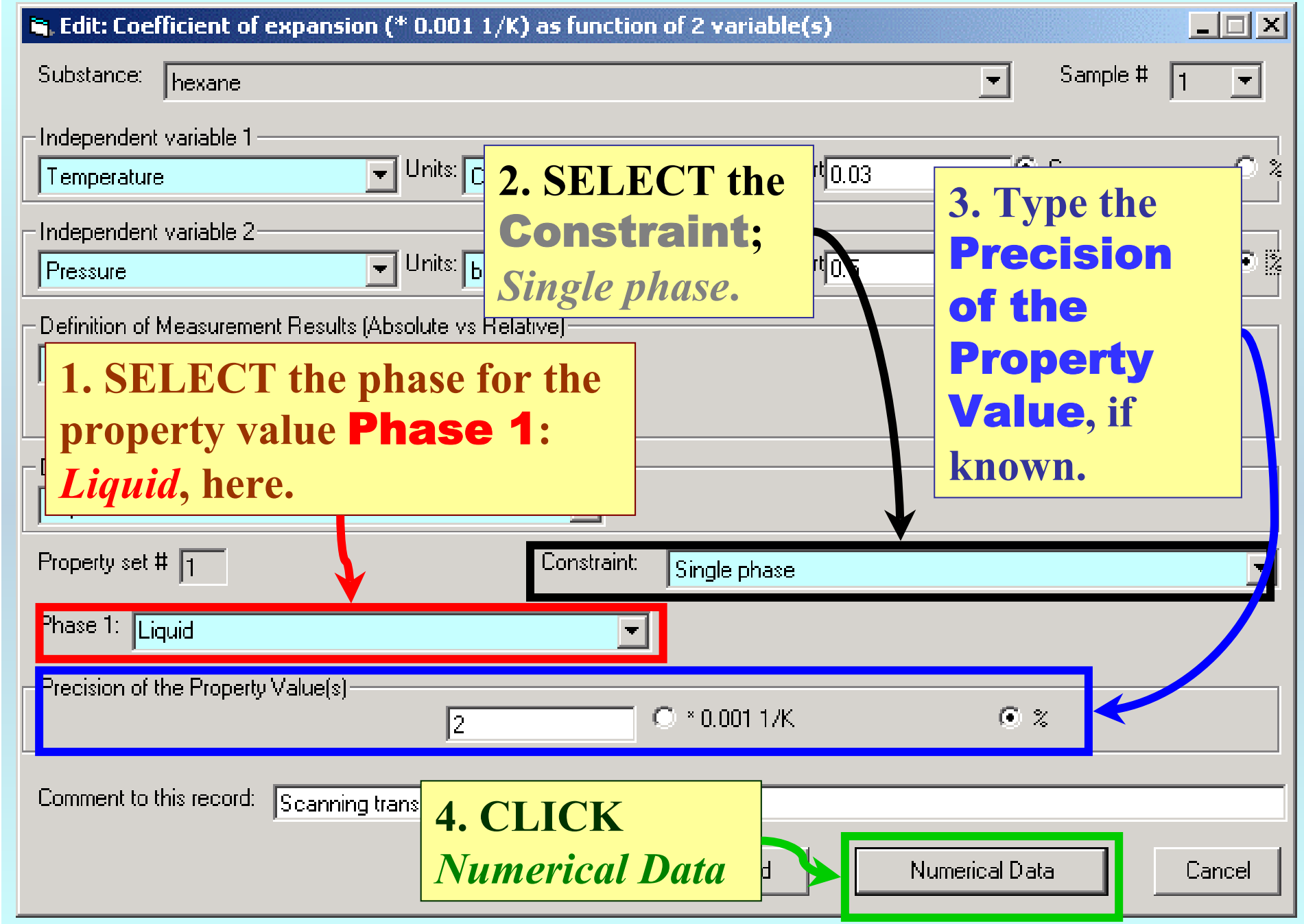

Property and experimental method for hexane
Help
Property group:
Volumetric properties
Property:
Coefficient of expansion
Units:
1/K
ALL OTHER UNITS
Method of measurement:
Experimental purpose:
Comment (optional)
1-Variable data
2-Variable data
One data point
Cancel
1. SELECT the Property Group: Volumetric properties from the menu.
2. SELECT the Property: Coefficient of expansion.
3. SELECT the Units from the menu. Choose "ALL OTHER UNITS" because the values are reported as (0.001·α) in the example.



ENTER the *Conversion Factor* to obtain (1/K). Here, it is 0.001.


Property and experimental method for hexane
Help
Property gr
Property:
Units:
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:
Other experimental method (please, describe in "Comments")
Experimental purpose:
Principal objective of the work
2. SELECT the Experimental Purpose from the list provided.
3. CLICK 2-Variable Data for the example
Comment (optional)
Scanning transiometry described in the article text.
1-Variable data
2-Variable data
One data point
Cancel


Edit: Coefficient of expansion (* 0.001 1/K) as function of 2 variable(s)
Substance:
hexane
Sample #
1
Temperature
Units:
C
Uncert
0.03
C
Independent variable 2
Pressure
Units:
bar
Uncert
0.5
bar
Definition of Measurement Results (Absolute vs Relative)
Direct value
Data presentation
Experimental values
Property set #
1
Constraint:
Phase 1:
Liquid
%
Numerical Data
Cancel
1. SELECT the Independent variables (Temperature and Pressure) and Units (C and bar) from the menus. Include the approximate Uncertainties, if known.
1. SELECT Direct value for the Definition of Measurement Results and Experimental values for Data Presentation, here.


Edit: Coefficient of expansion (* 0.001 1/K) as function of 2 variable(s)
Substance:
hexane
Sample #
1
Independent variable 1
Temperature
Units:
0.03
Independent variable 2
Pressure
Units:
Definition of Measurement Results (Absolute vs Relative)
2. SELECT the Constraint; Single phase.
3. Type the Precision of the Property Value, if known.
1. SELECT the phase for the property value Phase 1: Liquid, here.
Property set #
1
Constraint:
Single phase
Phase 1:
Liquid
Precision of the Property Value(s)
2
* 0.001 1/K
%
Comment to this record:
Scanning trans
4. CLICK Numerical Data
Numerical Data
Cancel

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

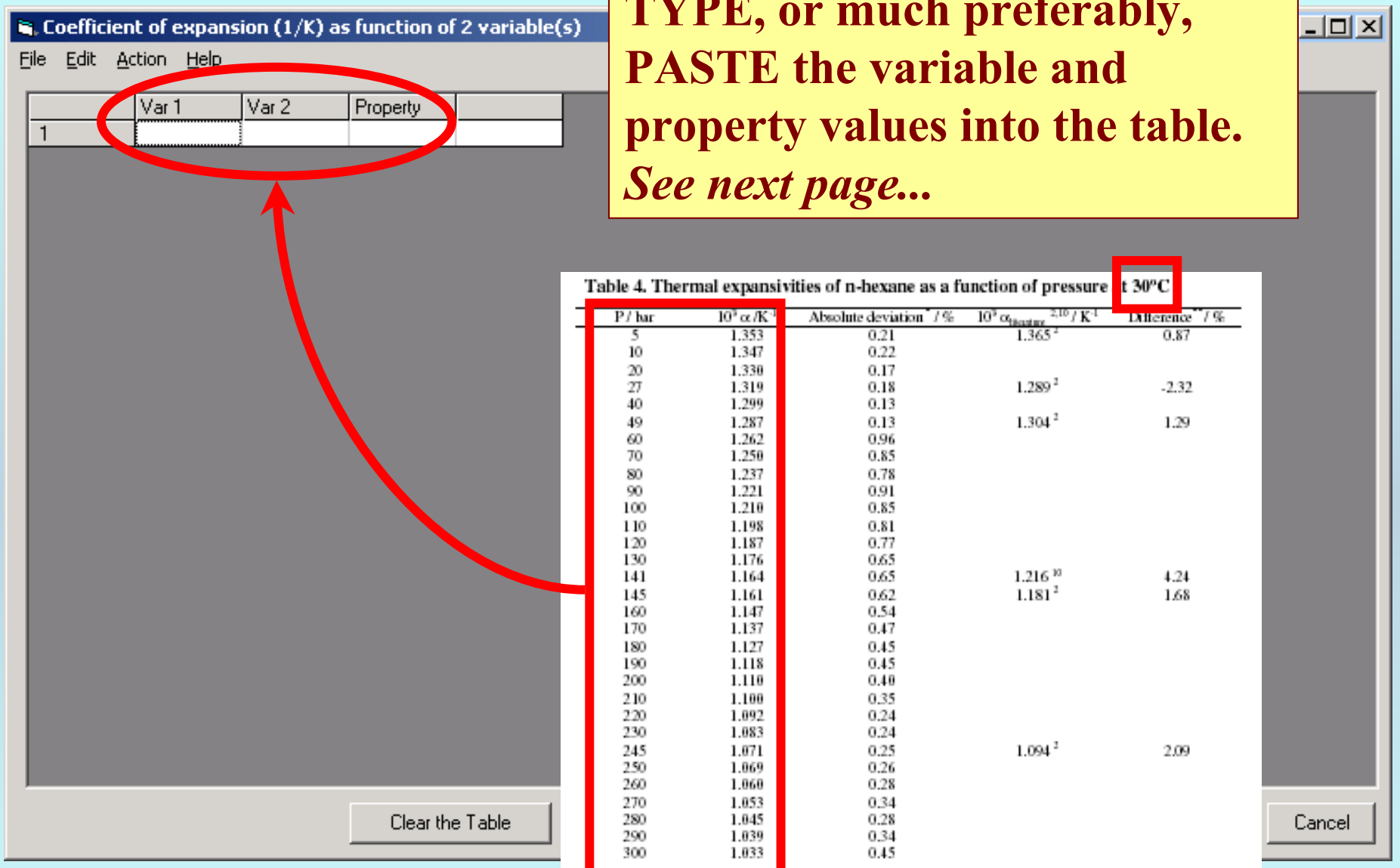


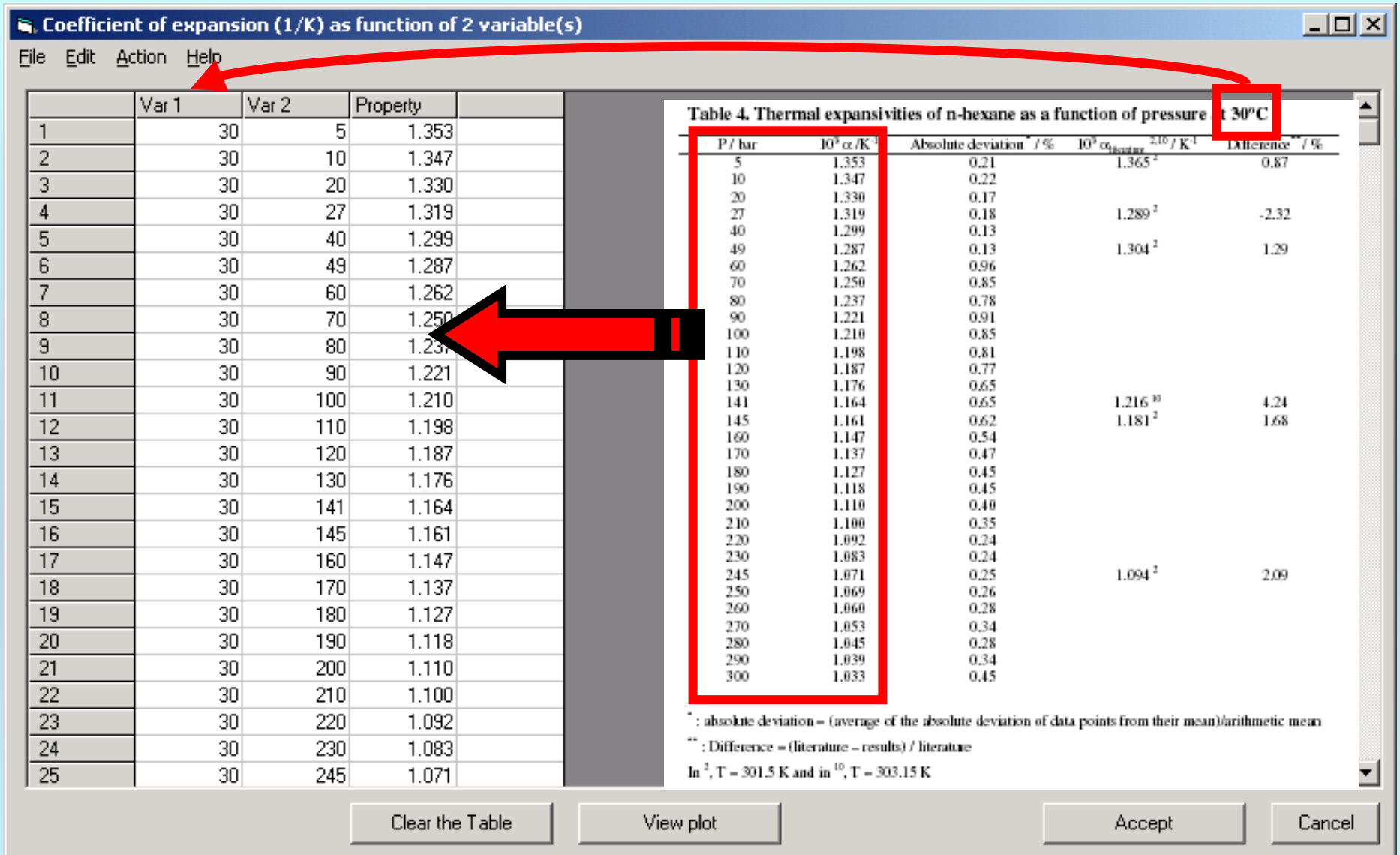
Table 4. Thermal expansivities of n-hexane as a function of pressure at 30°C

P / bar	$10^3 \alpha$ /K^{-1}	Absolute deviation* / %	$10^3 \alpha_{literature}$ [2,10] / K^{-1}	Difference** / %
5	1.353	0.21	1.365 [2]	0.87
10	1.347	0.22		
20	1.330	0.17		
27	1.319	0.18	1.289 [2]	-2.32
40	1.299	0.13		
49	1.287	0.13	1.304 [2]	1.29
60	1.262	0.96		
70	1.250	0.85		
80	1.237	0.78		
90	1.221	0.91		
100	1.210	0.85		
110	1.198	0.81		
120	1.187	0.77		
130	1.176	0.65		
141	1.164	0.65	1.216 [10]	4.24
145	1.161	0.62	1.181 [2]	1.68
160	1.147	0.54		
170	1.137	0.47		
180	1.127	0.45		
190	1.118	0.45		
200	1.110	0.40		
210	1.100	0.35		
220	1.092	0.24		
230	1.083	0.24		
245	1.071	0.25	1.094 [2]	2.09
250	1.069	0.26		
260	1.060	0.28		
270	1.053	0.34		
280	1.045	0.28		
290	1.039	0.34		
300	1.033	0.45		

*: absolute deviation = (average of the absolute deviation of data points from their mean)/arithmetic mean

**: Difference = (literature – results) / literature

In [2], T = 301.5 K and in [10], T = 303.15 K



	Var 1	Var 2	Property
1	30	5	1.353
2	30	10	1.347
3	30	20	1.330
4	30	27	1.319
5	30	40	1.299
6	30	49	1.287
7	30	60	1.262
8	30	70	1.250
9	30	80	1.237
10	30	90	1.221
11	30	100	1.210
12	30	110	1.198
13	30	120	1.187
14	30	130	1.176
15	30	141	1.164
16	30	145	1.161
17	30	160	1.147
18	30	170	1.137
19	30	180	1.127
20	30	190	1.118
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22	30	210	1.100
23	30	220	1.092
24	30	230	1.083
25	30	245	1.071

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245	1.071	0.25	1.094 [2]	2.09
250	1.069	0.26		
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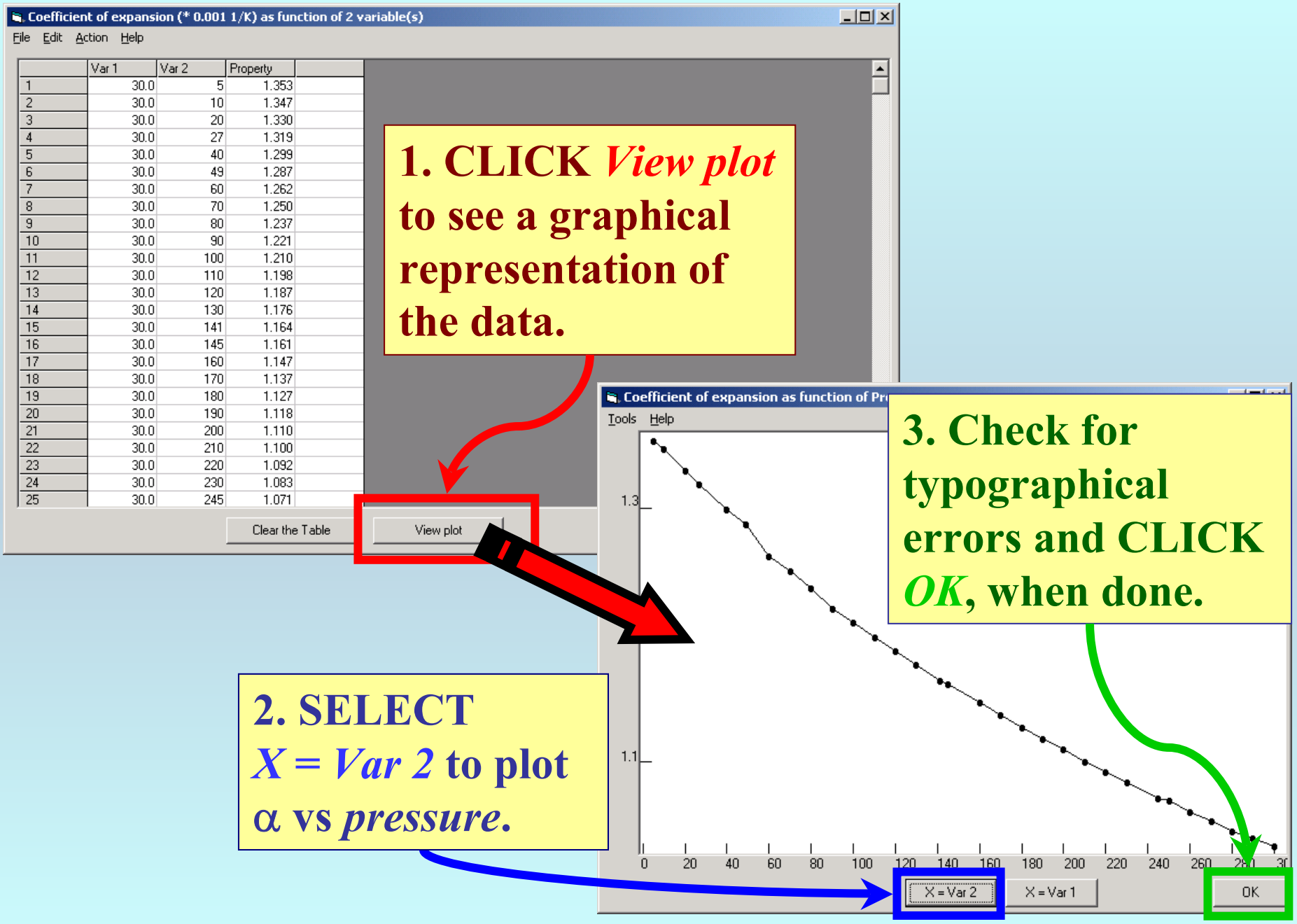
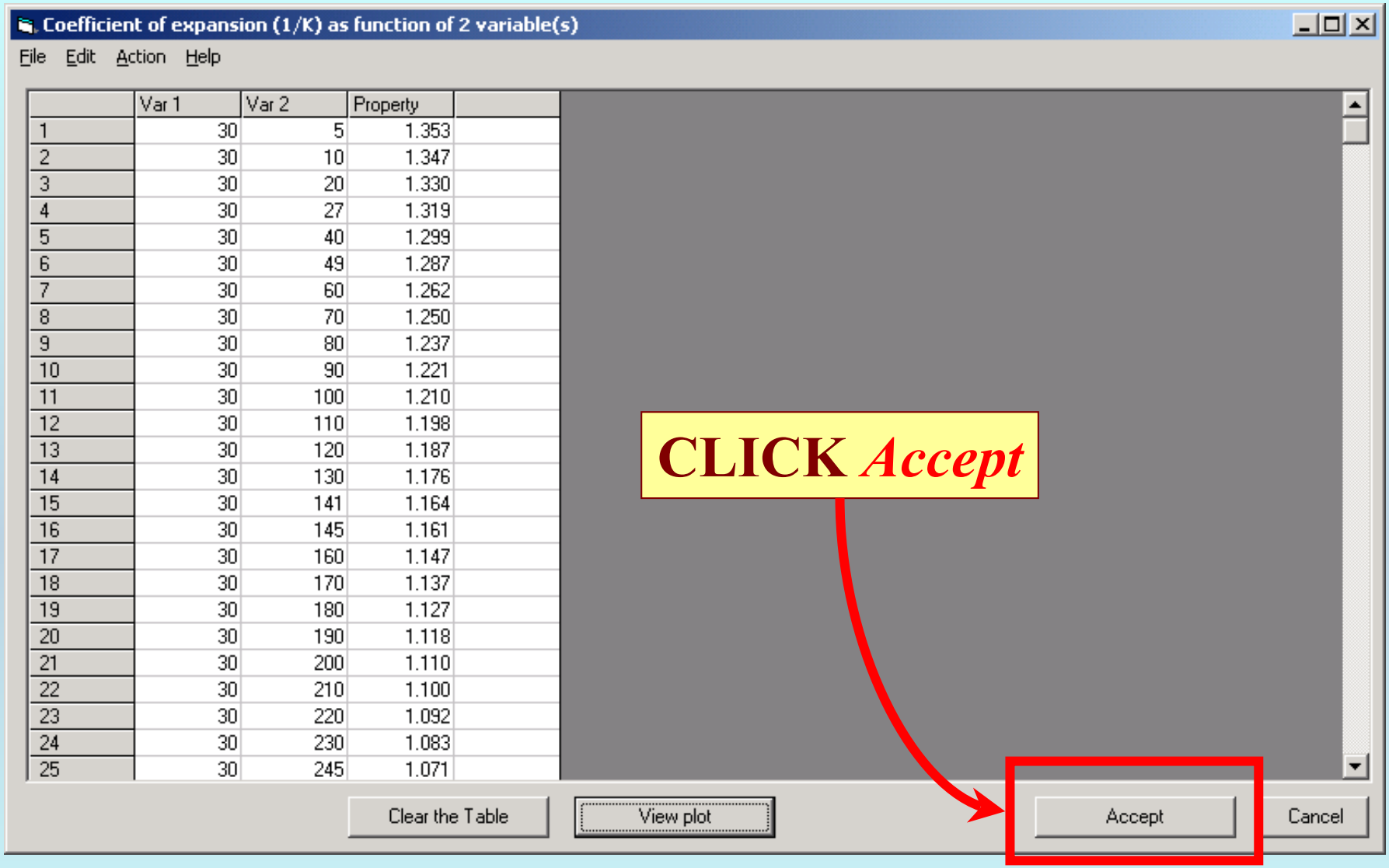
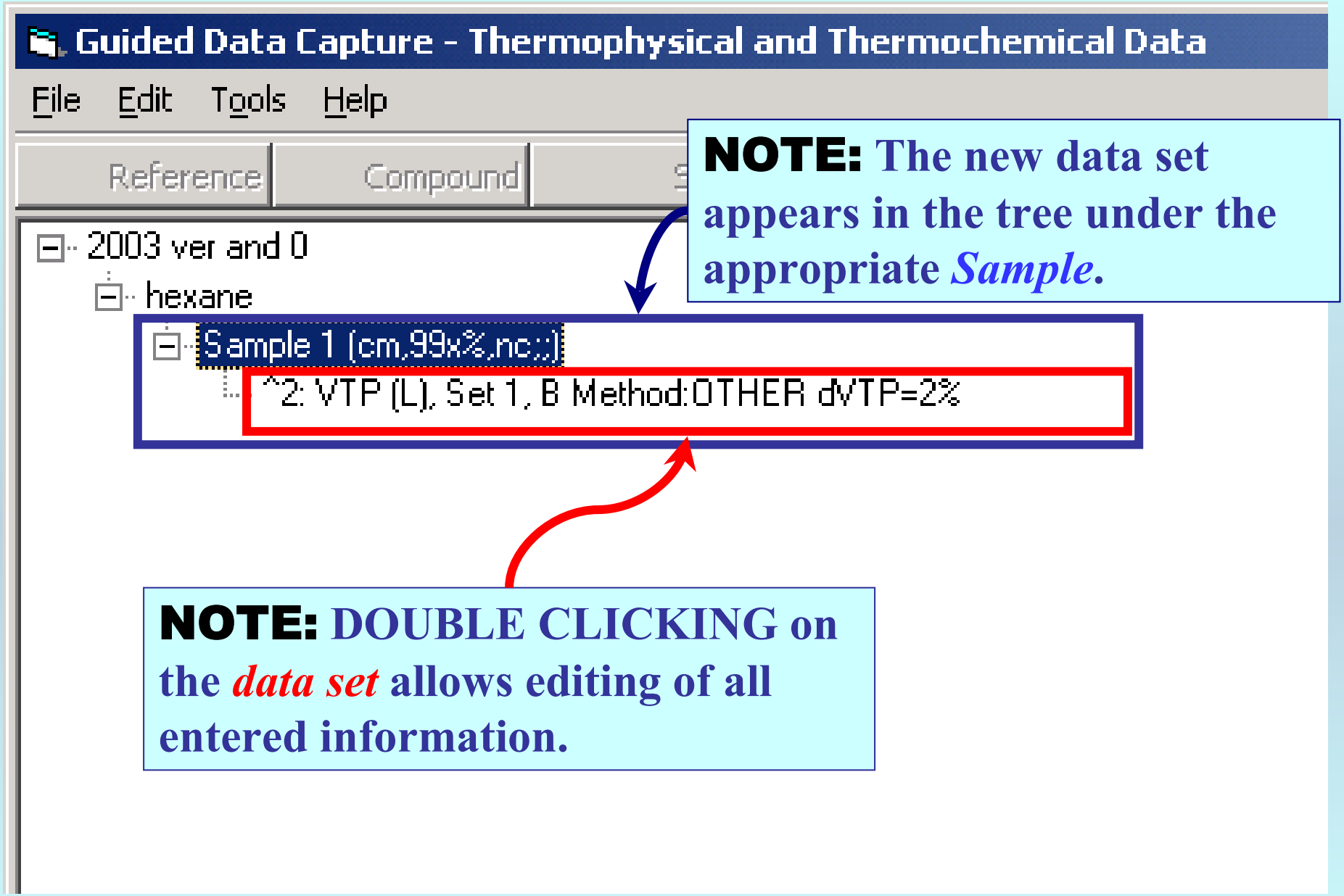
280	1.045	0.28		
290	1.039	0.34		
300	1.033	0.45		

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.)


Coefficient of expansion (* 0.001 1/K) as function of 2 variable(s)
File Edit Action Help
Var 1 Var 2 Property
1 30.0 5 1.353
2 30.0 10 1.347
3 30.0 20 1.330
4 30.0 27 1.319
5 30.0 40 1.299
6 30.0 49 1.287
7 30.0 60 1.262
8 30.0 70 1.250
9 30.0 80 1.237
10 30.0 90 1.221
11 30.0 100 1.210
12 30.0 110 1.198
13 30.0 120 1.187
14 30.0 130 1.176
15 30.0 141 1.164
16 30.0 145 1.161
17 30.0 160 1.147
18 30.0 170 1.137
19 30.0 180 1.127
20 30.0 190 1.118
21 30.0 200 1.110
22 30.0 210 1.100
23 30.0 220 1.092
24 30.0 230 1.083
25 30.0 245 1.071
Clear the Table
View plot
1. CLICK View plot to see a graphical representation of the data.
Coefficient of expansion as function of Pr
Tools Help
1.3
1.1
0 20 40 60 80 100 120 140 160 180 200 220 240 260
X = Var 2
X = Var 1
OK
3. Check for typographical errors and CLICK OK, when done.
2. SELECT X = Var 2 to plot α vs pressure.


Coefficient of expansion (1/K) as function of 2 variable(s)
File Edit Action Help
Var 1 Var 2 Property
1 30 5 1.353
2 30 10 1.347
3 30 20 1.330
4 30 27 1.319
5 30 40 1.299
6 30 49 1.287
7 30 60 1.262
8 30 70 1.250
9 30 80 1.237
10 30 90 1.221
11 30 100 1.210
12 30 110 1.198
13 30 120 1.187
14 30 130 1.176
15 30 141 1.164
16 30 145 1.161
17 30 160 1.147
18 30 170 1.137
19 30 180 1.127
20 30 190 1.118
21 30 200 1.110
22 30 210 1.100
23 30 220 1.092
24 30 230 1.083
25 30 245 1.071
CLICK Accept
Clear the Table
View plot
Accept
Cancel


Guided Data Capture - Thermophysical and Thermochemical Data
File
Edit
Tools
Help
Reference
Compound
2003 ver and 0
hexane
Sample 1 (cm,99x%,nc;;)
^2: VTP (L), Set 1, B Method:OTHER dVTP=2%
NOTE: The new data set appears in the tree under the appropriate Sample.
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.**