METADATA AND NUMERICAL DATA CAPTURE:
EUTECTIC COMPOSITION
2 – Components: *Solid / Liquid*

$\mathcal{G}$uided $\mathcal{D}$ata

$\mathcal{C}$apture (GDC)

This tutorial describes
METADATA AND NUMERICAL DATA CAPTURE:
for **2-components: Solid/Liquid**
EUTECTIC COMPOSITION (x)
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:

Solubility of Benzimidazoles in Alcohols

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The solid-liquid equilibrium (SLE) has been measured from 270 K to 445 K for 10 binary mixtures of benzimidazoles (benzimidazole and 2-methylbenzimidazole) with alcohols (1-propanol, 1-butanol, 2-butanol, 2-methyl-2-propanol, 1-hexanol) using a dynamic method. The melting point, enthalpy of fusion, and heat capacity change at the melting temperature were determined by differential scanning calorimetry (DSC). The solubility of benzimidazoles in alcohols (C_3-C_6) is higher than in water and in 1-octanol and generally decreases with an increase of the alkyl chain length of the alcohol. The intermolecular solute-solvent interaction is higher for the 1-alcohol than for the secondary or tertiary alcohol. The solubility of 2-methylbenzimidazole in alcohols (C_3-C_6) is higher than that of benzimidazole. Experimental results of solubility were correlated by means of the Wilson, UNIQUAC ASM, and NRTL 1 equations utilizing parameters derived from SLE results. The existence of a solid-solid first-order phase transition in benzimidazole and 2-methylbenzimidazole has been observed in the DSC measurements and has been taken into consideration in the solubility calculation. The best correlation of the solubility data has been obtained by the NRTL 1 equation.

EUTECTIC COMPOSITION
(2 ñ Components)
2-methyl-2-propanol & benzimidazole

Table 4. Eutectic Temperatures, $T_{1,e}$, and Composition, $x_{1,e}$, Detected Graphically for Systems of {Benzimidazole or 2-Methylbenzimidazole (1) + 2-Methyl-2-propanol(2)}

system	$x_{1,e}$	T_{1e} /K
benzimidazole + 2-methyl-2-propanol	0.09 ± 0.01	286.60 ± 0.1
2-methylbenzimidazole + 2-methyl-2-propanol	0.10 ± 0.01	281.71 ± 0.1

This data set is considered here.

Experimental Method Info:

Graphical analysis of SLE results

Guided Data Capture - Thermophysical and Thermochemical Data

File   Edit   Tools   Help

Reference | Compound | Sample | Mixture | Reaction | **Property** | Data Tables

- 2003 dom bog 0
  - benzimadazole
    - Sample 1 (cm,98m%,nc;dv;98m%,glc)
  - 2-methyl-2-propanol
    - Sample 1 (cm,99.5m%,nc;dc;d;99.8m%,glc)
  - **benzimadazole + 2-methyl-2-propanol**
    - 2. TE (Cp1, Cp2, L, air, , Set 1), B Method; PHASDIA

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.)

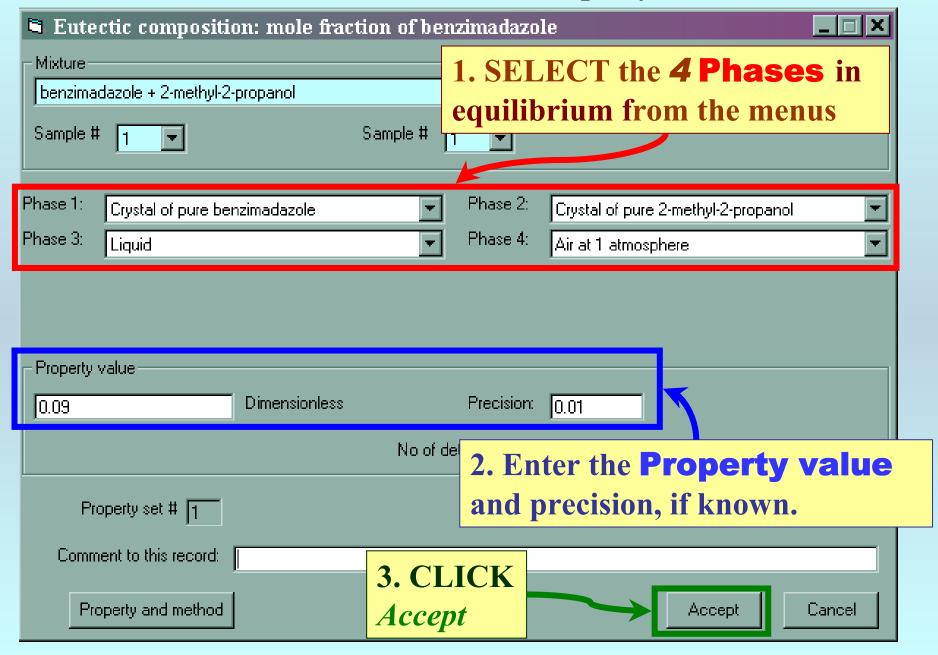**Property and experimental method for benzimadazole + 2-methyl-2-propanol**

Help

Property group: | Composition at phase equilibrium

Property: | Eutectic composition: mole fraction of benzimadazole

Units: | Dimensionless

Method of measurement:

Experimental purpose:

1. SELECT the Property Group: *Composition at phase equilibrium* **from the menu.**

2. SELECT the Property: *Eutectic composition.* **For the example, the composition is the** *mole fraction of benzimidazole.*

3. The Units (*Dimensionless*) are selected automatically by the GDC software

Invariant Property (No state variables) | Cancel

SELECTION of Phases & ENTRY of Property Value

Eutectic composition: mole fraction of benzimadazole

Mixture

benzimadazole + 2-methyl-2-propanol

Sample # 1

Sample # 1

1. SELECT the *4 Phases* in equilibrium from the menus

Phase 1:	Crystal of pure benzimadazole	Phase 2:	Crystal of pure 2-methyl-2-propanol
Phase 3:	Liquid	Phase 4:	Air at 1 atmosphere

Property value

0.09   Dimensionless   Precision: 0.01

No of de

2. Enter the Property value and precision, if known.

Property set # 1

Comment to this record:

Property and method

3. CLICK *Accept*

Accept   Cancel

END

Continue with other compounds, samples, properties, reactions, etc...

or save your file and exit the program.