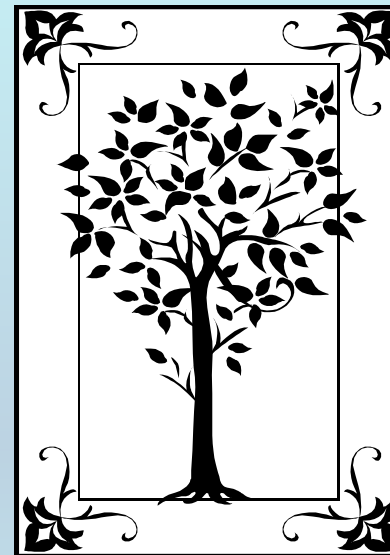


METADATA AND NUMERICAL DATA CAPTURE: **DENSITY** (2 component mixture)

Guided Data Capture (GDC)



This tutorial describes
METADATA AND NUMERICAL DATA CAPTURE:
for **DENSITIES (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 2002, 47, 811–815

811

Density and Refractive Index at 298.15 K and Vapor–Liquid Equilibria at 101.3 kPa for Four Binary Systems of Methanol, *n*-Propanol, *n*-Butanol, or Isobutanol with *N*-Methylpiperazine

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Department of Chemistry, Zhejiang University, Hangzhou 310027, Zhejiang, People's Republic of China

Density and refractive index data at 298.15 K, and isobaric vapor–liquid equilibrium (VLE) measurements at 101.3 kPa were reported for four binary systems of methanol, *n*-propanol, *n*-butanol, or isobutanol with *N*-methylpiperazine. Excess molar volumes and refractive index deviations were calculated. The measurement results exhibit no azeotropes for VLE, negative values for excess molar volume, and positive deviations from ideality for the refractive index over the whole mole fraction range. Liquid-phase activity coefficients and vapor-phase fugacity coefficients were estimated taking into account the nonideal nature of the vapor and liquid phases. The VLE data were shown to be thermodynamically consistent and were correlated by the UNIQUAC liquid-phase activity coefficient model with temperature-dependent parameters.

Densities (liquid phase) for (methanol + N-methylpiperazine) at T = 298.15 K and p = 101.3 kPa

Table 3. Density ρ and Excess Molar Volume V^E for Binary Mixtures of Alkanol (1) + N-Methylpiperazine (2) at 298.15 K

x_1	ρ g·cm ⁻³	V^E cm ³ ·mol ⁻¹	x_1	ρ g·cm ⁻³	V^E cm ³ ·mol ⁻¹
Methanol (1) + NMP (2)			<i>n</i> -Propanol (1) + NMP (2)		
0.0498	0.899 54	-0.225	0.0483	0.898 02	-0.187
0.1050	0.899 14	-0.463	0.1012	0.895 74	-0.361
0.1491	0.898 68	-0.641	0.1395	0.894 07	-0.492
0.2052	0.897 88	-0.848	0.1465	0.893 78	-0.519
0.2503	0.897 23	-1.020	0.1950	0.891 38	-0.661
0.2996	0.896 17	-1.178	0.2439	0.888 98	-0.815
0.3488	0.894 96	-1.330	0.2936	0.886 06	-0.930
0.3989	0.893 39	-1.465	0.3473	0.882 79	-1.056
0.4492	0.891 59	-1.593	0.3914	0.879 95	-1.153
0.5006	0.889 11	-1.686	0.4476	0.875 98	-1.255
0.5618	0.885 69	-1.787	0.4913	0.872 65	-1.323
0.6001	0.882 75	-1.807	0.5452	0.868 03	-1.370
0.6497	0.878 42	-1.822	0.5934	0.863 55	-1.395
0.7052	0.872 25	-1.789	0.6424	0.858 59	-1.399
0.7521	0.865 54	-1.707	0.6922	0.853 04	-1.372
0.8001	0.856 87	-1.563	0.7420	0.846 78	-1.299
0.8490	0.845 58	-1.340	0.7941	0.839 47	-1.177
0.8978	0.831 09	-1.023	0.8425	0.831 79	-1.006
0.9490	0.811 44	-0.571	0.8954	0.822 30	-0.749
			0.9474	0.811 76	-0.419

Experimental Method:

Densities of all the samples were measured by using a vibrating tube digital densimeter, model DMA 602 (Anton Paar), thermostated with a circulating-water bath with a precision of ± 0.01 K. Refractive indices were determined

The data set considered here.

Guided Data Capture - Thermophysical and Thermochemical Data

File Edit Tools Help

Reference Compound Sample Mixture Reaction Property Data

2002 che lei 0

- methanol
 - Sample 1 (cm,99.8x%,nc;x;99.8w%,gic)
- N-methylpiperazine
 - Sample 1 (cm,99.8x%,nc;mv;99.9w%,gic)
- methanol + N-methylpiperazine

1. SELECT the *mixture* for which the property is to be entered.

2. CLICK *Property*

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

Start | http://pubs... | N\TRC ... | Guided D... | N\TRC ... | Microsoft... | Table of ... | Guided ... | 12:00 PM

Property Group selection

1. **CLICK** in the **property group** field.

Property and experimental method for methanol + N-methylpiperazine

Help

Property group: [dropdown menu]

Property: [checkbox] Critical properties
[checkbox] Vapor pressure; Boiling temperature; and Azeotropic T & P
[checkbox] Phase transition properties
[checkbox] Composition at phase equilibrium
[checkbox] Activity; Fugacity; and Osmotic properties
[checkbox] **Volumetric properties**
[checkbox] Heat capacity and derived properties
[checkbox] Excess; partial; and apparent energetic properties

Units: [dropdown menu]

Method of measurement: [dropdown menu]

Experimental purpose: [dropdown menu]

Comment (optional) [text field]

Cancel

2. **SELECT Volumetric properties** from the menu.

Property selection

1. **CLICK** in the **Property** field.

Property and experimental method for methanol + N-methylpiperazine

Help

Property group: Volumetric properties

Property: **Specific density**

Units: Molar density

Method of measurement: 3rd virial coefficient

Experimental purpose:

Comment (optional)

Cancel

2. **SELECT specific density** from the menu.

Units selection

1. **CLICK** in the **Units** field.

Property and experimental method for methanol + N-methylpiperazine

Help

Property group: Volumetric properties

Property: Specific density

Units: **kg/m3**
g/cm3
lb/ft3
ALL OTHER UNITS

Method of measurement:

Experimental purpose:

Comment (optional)

Table of values

Single value

Cancel

2. **SELECT** the **Units** from the menu.

Method selection

1. **CLICK** in the **Method of measurement** field.

Property and experimental method for methanol + N

Help

Property group: Volumetric properties

Property: Specific density

Units: g/cm³

Method of measurement:

Experimental purpose:

- Pycnometric method
- Buoyancy method
- Vibrating tube method
- Anchoring PVT measurement
- Other PVT measurement
- Burnett expansion technique
- Constant-volume pycnometry
- Other experimental method (please, describe in "Comments")

Comment (optional)

Table of values

Single value

Cancel

2. **SELECT** a **Method** from the menu, which best describes your experiment

Note: *Other* is an option. A one sentence description or a reference is often adequate.

Method detail selection

Experiment details

Select the statements, which are true for the reported measurement

More than two calibration points used

Accept

Note: For a few methods, additional details are requested. **SELECT** those statements that apply, and **CLICK** *Accept*.

Experimental purpose selection

The screenshot shows a software window titled "Property and experimental method for me". It contains several input fields and a dropdown menu. A yellow box with a red border at the top right contains the text "1. CLICK in the Experimental purpose field." with a red arrow pointing to the dropdown menu. A blue oval highlights the first two items in the dropdown menu, and a blue arrow points from a yellow box at the bottom right to this oval. The yellow box at the bottom right contains the text "2. SELECT the purpose from the menu." The interface includes fields for "Property" (Specific density), "Units" (g/cm3), "Method of measurement" (Vibrating tube method), and "Experimental purpose" (Principal objective of the work). There are also radio buttons for "In original units (as in the source)" and "In system units (converted)", and a "Comment (optional)" field at the bottom.

Property: Specific density

Units: g/cm3

You are entering the data:

In original units (as in the source) In system units (converted)

Method of measurement: Vibrating tube method

Experimental purpose: Principal objective of the work
Principal objective of the work
Secondary purpose (by-product of other objective)
Determined for identification of a synthesized compound

Comment (optional)

1. CLICK in the **Experimental purpose** field.

2. SELECT the **purpose** from the menu.

Form is complete...

Property and experimental method for methanol + N-methylpiperazine

Help

Property group: Volumetric properties

Property: Specific density

Units: g/cm³

Method of measurement: Vibrating tube method Details...

Experimental purpose: Principal objective of the work

Comment (optional)

Table of values

Single value

Cancel

1. CLICK
Table of values

Specification of phases and constraints

Specific density as function of 1 variable(s)

Mixture: methanol + N-methylpiperazine

Phases in equilibrium: 1 Constraints: 0

Independent variables: Property set # 1 Sample # 1 Sample # 1

Phase of the Property Value(s) Precision of the Property Value(s)

0
1
2

g/cm3 %

1. SELECT # of **Phases** from the pulldown list:
(one here - liquid)

2. SELECT # of **Constraints** from the pulldown list:
(two here - T and p)

Definition of Measurement Results (Absolute vs Relative)

Data presentation
Experimental values

Comments (Optional):

Property and method Numerical Data Cancel

Specific density (kg/m³) as function of 1 variable(s)

Mixture: methanol + N-methylpiperazine

Phases in equilibrium: 1 Constraints: 2 Independent variables: 1 Property set #: 1 Sample #: 1 Sample #: 1

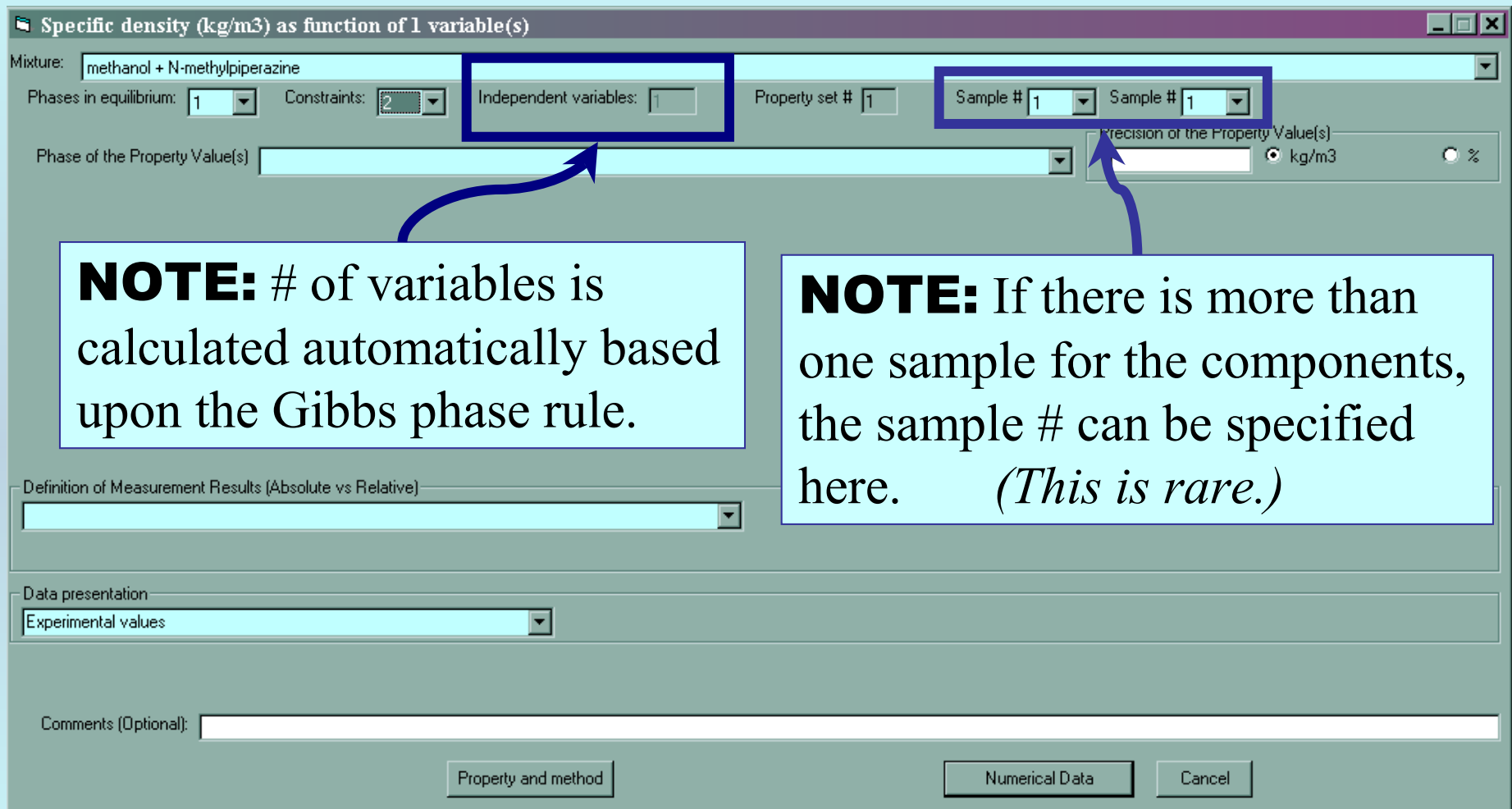
Phase of the Property Value(s) Precision of the Property Value(s) kg/m³ %

Definition of Measurement Results (Absolute vs Relative)

Data presentation: Experimental values

Comments (Optional):

Property and method Numerical Data Cancel



NOTE: # of variables is calculated automatically based upon the Gibbs phase rule.

NOTE: If there is more than one sample for the components, the sample # can be specified here. *(This is rare.)*

Phase of the property value selection

Mixture: methanol + N-methylpiperazine

Phases in equilibrium: 1 Constraints: 2 Independent variables: 1 Property set # 1 Sample # 1 Sample # 1

Phase of the Property Value(s):

- Glass
- Glass of pure methanol
- Glass of pure N-methylpiperazine
- Liquid
- Liquid of pure methanol
- Liquid of pure N-methylpiperazine
- Liquid mixture 1
- Liquid mixture 2

Precision of the Property Value(s): g/cm3 %

Data presentation: Experimental values

Comments (Optional):

Property and method Numerical Data Cancel

1. CLICK in the **Phase of the Property Values field**

2. SELECT the **Phase associated with the property values from the menu; (*liquid* here).**

Specific density (kg/m³) as function of 1 variable(s)

Mixture:

Phases in equilibrium: Constraints: Independent variables: Property set # Sample # Sample #

Phase of the Property Value(s) Precision of the Property Value(s) kg/m³ %

Constraint 1 (Fixed value of) of Units: Uncertainty:

Constraint 2 (Fixed value of) of Units: Uncertainty:

Independent variable 1 of Units: Uncertainty: %

Definition of Measurement Results (Absolute vs Relative)

Data presentation

Comments (Optional):

NOTE: Fields for specification of *constraints*, *variables*, *units*, and *uncertainties*, appear automatically based on the Gibbs Phase Rule.

Variable and constraint identification

Specific density (g/cm³) as function of 1 variable(s)

Mixture: methanol + N-methylpiperazine

Phases in equilibrium: 1 Constraints: 2 Independent variables: 1 Property set # 1 Sample # 1 Sample # 1

Phase of the Property Value(s) Liquid Precision of the Property Value(s) g/cm³ %

Constraint 1 (Fixed value of) Temperature of Liquid Value: Units: K Uncertainty: %

Constraint 2 (Fixed value of) Pressure of Liquid Value: Units: Uncertainty: %

Independent variable 1 of Liquid Units: Uncertainty: %

- Temperature
- Pressure
- Partial pressure of methanol
- Partial pressure of N-methylpiperazine
- Partial pressure of component 3
- Mole fraction of methanol
- Mole fraction of N-methylpiperazine
- Weight fraction of methanol

Data presentation Experimental values

Comments (Optional):

Property and method Numerical Data Cancel

Identify **Constraints** and **Variables** from the menus provided.

Entry of values for constraints

Specific density (g/cm³) as function of 1 variable(s)

Mixture: methanol + N-methylpiperazine

Phases in equilibrium: 1 Constraints: 2 Independent variables: 1 Property set # 1 Sample # 1 Sample # 1

Phase of the Property Value(s) Liquid Precision of the Property Value(s) g/cm³ %

Constraint 1 (Fixed value of) Temperature of Liquid Value: 298.15 Units: K Uncertainty: %

Constraint 2 (Fixed value of) Pressure of Liquid Value: 1 Units: kPa Uncertainty: %

Independent variable 1 Mole fraction of methanol of Liquid

Definition of Measurement Results (Absolute vs Relative)

Data presentation Experimental values

Comments (Optional):

Property a

TYPE Values for the constraints and **SELECT Units** from the menus.

Capture of precisions, if known

The screenshot shows a software window titled "Specific density (g/cm³) as function of 1 variable(s)". The interface includes several input fields and dropdown menus. A red box highlights the "Precision of the Property Value(s)" section, which contains a text input field and a radio button for "g/cm³". Three other red boxes highlight the "Uncertainty" input fields for "Temperature" (value 298.15, units K), "Pressure" (value 1, units bar), and "Mole fraction of methanol" (units Dimensionless). Red arrows point from a central yellow text box to these three uncertainty input fields.

TYPE Values for the
precisions of the properties,
variables, and constraints, if
known.

NOTE: Only the precision of temperature was provided by the authors in this example.

Define results: Absolute vs Relative

Specific density (g/cm³) as function of 1 variable(s)

Mixture: methanol + N-methylpiperazine

Phases in equilibrium: 1 Constraints: 2 Independent variables: 1 Property set #: 1 Sample #: 1 Sample #: 1

Phase of the Property Value(s): Liquid Precision of the Property Value(s): g/cm³

Constraint 1 (Fixed value of): Temperature of Liquid Value: 298.15 Units: K Uncertainty: 0.01 %

Constraint 2 (Fixed value of): Pressure of Liquid Uncertainty: %

Independent variable 1: Mole fraction of methanol of Liquid Uncertainty: %

Definition of Measurement Results (Absolute vs Relative)

- Direct value
- Rel. to ref. phase with same composition at FIXED T and P
- Rel. to ref. phase with SAME composition, T and P
- Rel. to mixture in EQUIL. with primary phase at same T and P
- Rel. to pure COMPONENTS in same proportion at same T and P
- Rel. to pure SOLVENT at T of same phase EQUILIBRIUM
- Rel. to pure SOLVENT at same T and P
- Rel. to pure SOLUTE at same T and P

Comments (Optional):

Property and method Numerical Data Cancel

SELECT *Direct* values from the menu.

NOTE: Other options are typically for data reported as relative values (e.g., relative to the density of the pure solvent). These are not common.

Form is complete...

Specific density (g/cm³) as function of 1 variable(s)

Mixture:

Phases in equilibrium: Constraints: Independent variables: Property set # Sample # Sample #

Phase of the Property Value(s) Precision of the Property Value(s) g/cm³ %

Constraint 1 (Fixed value of) of Value: Units: Uncertainty: %


Constraint 2 (Fixed value of) of Value: Units: Uncertainty: %

Independent variable 1 of Units: Uncertainty: %

Definition of Measurement Results (Absolute vs Relative)

Data presentation

Comments (Optional):



Specific density (kg/m³) as function of 1 variable(s)

File Edit Action Help

Var 1	Property
1	

TYPE or (preferably) PASTE (from WORD, EXCEL, etc.) the **Variable** (mole fraction of methanol) and **Property** (density) values.

Clear the Table View plot Accept Cancel

Specific density (g/cm³) as function of 1 variable(s)

File Edit Action Help

	Var 1	Property
1	0.0498	0.89954
2	0.1050	0.89914
3	0.1491	0.89868
4	0.2052	0.89788
5	0.2503	0.89723
6	0.2996	0.89617
7	0.3488	0.89496
8	0.3989	0.89339
9	0.4492	0.89159
10	0.5006	0.88911
11	0.5618	0.88569
12	0.6001	0.88275
13	0.6497	0.87842
14	0.7052	0.87225
15	0.7521	0.86554
16	0.8001	0.85687
17	0.8490	0.84558
18	0.8978	0.83109
19	0.9490	0.81144



Table 3. Density ρ and Excess Molar Volume V^E for Binary Mixtures of Alkanol (1) + *N*-Methylpiperazine (2) at 298.15 K

	ρ		V^E			ρ		V^E	
x_1	g·cm ⁻³		cm ³ ·mol ⁻¹		x_1	g·cm ⁻³		cm ³ ·mol ⁻¹	
Methanol (1) + NMP (2)					<i>n</i> -Propanol (1) + NMP (2)				
0.0498	0.899 54		-0.225		0.0483	0.898 02		-0.187	
0.1050	0.899 14		-0.463		0.1012	0.895 74		-0.361	
0.1491	0.898 68		-0.641		0.1395	0.894 07		-0.492	
0.2052	0.897 88		-0.848		0.1465	0.893 78		-0.519	
0.2503	0.897 23		-1.020		0.1950	0.891 38		-0.661	
0.2996	0.896 17		-1.178		0.2439	0.888 98		-0.815	
0.3488	0.894 96		-1.330		0.2936	0.886 06		-0.930	
0.3989	0.893 39		-1.465		0.3473	0.882 79		-1.056	
0.4492	0.891 59		-1.593		0.3914	0.879 95		-1.153	
0.5006	0.889 11		-1.686		0.4476	0.875 98		-1.255	
0.5618	0.885 69		-1.787		0.4913	0.872 65		-1.323	
0.6001	0.882 75		-1.807		0.5452	0.868 03		-1.370	
0.6497	0.878 42		-1.822		0.5934	0.863 55		-1.395	
0.7052	0.872 25		-1.789		0.6424	0.858 59		-1.399	
0.7521	0.865 54		-1.707		0.6922	0.853 04		-1.372	
0.8001	0.856 87		-1.563		0.7420	0.846 78		-1.299	
0.8490	0.845 58		-1.340		0.7941	0.839 47		-1.177	
0.8978	0.831 09		-1.023		0.8425	0.831 79		-1.006	
0.9490	0.811 44		-0.571		0.8954	0.822 30		-0.749	
					0.9474	0.811 76		-0.419	

Clear the Table

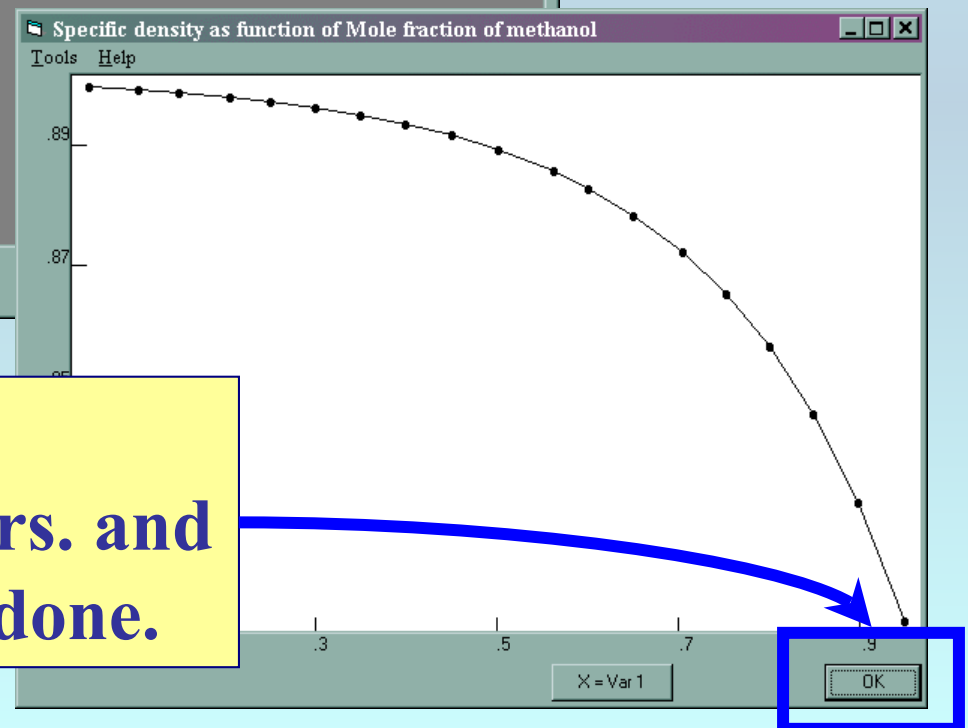
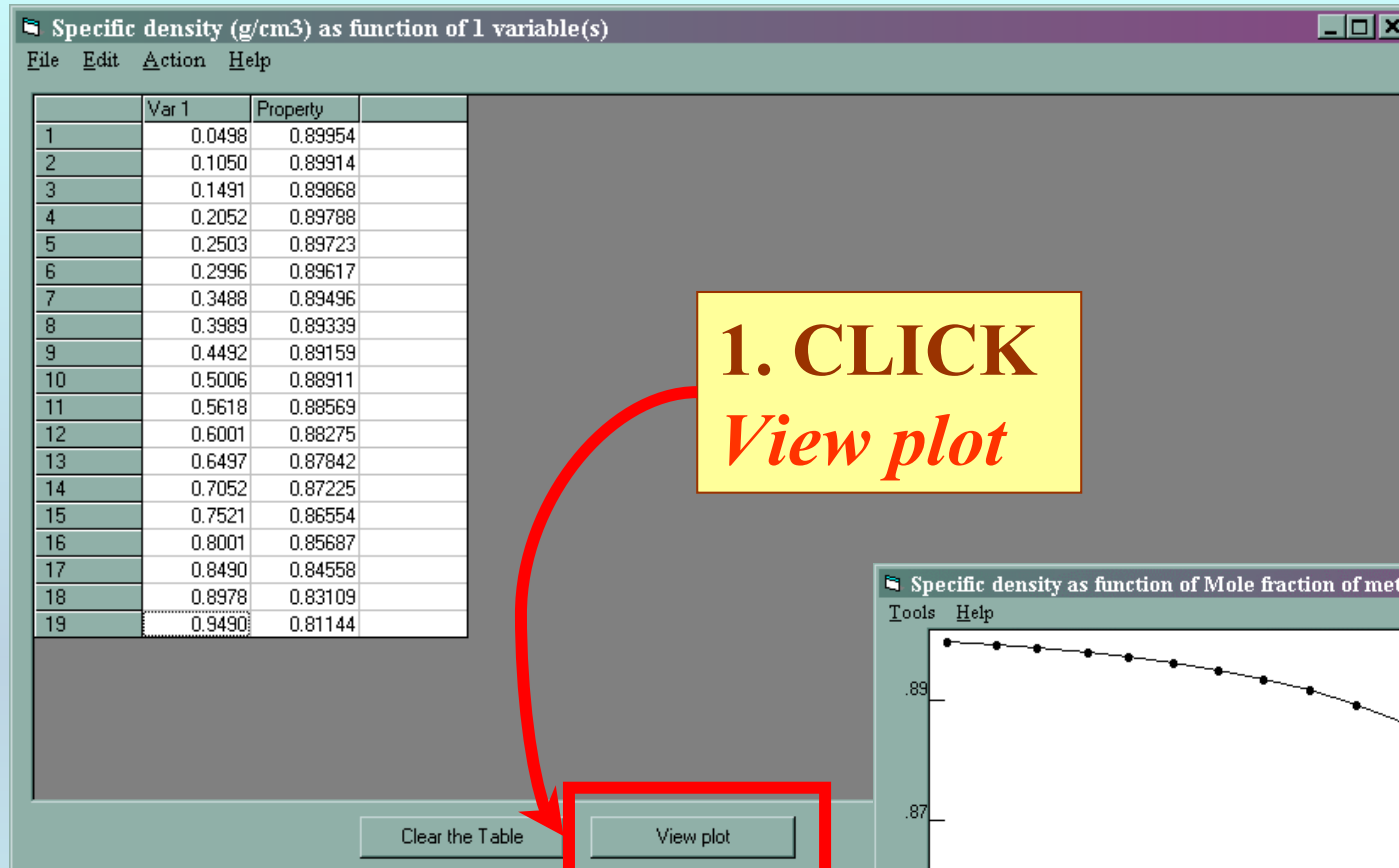
View plot

Accept

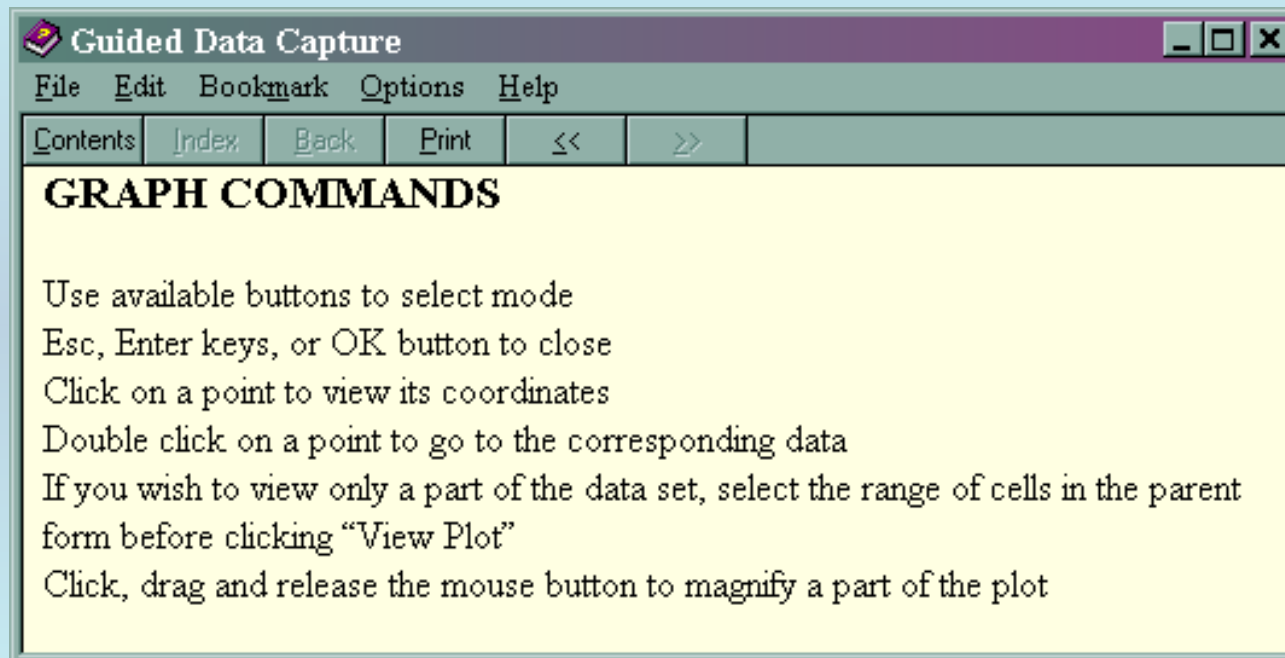
Cancel

Type or (preferably) Paste from WORD, EXCEL, etc.

Graphical check for typographical errors



NOTE: The plots have several useful features. See the *HELP* screen on the plot.



Final acceptance

Specific density (g/cm³) as function of 1 variable(s)

File Edit Action Help

	Var 1	Property
1	0.0498	0.89954
2	0.1050	0.89914
3	0.1491	0.89868
4	0.2052	0.89788
5	0.2503	0.89723
6	0.2996	0.89617
7	0.3488	0.89496
8	0.3989	0.89339
9	0.4492	0.89159
10	0.5006	0.88911
11	0.5618	0.88569
12	0.6001	0.88275
13	0.6497	0.87842
14	0.7052	0.87225
15	0.7521	0.86554
16	0.8001	0.85687
17	0.8490	0.84558
18	0.8978	0.83109
19	0.9490	0.81144

Clear the Table View plot **Accept** Cancel

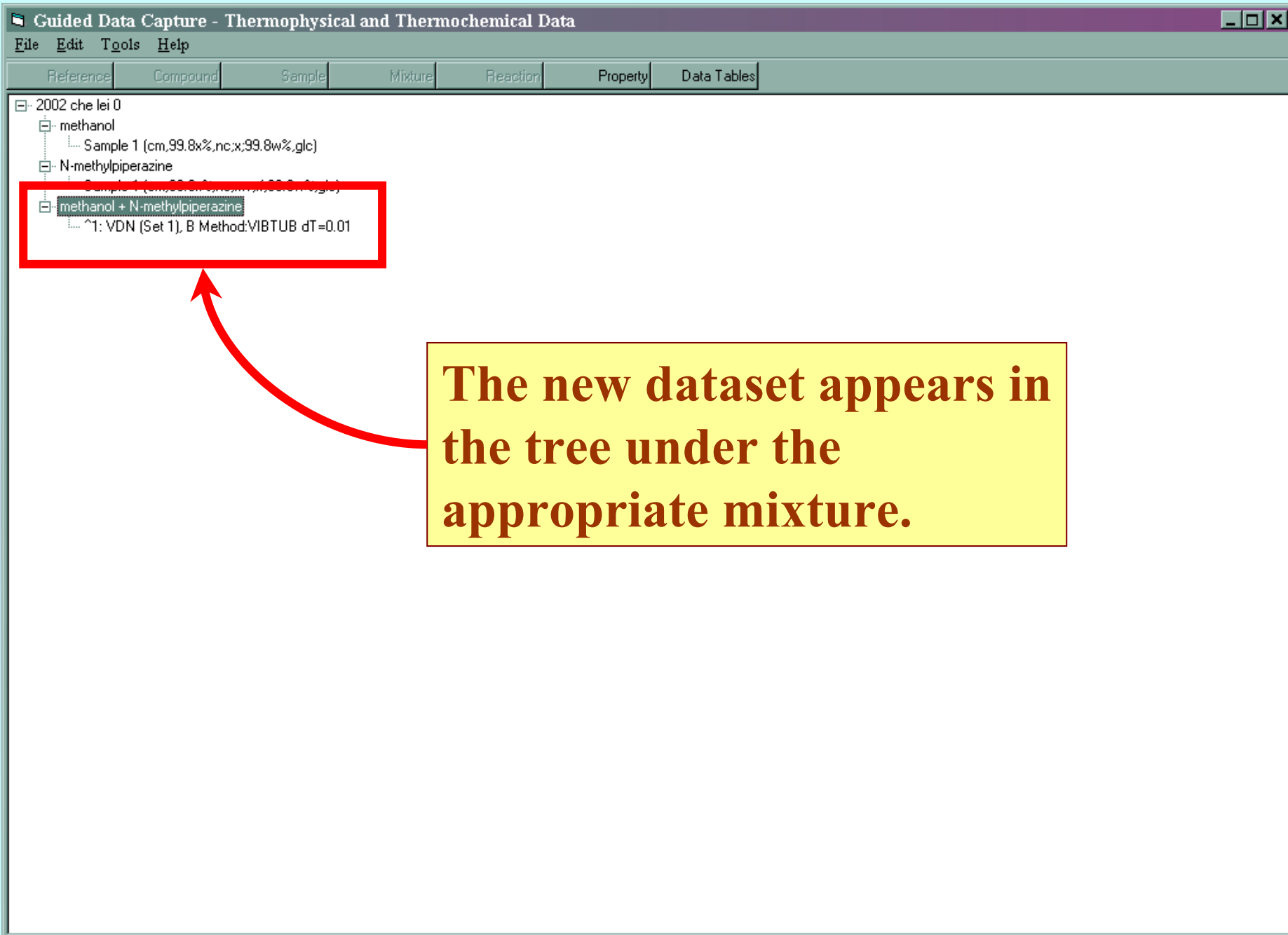
CLICK Accept

Guided Data Capture - Thermophysical and Thermochemical Data

File Edit Tools Help

Reference Compound Sample Mixture Reaction Property Data Tables

- 2002 che lei 0
 - methanol
 - Sample 1 (cm,99.8x%,nc,x;99.8w%,glc)
 - N-methylpiperazine
 - Sample 1 (cm,99.8x%,nc,x;99.8w%,glc)
 - methanol + N-methylpiperazine
 - ^1: VDN (Set 1), B Method:VIBTUB dT=0.01



The new dataset appears in the tree under the appropriate mixture.

Guided Data Capture - Thermophysical and Thermochemical Data

File Edit Tools Help

Reference	Compound	Sample
-----------	----------	--------

- 2002 che lei 0
 - methanol
 - Sample 1 (cm,99.8x%,nc,99.8w%,glc)
 - N-methylpiperazine
 - Sample 1 (cm,99.8x%,nc,99.9w%,glc)
 - methanol + N-methylpiperazine
 - ^1: VDN (Set 1), B Method:VIBTUB dT=0.01

The new data set 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.