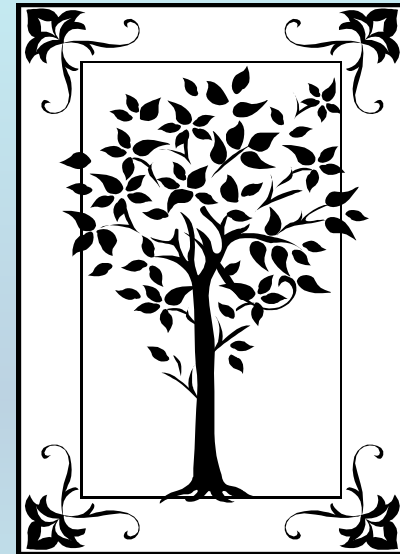


**METADATA AND NUMERICAL DATA CAPTURE:
Liquid-Liquid Equilibrium - Binary
(Conjugate phase compositions - 2 Phases)**

**Guided Data
Capture (GDC)**



This tutorial describes
METADATA AND NUMERICAL DATA CAPTURE:
for **Liquid-Liquid Equilibrium (2 components)**
Conjugate Phase Compositions (2 Phases)
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:

152

J. Chem. Eng. Data 2003, 48, 152–157

Liquid–Liquid Equilibrium and Excess Enthalpies in Binary Systems Methylcyclohexane + Methanol and Methylcyclohexane + *N,N*-Dimethylformamide

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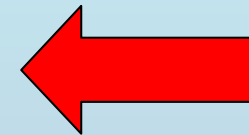
Liquid–liquid equilibrium and excess enthalpies were studied for the two binary systems: methylcyclohexane + methanol and methylcyclohexane + *N,N*-dimethylformamide. Points of the binodal curve in the vicinity of the critical point were established in both of the systems by means of the cloud-point method. Equilibrium compositions were determined at different temperatures using the direct analytical method and the volume method. Excess enthalpies as functions of composition were determined at 298.15 K and 313.15 K using a Hart 4410 microcalorimeter with continuous-flow mixing cells. The results were correlated by the modified Wilson equation. A prediction of the liquid–liquid equilibrium and the excess enthalpy by the modified UNIFAC contribution method (Dortmund) was compared to the experimental values.

Conjugate phase compositions for (methylcyclohexane + methanol) at $p = 101.3$ kPa

Table 3. Conjugated Phases Mole Fractions for the Systems Methylcyclohexane (1) + Methanol (2) and Methylcyclohexane (1) + *N,N*-DMF(2)

T/K	solvent phase	alkane phase
	x_1'	x_1''
Direct Analytical Method		
Methylcyclohexane (1) + Methanol (2)		
293.15	0.135	0.831
298.15	0.150	0.812
303.15	0.174	0.792
308.15	0.202	0.750
313.15	0.251	0.680

**This data set is
considered here.**



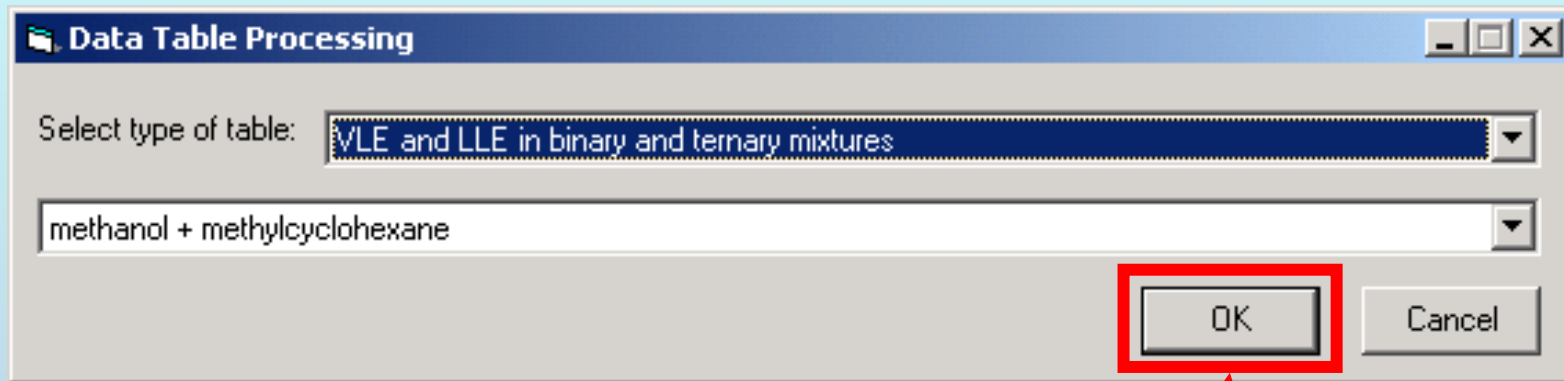
Experimental Method Info:

The direct analytical method consists of analyzing samples of the conjugated phases. In this work, capillary gas chromatography was employed. In the system methylcyclohexane + methanol, the concentration of methylcyclohexane was determined in both phases, because methanol was used as the GC solvent.

1. SELECT the *mixture* for which the data are to be captured.

2. CLICK *Data Tables*

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.)



CLICK *OK*

VLE and LLE in methanol + methylcyclohexane

File Edit Help

Property			
Units			
Phase			
1			

NOTE: This form appears.

The next pages of this tutorial show you how to

(1) PASTE your data in the *Data Table*, and to

(2) SELECT the **Property, Units,** and **Phase** for each column.

Clear the Table View plot ... Process Cancel

VLE and LLE in methanol + methylcyclohexane

File Edit Help

Property			
Units			
Phase			
1	293.15	0.135	0.831
2	298.15	0.150	0.812
3	303.15	0.174	0.792
4	308.15	0.202	0.750
5	313.15	0.251	0.680
6			

Clear the Table View plot ... Process Cancel

Table 3. Conjugated Phases Mole Fractions for the Systems Methylcyclohexane (1) + Methanol (2) and Methylcyclohexane (1) + *N,N*-DMF(2)

<i>T</i> /K	solvent phase	alkane phase
	x_1'	x_1''
Direct Analytical Method		
Methylcyclohexane (1) + Methanol (2)		
293.15	0.135	0.831
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303.15	0.174	0.792
308.15	0.202	0.750
313.15	0.251	0.680

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

VLE and LLE in methanol + methylcyclohexane

File Edit Help

Property	Units	Phase		
1	293.15	0.135	0.831	
2	298.15	0.150	0.812	
3	303.15	0.174	0.792	
4	308.15	0.202	0.750	
5	313.15	0.251	0.680	
6				

DOUBLE CLICK in each of the *3 boxes* above each column to **SELECT** the (1) **Property**, (2) **Units**, and (3) **Phase** from menus.

Clear the Table View plot ... Process Cancel

VLE and LLE in methanol + methylcyclohexane

File Edit Help

Property	Temperature	Mole fraction of methylcyclohexane	
Units	K	Dimensionless	
Phase	Liquid mixture 1	Liquid mixture 1	Liquid mixture 2
1	293.15	0.135	0.831
2	298.15	0.150	0.812
3	303.15	0.174	0.792
4	308.15	0.202	0.750
5	313.15	0.251	0.680
6			

The completed table looks as shown here.

The **Phase** specifications for the 2 liquid mixtures are *Liquid Mixture 1* and *Liquid Mixture 2*.

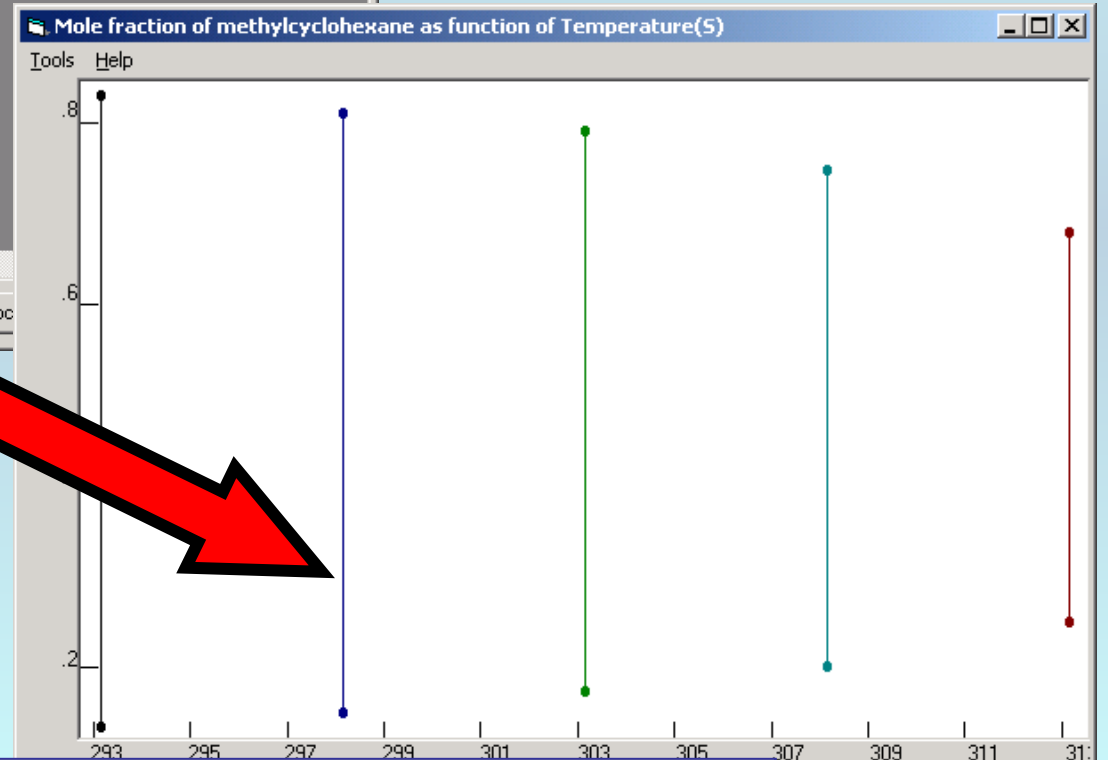
The **Phase** specification for *Temperature* is arbitrary, but must be one of the two specified phases.

Clear the Table View plot ... Process Cancel

VLE and LLE in methanol + methylcyclohexane

Property	Temperature	Mole fraction of methylcyclohexane	Mole fraction of methylcyclohexane
Units	K	Dimensionless	Dimensionless
Phase	Liquid mixture 1	Liquid mixture 1	Liquid mixture 2
1	293.15	0.135	0.831
2	298.15	0.150	0.812
3	303.15	0.174	0.792
4	308.15	0.202	0.750
5	313.15	0.251	0.680
6			

1. CLICK *View plot* to see a plot and check for typographical errors.



2. CLICK *OK*, when done



VLE and LLE in methanol + methylcyclohexane

File Edit Help

Property	Temperature	Mole fraction of methylcyclohexane	Mole fraction of methylcyclohexane
Units	K	Dimensionless	Dimensionless
Phase	Liquid mixture 1	Liquid mixture 1	Liquid mixture 2
1	293.15	0.135	0.831
2	298.15	0.150	0.812
3	303.15	0.174	0.792
4	308.15	0.202	0.750
5	313.15	0.251	0.680
6			

CLICK
Process

Clear the Table View plot ... **Process** Cancel

Property and experimental method for methanol + methylcyclohexane

Help

Proper

Units:

You are entering the data:

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

Method of measurement: Chromatography

Experimental purpose: Principal objective of the work

Comment (optional)

OK Cancel

1. SELECT **Method of Measurement** from the list.

NOTE: *Other* is a valid selection and should include a brief description in the **Comment** field, as shown below.

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

3. CLICK **OK**

Edit: Mole fraction of methylcyclohexane (Liquid mixture 1) (Dimensionless) as function of 1 variable(s)

Mixture: methanol + methylcyclohexane

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

Phase of the Property Value: Liquid mixture 1 Precision of the Property Value(s): Dimensionless

Phase 2: Liquid mixture 2

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

Comments (Optional):

Property and method Numerical Data Cancel

The # of **Phases in Equilibrium** and # of **Constraints** are determined by the software based upon the *Data Table* entries.

*Multiple **Samples*** for a given component can be accommodated, but this is rarely needed.

1. TYPE the **Value** (*101.3*, here) and **SELECT** the **Units** (*kPa*, here) for the **Constraint** (if required).

NOTE: The identity of the constraint was assumed by the software.

The screenshot shows a software window titled 'Edit: M...'. It contains several sections:

- Constraint 1 (Fixed value of):** A dropdown menu shows 'Pressure' selected, with 'of Liquid mixture 1' next to it. To the right, a text box contains 'Value: 101.3' and a dropdown menu shows 'Units: kPa' selected. A red box highlights these two fields.
- Independent variable 1:** A dropdown menu shows 'Temperature' selected, with 'of Liquid mixture 1' next to it. To the right, a text box is empty and a dropdown menu shows 'Units: K' selected. A blue box highlights the 'Uncertainty' field next to it.
- Precision of the Property Value(s):** A text box is empty and a radio button is selected for 'Dimensionless'. A blue box highlights this section.
- Definition of Measurement Results (Absolute vs Relative):** A dropdown menu shows 'Direct value' selected.
- Data presentation:** A dropdown menu shows 'Experimental values' selected.
- Comments (Optional):** A text box is empty.
- Buttons:** At the bottom, there are three buttons: 'Property and method', 'Numerical Data' (highlighted with a green box), and 'Cancel'.

2. ENTER the **Precision of the Property** and the **Uncertainties** for the **Constraint(s)** and **Independent Variable(s)**, if known.

3. **CLICK Numerical Data**

Note: The numerical data shown here were transferred by the software from the *Data Table* entered previously.

The screenshot shows a software window titled "Mole fraction of methylcyclohexane (Dimensionless) as function of 1 variable(s)". The window contains a menu bar with "File", "Edit", "Action", and "Help". Below the menu bar is a table with the following data:

	Var 1	Property
1	293.15	0.135
2	298.15	0.150
3	303.15	0.174
4	308.15	0.202
5	313.15	0.251

At the bottom of the window, there are four buttons: "Clear the Table", "View plot", "Accept", and "Cancel". The "View plot" button is highlighted with a red box, and the "Accept" button is highlighted with a blue box. A red arrow points from a yellow text box to the "View plot" button, and a blue arrow points from another yellow text box to the "Accept" button.

1. CLICK *View plot* to see a plot, if desired, but typographical errors were checked earlier.

2. CLICK *Accept* to accept this **first data set derived from the entered *Data Table*.**

Edit: Mole fraction of methylcyclohexane (Liquid mixture 2) (Dimensionless) as function of 1 variable(s)

Mixture: methanol + methylcyclohexane

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

Phase of the Property Value(s) Liquid mixture 2 Precision of the Property Value(s) Dimensionless %

Phase 2 Liquid mixture 1

Constraint 1 (Fixed value of) Pressure of Liquid mixture 1 Value: 101.3 Units: kPa Uncertainty: %

Independent variable 1 Temperature of Liquid mixture 1 Units: K Uncertainty: %

Property and method Numerical Data Cancel

1. NOTE: Information such as the **Constraint** value and **Uncertainties** are transferred from the first data set by the GDC software.

2. CLICK Numerical Data

Note: The numerical data shown here were, *also*, transferred by the software from the *Data Table* entered previously.

	Var 1	Property	
1	293.15	0.831	
2	298.15	0.812	
3	303.15	0.792	
4	308.15	0.750	
5	313.15	0.680	

1. CLICK *View plot* to see a plot, if desired, but typographical errors were checked earlier.

2. CLICK *Accept* to accept this **second data set derived from the entered *Data Table*.**

Clear the Table View plot Accept Cancel

Guided Data Capture - Thermophysical and Thermochemical Data

File Edit Tools Help

Reference

Compound

2003 ben reh 0

methylocyclohexane

Sample 1 (cm,99m%,nc,;0.005h%,(Karl Fischer titration))

methanol

Sample 1 (cm,99n%,nc,;0.006h%,(Karl Fischer titration))

methanol + methylocyclohexane

^1: Ile, X2 (L1, Set 1), B Method:CHROM

^1: Ile, X2 (L2, Set 2), B Method:CHROM

NOTE: The 2 new data sets appear in the tree under the appropriate mixture.

NOTE: DOUBLE CLICKING on a **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.