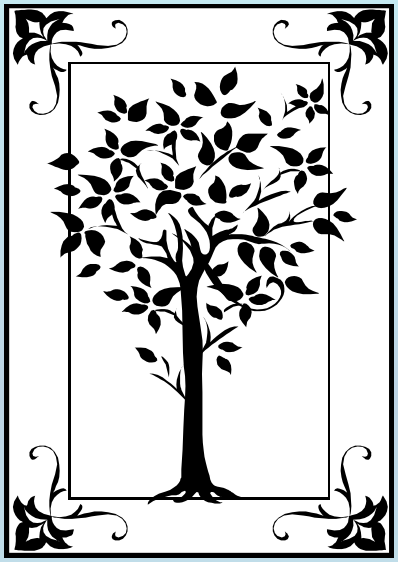
METADATA AND NUMERICAL DATA CAPTURE:

Common pure-component properties

Refractive index η_D at 1 temperature and pressure

Guided Data Capture (GDC)



This tutorial describes
METADATA AND NUMERICAL DATA CAPTURE:
for **Common pure-component properties:**
Refractive index η_D at 1 temperature and pressure
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 1999, *44*, 441−445

Density, Viscosity, Refractive Index, and Speed of Sound in Binary Mixtures of 2-Chloroethanol with Methyl Acetate, Ethyl Acetate, *n*-Propyl Acetate, and *n*-Butyl Acetate

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Experimental values of density, viscosity, and refractive index at 298.15, 303.15, and 308.15 K and the speed of sound at 298.15 K in the binary mixtures of 2-chloroethanol with methyl acetate, ethyl acetate, propyl acetate, and butyl acetate are presented over the whole range of mixture composition. From these data, excess molar volume, deviations in viscosity, speed of sound, isentropic compressibility, and Lorenz−Lorentz molar refraction have been calculated. These results are fit to a Redlich−Kister type polynomial equation of the third degree to derive the binary coefficients. The values of standard deviations are estimated for the calculated and experimental data.

Refractive Index η_D

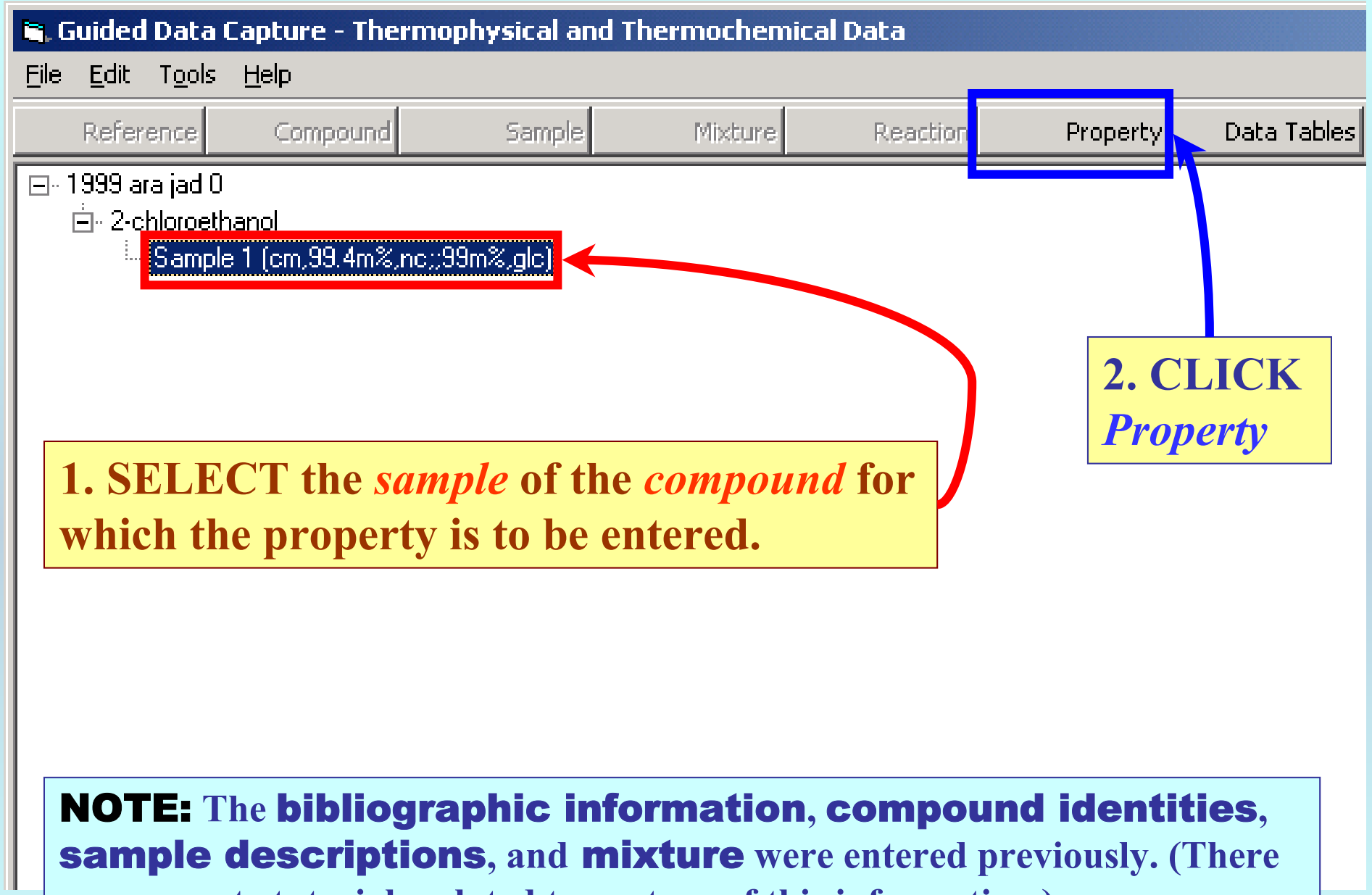
for T = 298.15 K and p = 101.3 kPa

for 2-chloroethanol

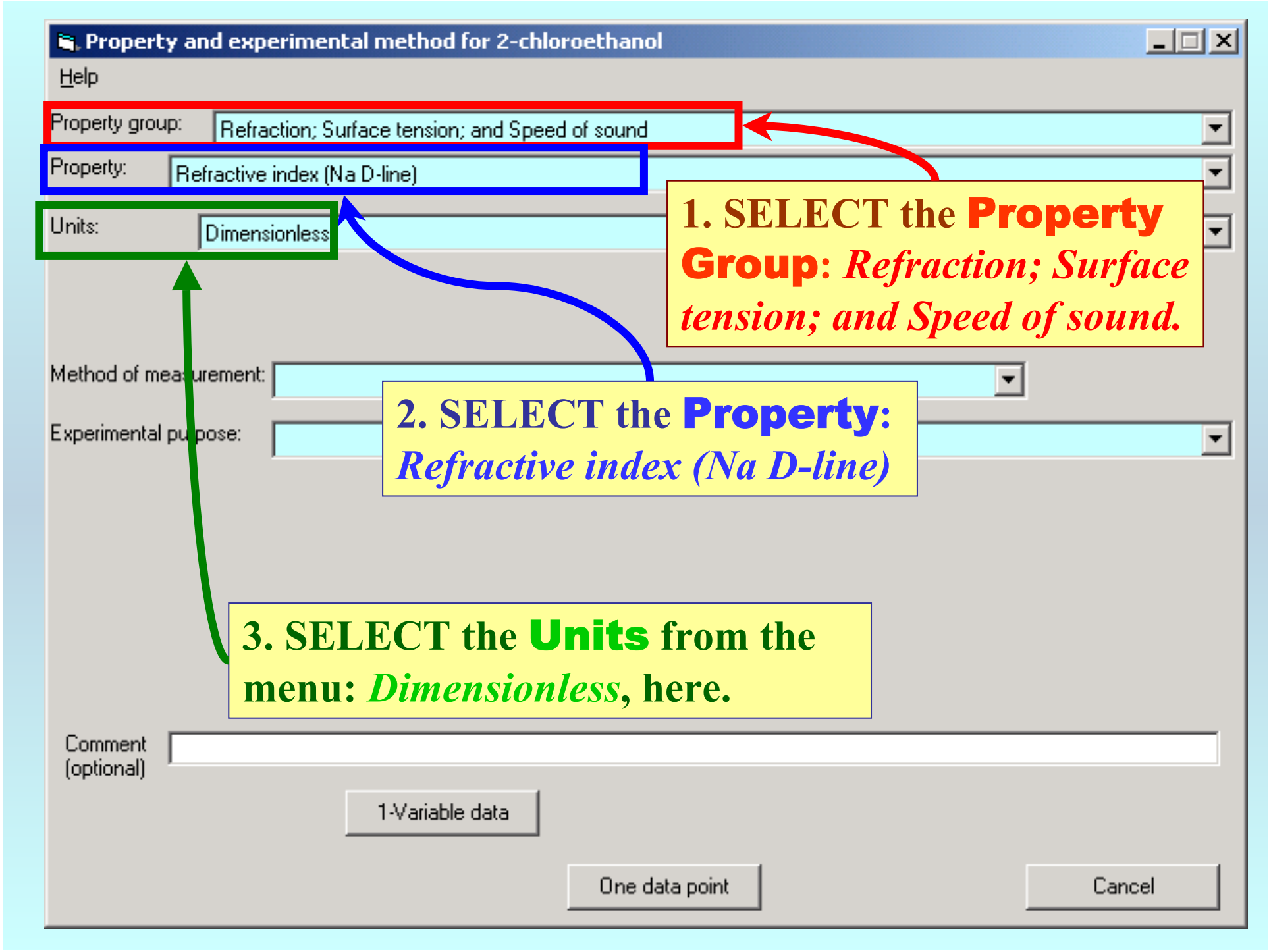
Table 1. Comparison of Experimental Densities (ρ) and Refractive Indices (n_D) of the Pure Liquids with Literature Values at 298.15 K

	ρ/g^{-1} cm^{-3}		n_D	
liquids (mol % purity)	expt	lit.	expt	lit.
2-chloroethanol (99.4)	1.1976	1.1965[a]	1.4402	1.4418[a]
methyl acetate (99.2)	0.9285	0.9282[b]	1.3602	1.3606[b]
ethyl acetate (99.4)	0.8948	0.8946[c]	1.3710	1.3714[d]
propyl acetate (99.3)	0.8831	0.8830[e]	1.3835	1.3828[e]
butyl acetate (99.5)	0.8757	0.8758[f]	1.3931	1.3929[f]

The data considered here.

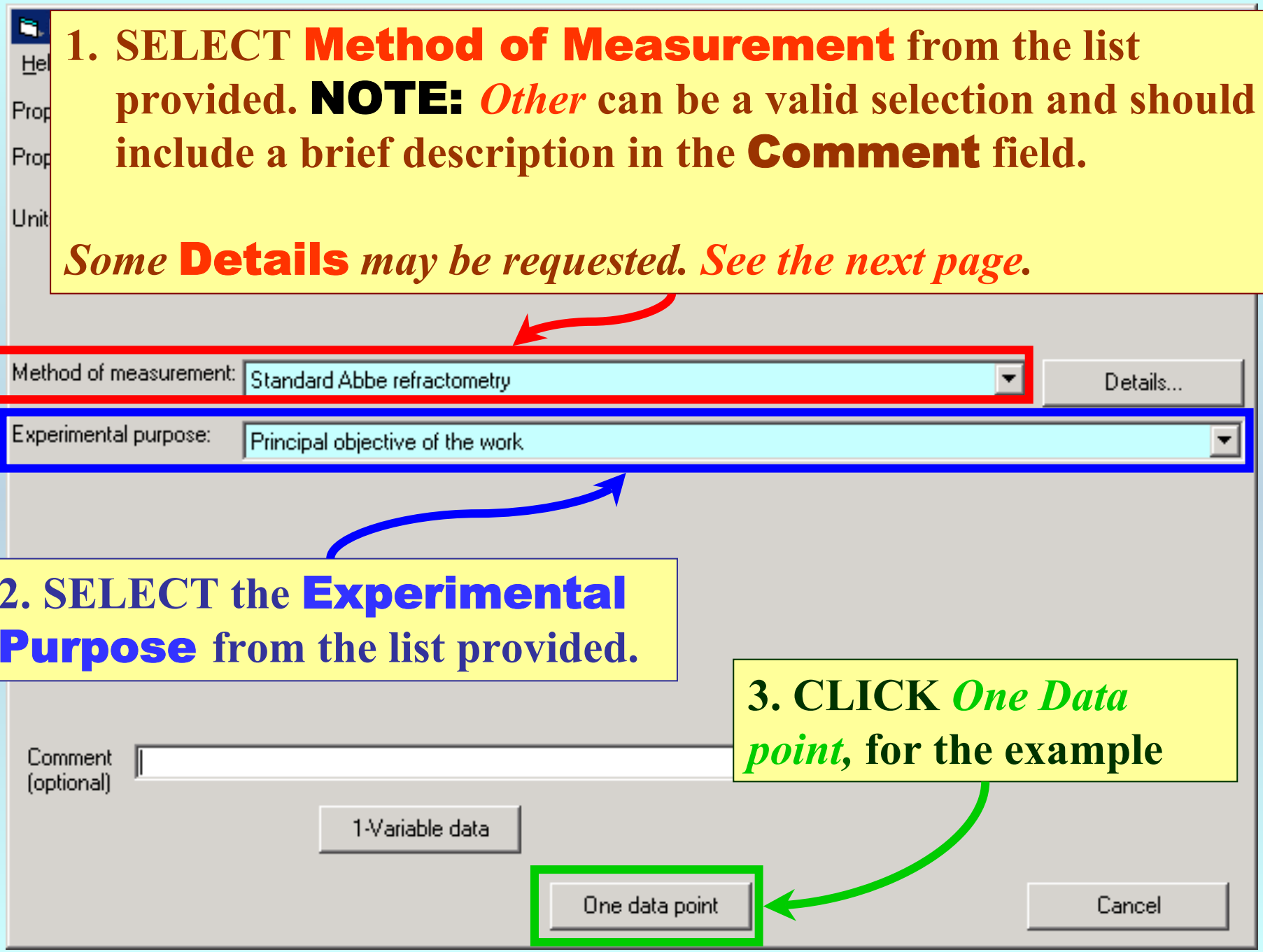


NOTE: The **bibliographic information**, **compound identities**, **sample descriptions**, and **mixture** were entered previously. (There are separate tutorials related to capture of this information.)


Property and experimental method for 2-chloroethanol
Help
Property group:
Refraction; Surface tension; and Speed of sound
Property:
Refractive index (Na D-line)
Units:
Dimensionless
Method of measurement:
Experimental purpose:
1. SELECT the Property Group: Refraction; Surface tension; and Speed of sound.
2. SELECT the Property: Refractive index (Na D-line)
3. SELECT the Units from the menu: Dimensionless, here.
Comment (optional)
1-Variable data
One data point
Cancel

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.

Some **Details** *may be requested. See the next page.*

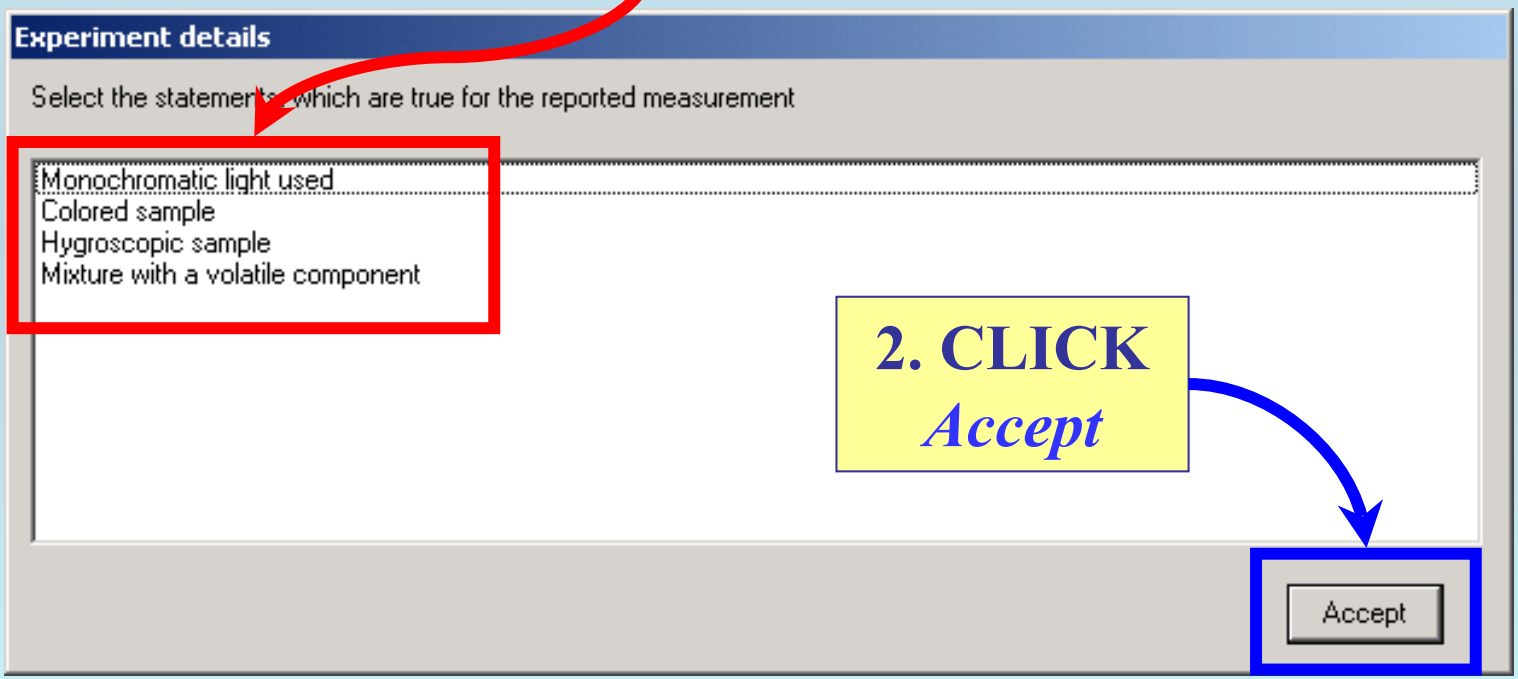


2. SELECT the **Experimental Purpose** from the list provided.

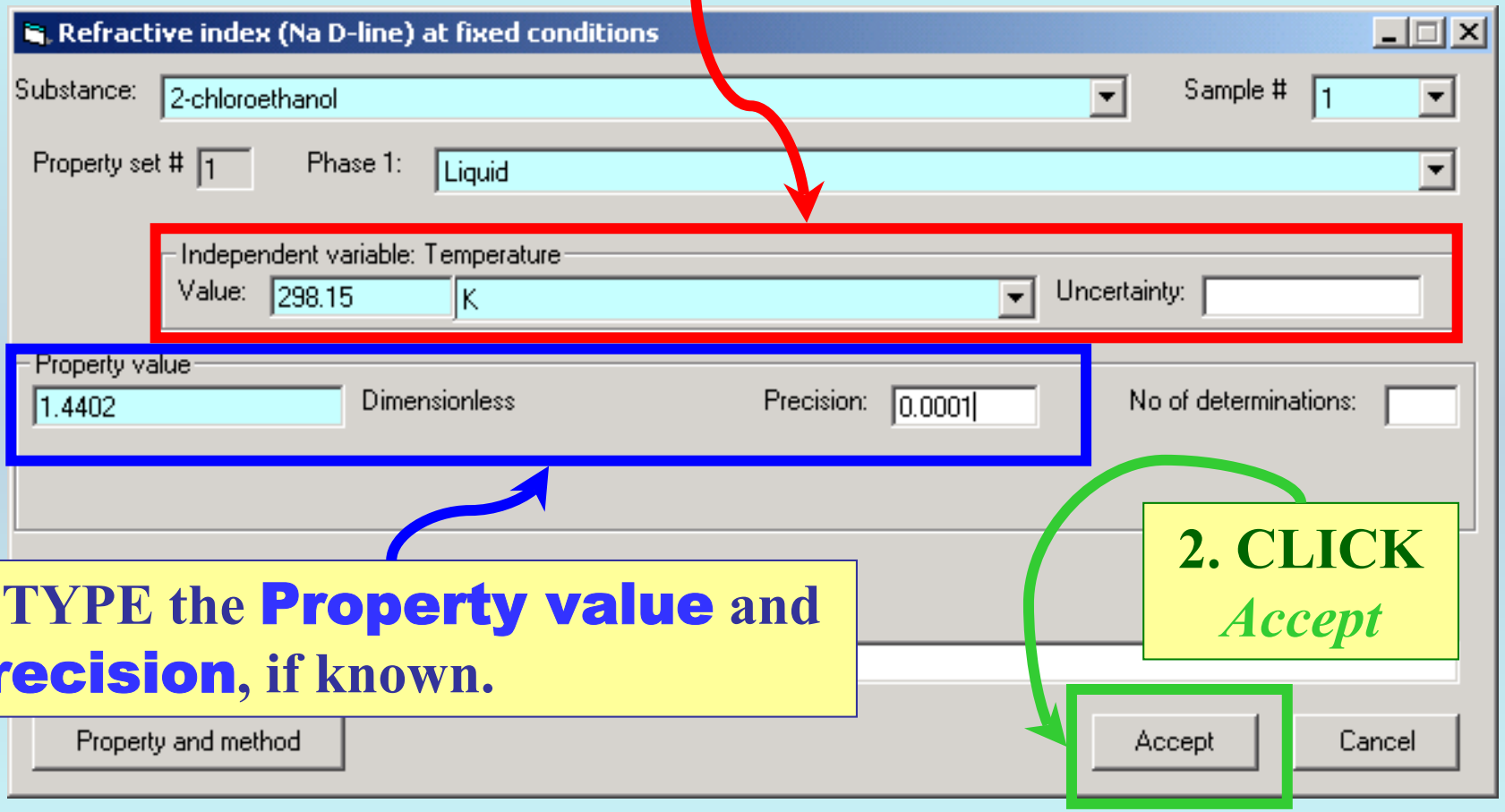
3. CLICK *One Data point*, for the example

Experimental Details

1. **SELECT all statements, which apply to the method used.**



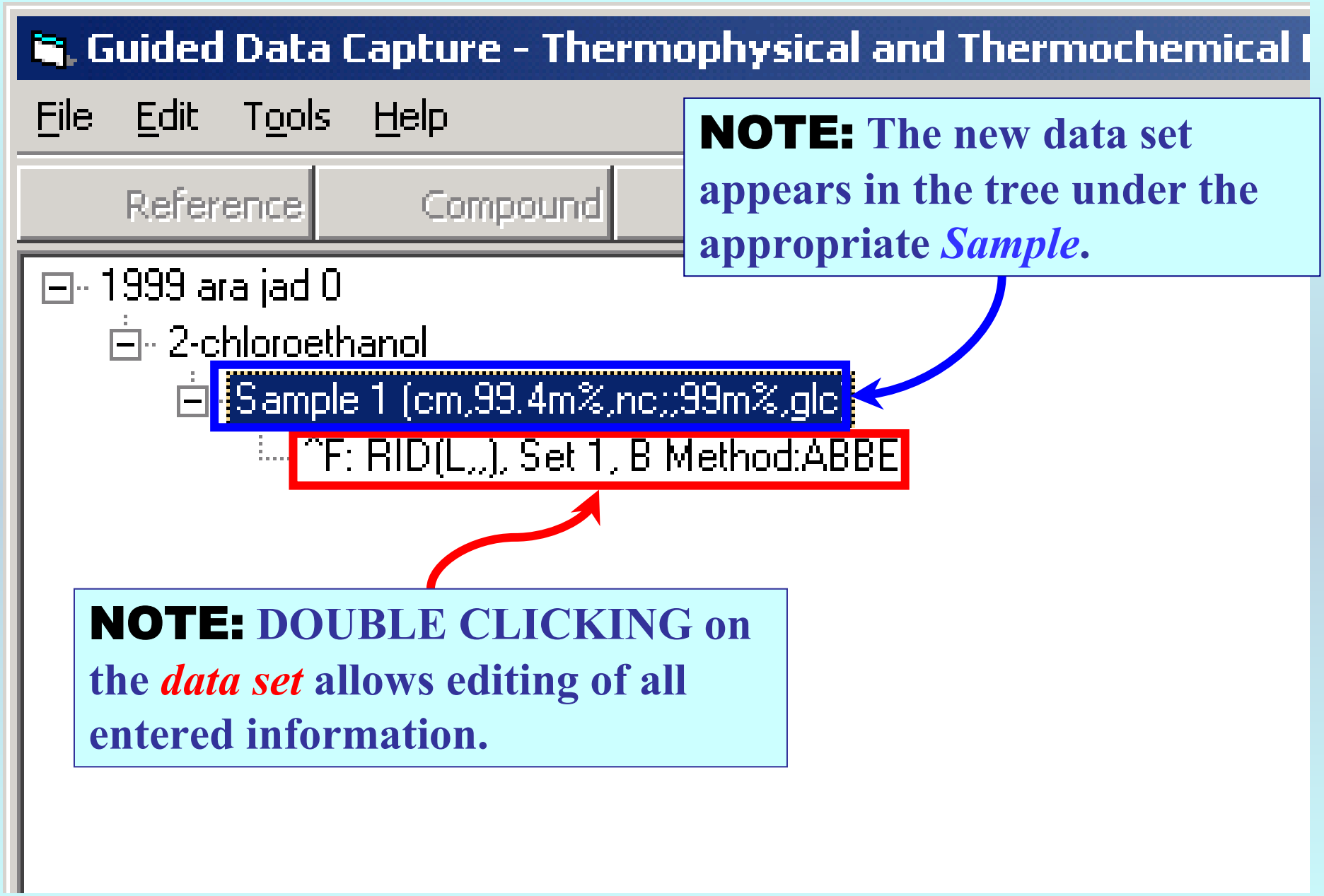
1. TYPE the **Value** and SELECT the **Units** for the **Independent variable** (Temperature). Include the **Uncertainty**, if known.



2. TYPE the **Property value** and **Precision**, if known.

2. CLICK *Accept*

NOTE: For a single η_D value, the pressure is assumed to be p = 101.3 kPa.


Guided Data Capture - Thermophysical and Thermochemical
File Edit Tools Help
Reference
Compound
1999 ara jad 0
2-chloroethanol
Sample 1 (cm,99.4m%,nc;;99m%,glc
^F: RID(L,,), Set 1, B Method:ABBE
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.**