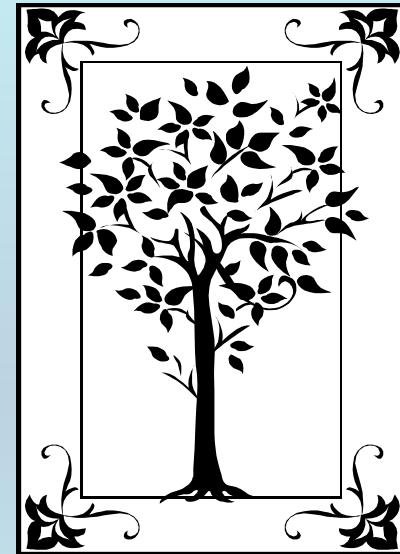


METADATA AND NUMERICAL DATA CAPTURE:

Excess Enthalpy: $H^E_{m,12}$
(2 – Components)

Guided Data
Capture (GDC)



This tutorial describes
METADATA AND NUMERICAL DATA CAPTURE:
for **2-component**
EXCESS ENTHALPY: $H^E_{m,12}$
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:

768

J. Chem. Eng. Data 2002, 47, 768–771

Excess Molar Enthalpies of 1-Octanol with Ethylbenzene, Ethyl Benzoate, Acetophenone, Anisole, or Methanol at 298.15 K

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Department of Chemical Engineering, National Taiwan University of Science and Technology,
43 Keelung Road, Section 4, Taipei 106-07, Taiwan

Excess molar enthalpies, H^E , of binary mixtures of 1-octanol with ethylbenzene, ethyl benzoate, acetophenone, anisole, or methanol have been measured at 298.15 K under atmospheric pressure using an isothermal microcalorimeter. The experimental H^E values are positive for all the binary mixtures over the entire range of compositions. The experimental data have been correlated with the modified Redlich–Kister polynomial equation. The results were qualitatively interpreted in terms of thermodynamic molecular interactions between the mixing components.

**Excess Enthalpy ($H^E_{m,12}$) for the binary system
1-octanol + ethylbenzene
at $p = 101.3$ kPa and $T = 298.15$ K**

**Table 2. Experimental Excess Enthalpies, H^E , of
1-Octanol (1) + Solvents (2) as a Function of Mole
Fraction, x_1 , of 1-Octanol at 298.15 K**

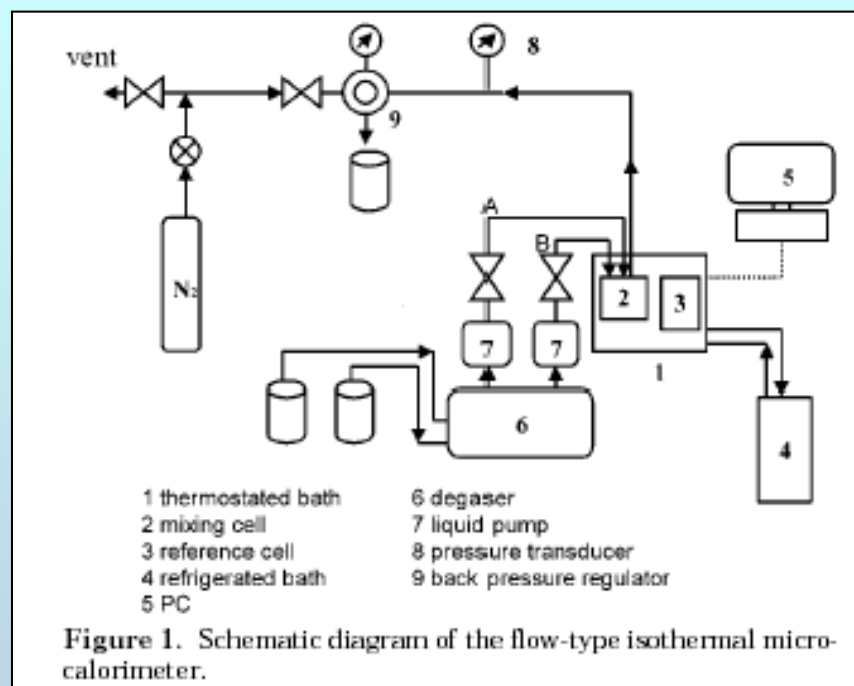
x_1	$H^E/\text{J}\cdot\text{mol}^{-1}$	x_1	$H^E/\text{J}\cdot\text{mol}^{-1}$
1-Octanol (1) + Ethylbenzene (2)			
0.0495	534.9	0.4987	895.7
0.1004	743.0	0.5996	777.2
0.2001	907.8	0.6978	625.7
0.2985	971.1	0.7979	421.0
0.3492	976.0	0.8997	202.2
0.3997	961.8		

This data set is considered here.

Experimental Method Info:

Apparatus and Procedure. The excess molar enthalpies have been measured using the isothermal microcalorimeter (model 4400 IMC) available commercially from Calorimeter Science Corporation, USA. A schematic diagram of the microcalorimeter is shown in Figure 1. The

temperature of the bath is controlled to within ± 0.05 K.



Uncertainty estimate:

The accuracy of the reported H^E values in this study is estimated approximately to be within $\pm 2\%$.

Guided Data Capture - Thermophysical and Thermochemical Data

File Edit Tools Help

Reference Compound Sample Mixture Elasticity **Property** Data Tables

2002 lie ven 0

- 1-octanol
 - Sample 1 (cm,99w%,nc;x;)
 - ^F: VDN(L,.) Set 2, C Method:VIBTUB UFactor 2
- ethylbenzene
 - Sample 1 (cm,99w%,nc;x;)
 - ^F: VDN(L,.) Set 2, C Method:VIBTUB UFactor 2
- ethylbenzene + 1-octanol**

2. CLICK *Property*

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

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 ethylbenzene + 1-octanol

Help

Property group: Excess; partial; and apparent energetic properties

Property:

Units:

Method of me

Experimental purpose:

Comment (optional)

Cancel

1. SELECT the **Property Group:**
Excess; partial; and apparent energetic properties from the menu.

2. SELECT the **Property:**
Excess enthalpy for this example.

Property and experimental method for ethylbenzene + 1-octanol

Help

Property group: Excess; partial; and apparent energetic properties

Property: Excess enthalpy

Units: J/mol

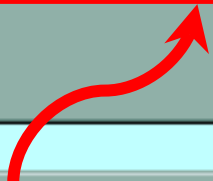
Method of measurement:

Experimental purpose:

Comment (optional)

OK Cancel

SELECT the Units:
J/mol here.



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.

Units: J/mol

Method of measurement: Flow calorimetry

Experimental purpose: Principal objective of the work

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

Comment (optional)

3. CLICK **OK**

OK

Cancel

SELECTION of # of Phases in Equilibrium and # of Constraints

Excess enthalpy (J/mol) as function of 1 variable(s)

Mixture: ethylbenzene + 1-octanol

Phases in equilibrium: 1 Constraints: 2 Independent variables: 1

Phase of the Property Value(s)

SELECT the # of phases
in equilibrium.

There is **1** phase (liquid).

SELECT the # of Constraints.

There are **2** constraints in the
present example;
 $T = 298.15$ K and $p = 101$ kPa.

Excess enthalpy (J/mol) as function of 1 variable(s)

Mixture: ethylbenzene + 1-octanol

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

Sample #: 1 Sample #: 1

Phase of the Property Value(s):

Definition of Measurement Results (Absolute vs Relative):

Data presentation: Experimental values

Comments (Optional):

Property and method Numerical Data Cancel

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

Excess enthalpy (J/mol) as function of 1 variable(s)

Mixture: ethylbenzene + 1-octanol

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) J/mol

Constraint 1 (Fixed value of)

Constraint 2 (Fixed value of)

Independent variable 1

Definition of Measurement Results (Absolute Relative)

NOTE: Constraint and Independent Variable field(s) appear automatically based on the Gibbs Phase Rule.

1) SELECT *Liquid* from the list provided for the **Phase of the Property Value**

Specification of constraints, constraint values, and constraint units

1. SELECT the **Constraint(s)** (T and p here) and the **Independent Variable(s)** (T here) from the lists provided.

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) 2 J/mol

Constraint 1 (Fixed value of) Temperature of Liquid Value: 298.15 Units: K Uncertainty: 0.05 %

Constraint 2 (Fixed value of) Pressure of Liquid Value: 101.3 Units: kPa Uncertainty: %

Independent variable 1 Mole fraction of 1-octanol of Liquid Units: Dimensionless Uncertainty: %

Definition of ...

Data presentation Experiment

Comments

Property and method Numerical Data Cancel

2. TYPE the Constraint **Values** and **SELECT Units** for the Variable(s) and **Constraint(s)**. Include **Uncertainties**, if known.

Measurement definition and Data presentation

Excess enthalpy (J/mol) as function of 1 variable(s)

Mixture: ethylbenzene + 1-octanol

Phases in equilibrium: 1 Constraints: 2 Independent variable

Phase of the Property Value(s) Liquid

Constraint 1 (Fixed value of) Temperature of Liquid

Constraint 2 (Fixed value of) Pressure of Liquid

Independent variable 1 Mole fraction of 1-octanol of Liquid

Units: Dimensionless Uncertainty: %

Definition of Measurement Results (Absolute vs Relative)
Direct value

Data presentation
Experimental values

Comments (Optional):

Property and method Numerical Data Cancel

1. SELECT *Direct Value* (as compared with Relative Value) from the list defining the **Measurement Results**

2. SELECT the appropriate **Data presentation** method. *Experimental values* here.

3. CLICK *Numerical Data*

Excess enthalpy (J/mol) as function of 1 variable(s)

File Edit Action Help

	Var 1	Property
1		

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

Table 2. Experimental Excess Enthalpies, H^E , of 1-Octanol (1) + Solvents (2) as a Function of Mole Fraction, x_1 , of 1-Octanol at 298.15 K

x_1	$H^E/\text{J}\cdot\text{mol}^{-1}$	x_1	$H^E/\text{J}\cdot\text{mol}^{-1}$
1-Octanol (1) + Ethylbenzene (2)			
0.0495	534.9	0.4987	895.7
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0.2985	971.1	0.7979	421.0
0.3492	976.0	0.8997	202.2
0.3997	961.8		

Clear Cancel

Table 2. Experimental Excess Enthalpies, H^E , of 1-Octanol (1) + Solvents (2) as a Function of Mole Fraction, x_1 , of 1-Octanol at 298.15 K

x_1	$H^E/\text{J}\cdot\text{mol}^{-1}$	x_1	$H^E/\text{J}\cdot\text{mol}^{-1}$
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0.2985	971.1	0.7979	421.0
0.3492	976.0	0.8997	202.2
0.3997	961.8		

Excess enthalpy (J/mol) as function of 1 variable(s)

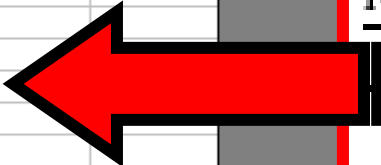
File Edit Action Help

	Var 1	Property
1	0.0495	534.9
2	0.1004	743.0
3	0.2001	907.8
4	0.2985	971.1
5	0.3492	976.0
6	0.3997	961.8
7	0.4987	895.7
8	0.5996	777.2
9	0.6978	625.7
10	0.7979	421.0
11	0.8997	202.2
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Clear the Table View plot Accept Cancel

Table 2. Experimental Excess Enthalpies, H^E , of 1-Octanol (1) + Solvents (2) as a Function of Mole Fraction, x_1 , of 1-Octanol at 298.15 K

x_1	$H^E/\text{J}\cdot\text{mol}^{-1}$	x_1	$H^E/\text{J}\cdot\text{mol}^{-1}$
1-Octanol (1) + Ethylbenzene (2)			
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0.2001	907.8	0.6978	625.7
0.2985	971.1	0.7979	421.0
0.3492	976.0	0.8997	202.2
0.3997	961.8		



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.)

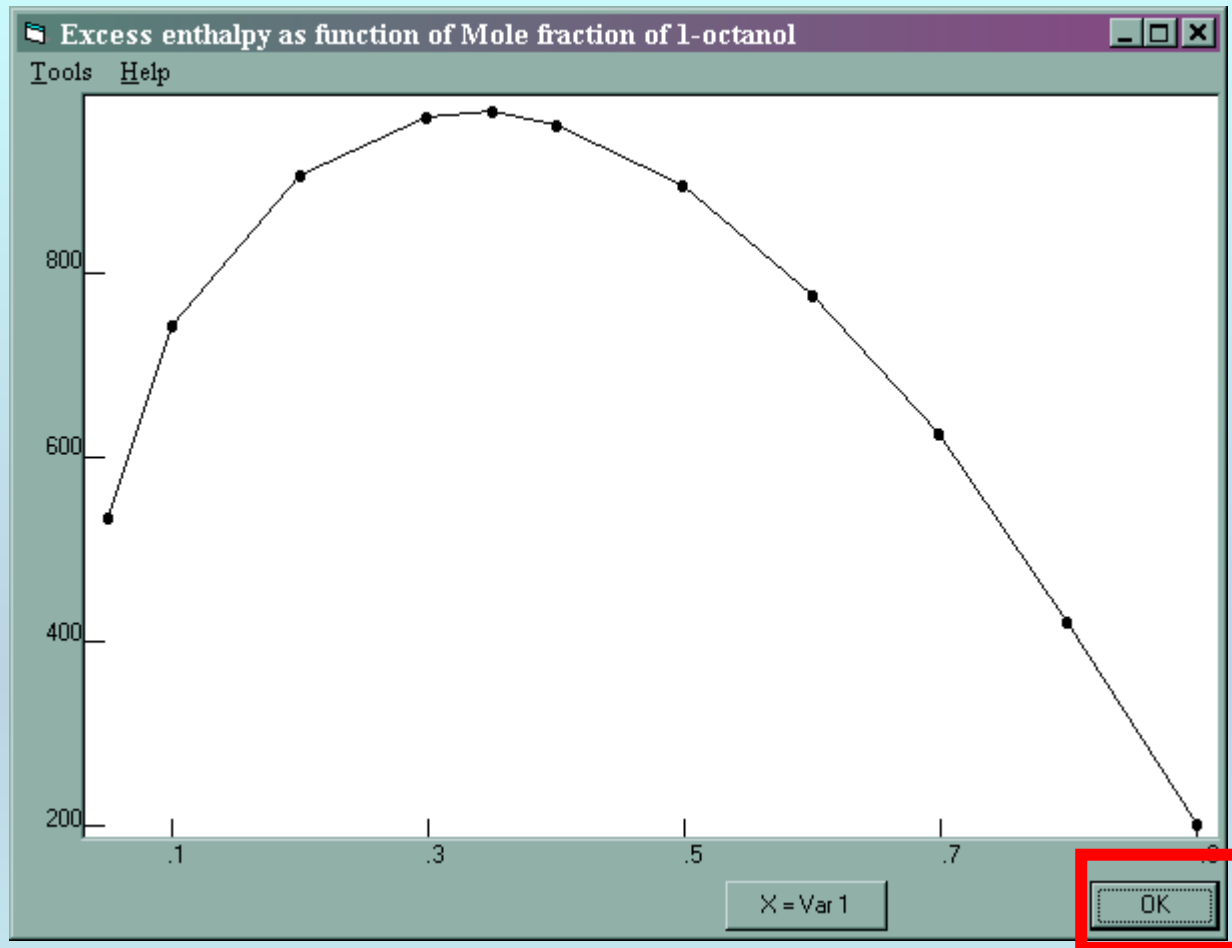
Excess enthalpy (J/mol) as function of 1 variable(s)

File Edit Action Help

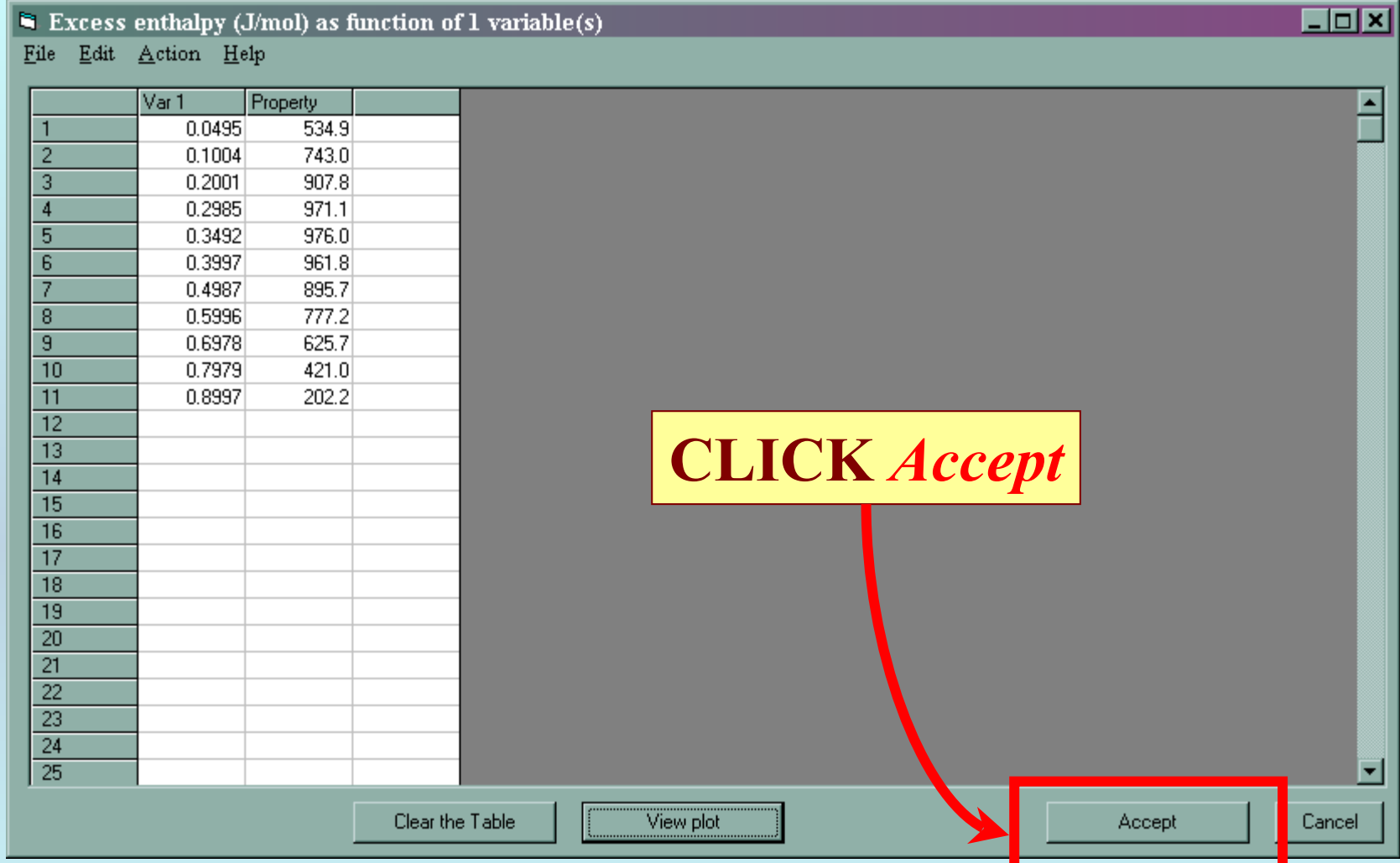
	Var 1	Property
1	0.0495	534.9
2	0.1004	743.0
3	0.2001	907.8
4	0.2985	971.1
5	0.3492	976.0
6	0.3997	961.8
7	0.4987	895.7
8	0.5996	777.2
9	0.6978	625.7
10	0.7979	421.0
11	0.8997	202.2
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CLICK *View plot* to see a graphical representation of the data.

Clear the Table View plot Accept Cancel



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



Guided Data Capture - Thermophysical and Thermochemical Data

File Edit Tools Help

Reference Compound Sample

2002 lie ven 0

- 1-octanol
 - Sample 1 (cm,99w%,nc;x)
 - ^F: VDN(L..), Set 2, C Method:VIBTUB UFactor 2
- ethylbenzene
 - Sample 1 (cm,99w%,nc;x)
 - ^F: VDN(L..), Set 2, C Method:VIBTUB UFactor 2
- ethylbenzene + 1-octanol
 - ^1: HEX (Set 1), B Method:FLOW dHEX=2% dT=0.05

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.