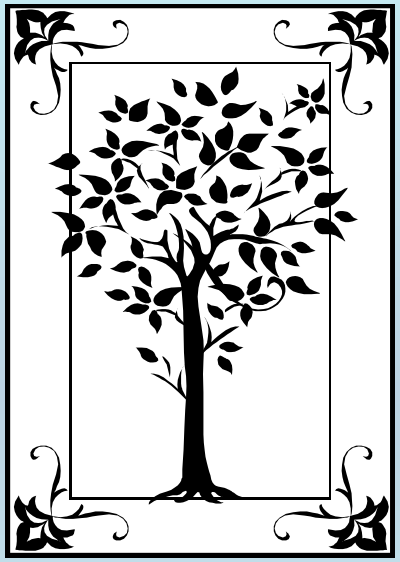
METADATA AND NUMERICAL DATA CAPTURE:
Energy of Combustion $\Delta_c u^o$ (J/g)

Guided Data Capture (GDC)



This tutorial describes
METADATA AND NUMERICAL DATA CAPTURE:
for **Energy of Combustion in O_2(g)**
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:

700 *J. Chem. Eng. Data* 2002, *47*, 700−714

Thermodynamic Properties and Ideal-Gas Enthalpies of Formation for *trans*-Methyl Cinnamate, α-Methyl Cinnamaldehyde, Methyl Methacrylate, 1-Nonyne, Trimethylacetic Acid, Trimethylacetic Anhydride, and Ethyl Trimethyl Acetate

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The results of a study aimed at improvement of group-contribution methodology for estimation of thermodynamic properties of organic substances are reported. Specific weaknesses where particular group-contribution terms were unknown, or estimated because of lack of experimental data, are addressed by experimental studies of enthalpies of combustion in the condensed phase, vapor-pressure measurements, and differential scanning calorimetric heat-capacity measurements. Ideal-gas and condensed-phase enthalpies of formation of *trans*-methyl cinnamate, α-methyl cinnamaldehyde, methyl methacrylate, 1-nonyne, trimethylacetic acid, trimethylacetic anhydride, and ethyl trimethyl acetate are reported. Enthalpies of fusion were determined for *trans*-methyl cinnamate and trimethylacetic acid. Two-phase (solid + vapor) or (liquid + vapor) heat capacities were determined from 300 K to the critical region or earlier decomposition temperature for all the compounds. For ethyl trimethyl acetate, the values of the critical temperature and critical density were determined from the DSC results and the corresponding critical pressure was derived from the fitting procedures. The results of all the measurements were combined to derive a series of thermophysical properties including critical temperature, critical density, critical pressure, acentric factor, enthalpies of vaporization (restricted to within ±50 K of the temperature range of the vapor pressures), and heat capacities along the saturation line. Wagner-type vapor-pressure equations were derived for each compound. Group-additivity enthalpy of formation parameters and strain energies useful in the application of ideal-gas group-contribution correlations were derived.

Energy of Combustion in $O_2(g)$
methyl methacrylate at $T = 298.15$ K and $p = 101.3$ kPa

Table 5. Energy of Combustion Results ($T = 298.15$ K and $p^\circ = 101.325$ kPa)[a,b]

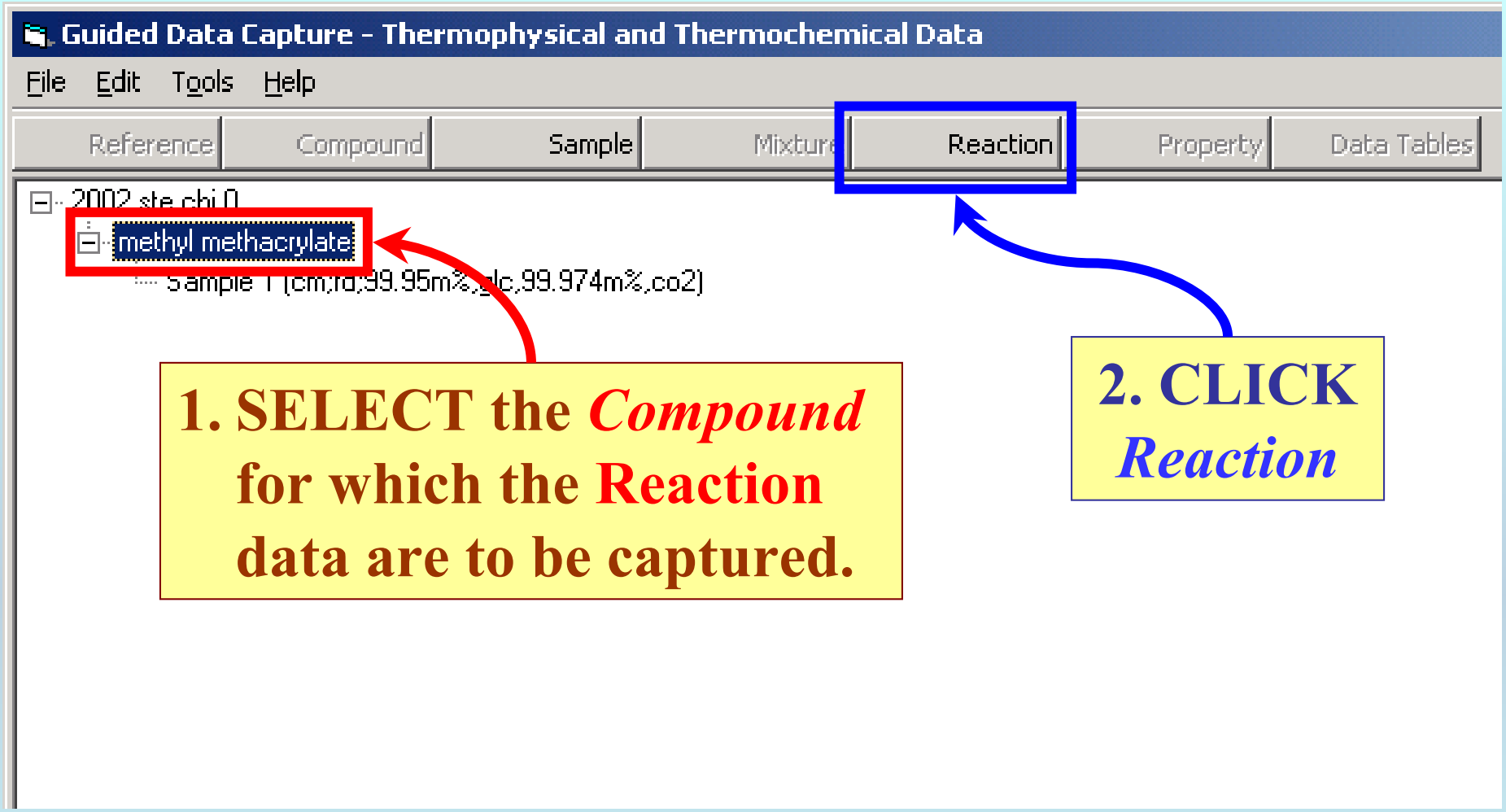
compd	$\{(\Delta_c U^\circ_m/M)(\text{compd})\}/(\text{J}\cdot\text{g}^{-1})$	$\langle\{(\Delta_c U^\circ_m/M)(\text{compd})\}/(\text{J}\cdot\text{g}^{-1})\rangle$
methyl methacrylate	−27 298.7, −27 306.2, −27 301.7, −27 305.4, −27 299.4, −27 298.7, −27 297.6	−27 301.1 ± 1.3
trans-methyl cinnamate	−31 187.3, −31 187.5, −31 186.3, −31 186.2, −31 188.3, −31 187.7, −31 189.5, −31 190.0	−31 187.9 ± 0.5
α-methyl cinnamaldehyde	−36 168.7, −36 157.5, −36 171.0, −36 [illegible]52.7, −36 155.5, −36 156.3, −36 178.9, −36 159.8, −36 155.0	−36 159.5 ± 2.1
1-nonyne	[illegible], −46 956.3, −46 971.0, −46 960.4, −46 967.2, −46 959.3, [illegible]8.4, −46 [illegible]0.7	−46 962.3 ± 1.7
trimethyla	[illegible]55.8, −27 654.7, −27 645.0, −27 651.3	−27 650.7 ± 1.7
trimethyla	[illegible], −30 680.8, −30 681.4, −30 675.2, −30 677.0	−30 678.7 ± 1.1
ethyl trim	[illegible], −32 176.0, −32 180.9, −32 169.5, −32 179.4, −32 175.4	−32 177.9 ± 1.7

[a] The uncertainties shown are one standard deviation of the mean. [b] All the energy of combustion measurements made for each compound are listed in this table.

This data set is considered here.

Experimental Method Info:

Rotating Combustion Bomb Calorimetry

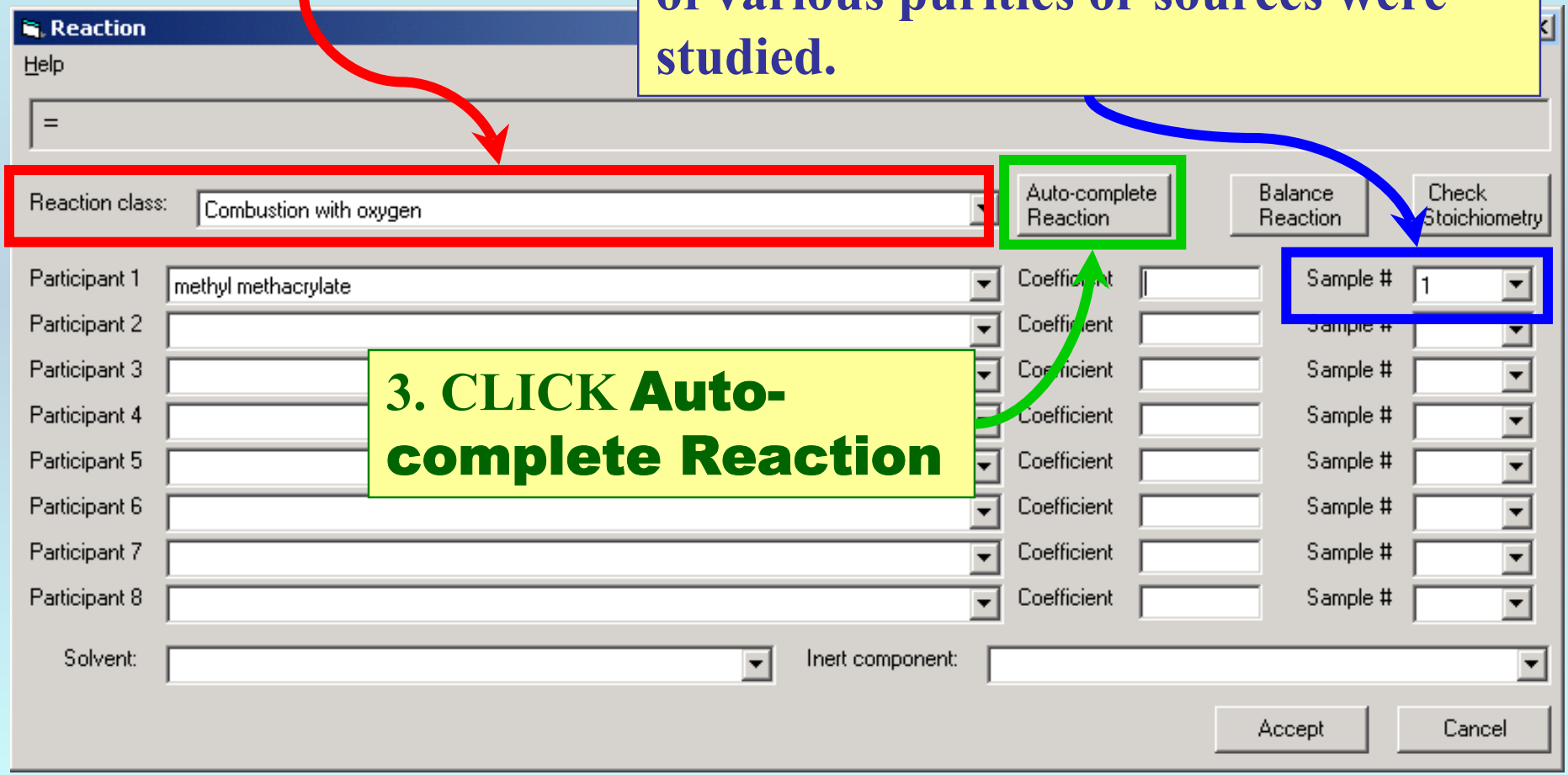


NOTE: The **bibliographic information**, **compound identities**, **sample descriptions**, and **mixture** were entered previously. (There are separate tutorials, which describe capture of this information, if needed.)

1. SELECT the **Reaction Class**: *Combustion with oxygen*, here.

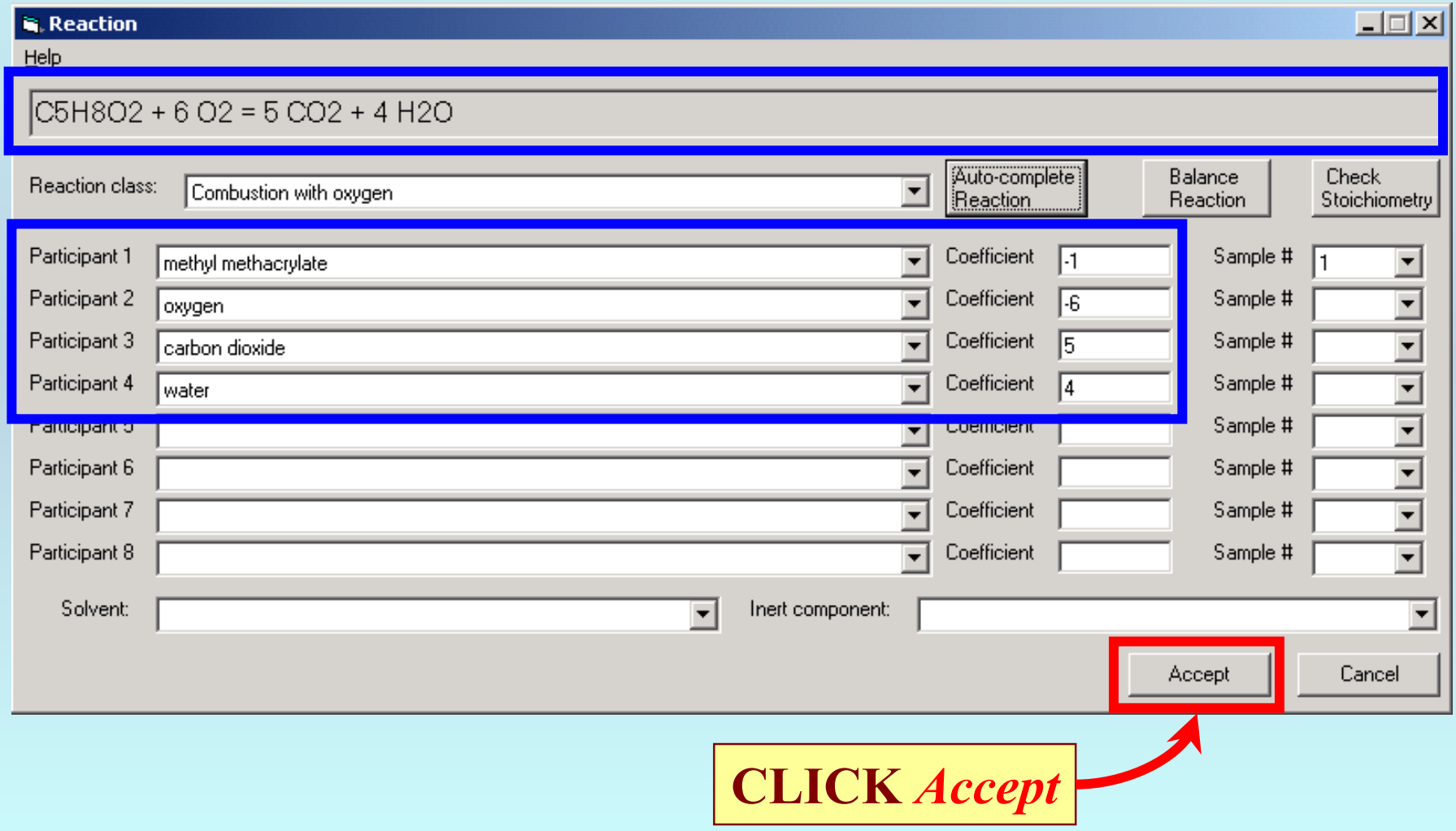
2. SELECT the **Sample #**: *1*, here.

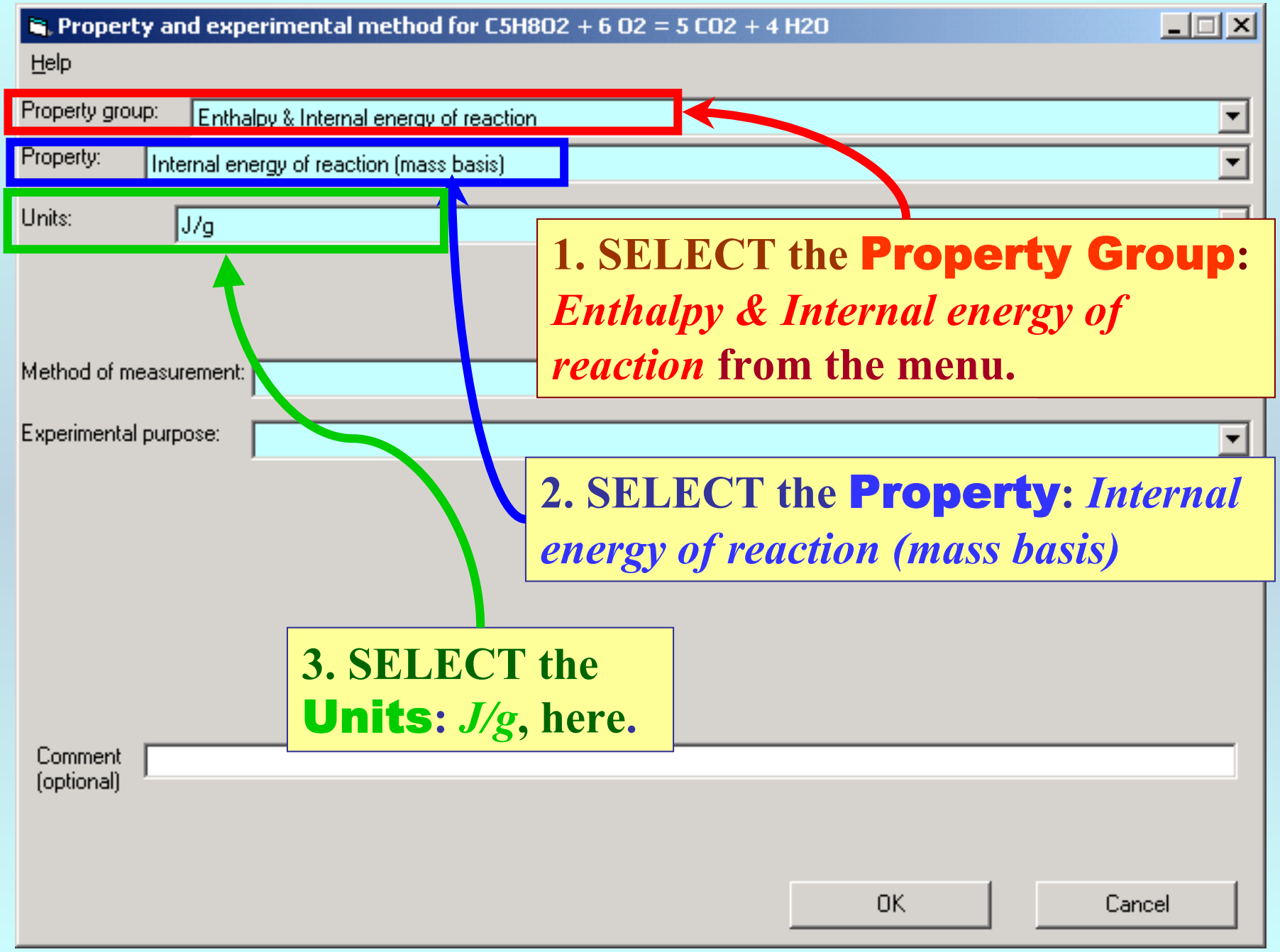
NOTE: The sample number will nearly always be "1", unless samples of various purities or sources were studied.

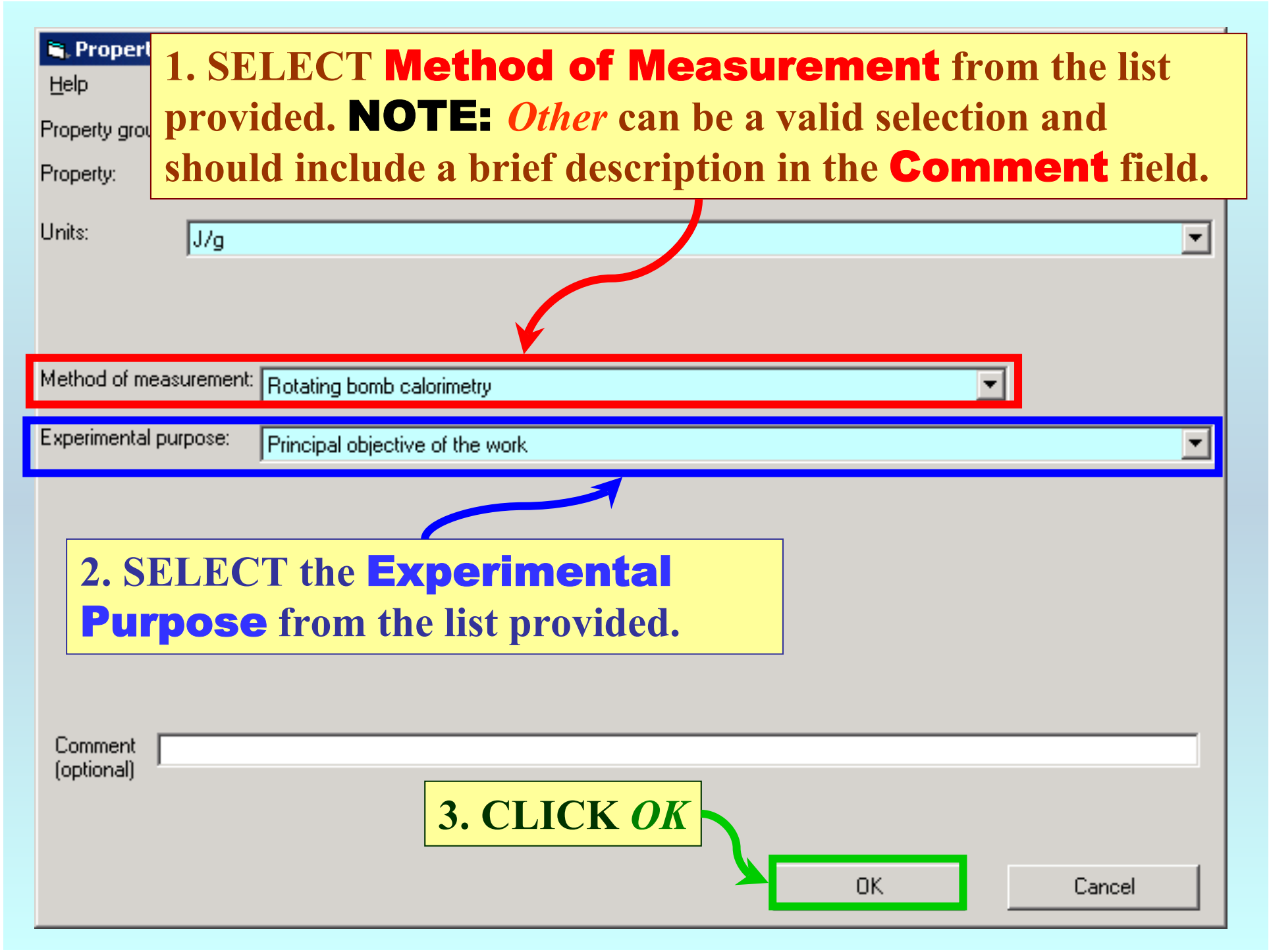


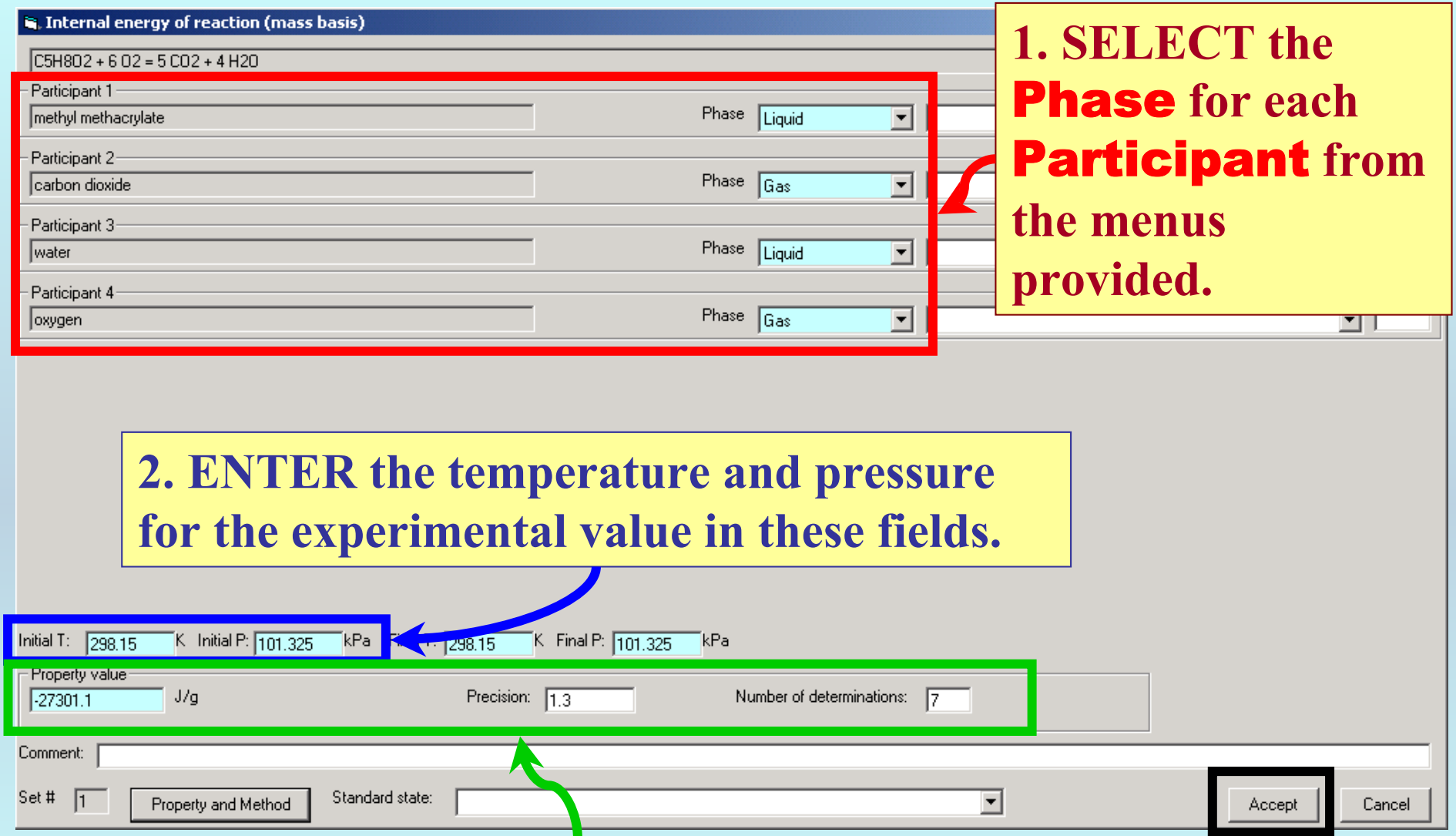
3. CLICK **Auto-complete Reaction**

The other reaction **Participants** and the stoichiometry **Coefficients** are added automatically based upon the **Reaction class** and the elements of the compound combusted.




Property and experimental method for C5H8O2 + 6 O2 = 5 CO2 + 4 H2O
Help
Property group:
Enthalpy & Internal energy of reaction
Property:
Internal energy of reaction (mass basis)
Units:
J/g
Method of measurement:
Experimental purpose:
Comment (optional)
OK
Cancel
1. SELECT the Property Group: Enthalpy & Internal energy of reaction from the menu.
2. SELECT the Property: Internal energy of reaction (mass basis)
3. SELECT the Units: J/g, here.


Properl
Help
Property grou
Property:
Units:
J/g
Method of measurement:
Rotating bomb calorimetry
Experimental purpose:
Principal objective of the work
Comment
(optional)
OK
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.
2. SELECT the Experimental Purpose from the list provided.
3. CLICK OK

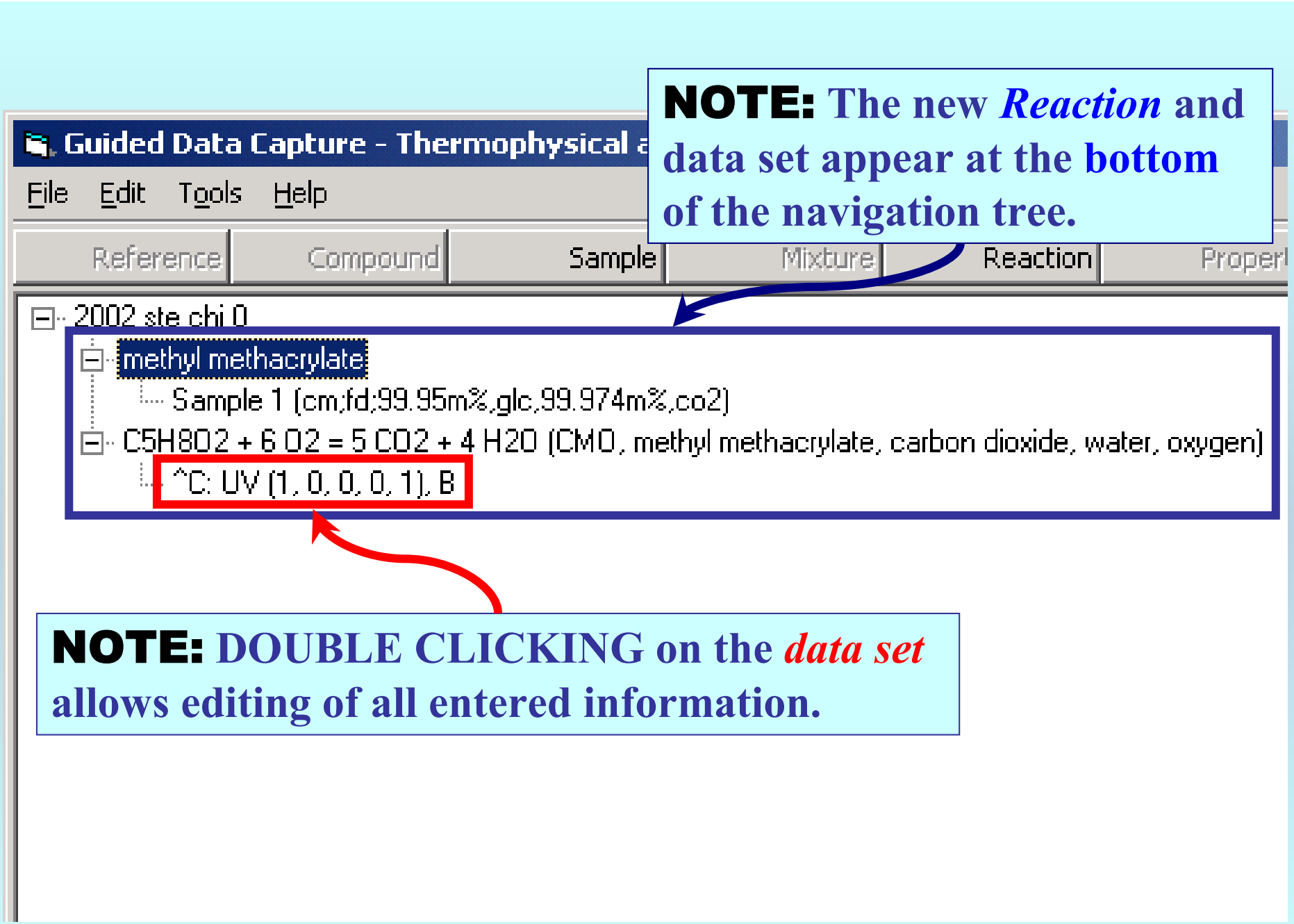


1. SELECT the Phase for each Participant from the menus provided.

2. ENTER the temperature and pressure for the experimental value in these fields.

3. ENTER the Property value, the Precision, and the Number of determinations

4. CLICK *Accept*


NOTE: The new Reaction and data set appear at the bottom of the navigation tree.
Guided Data Capture - Thermophysical a
File Edit Tools Help
Reference Compound Sample Mixture Reaction Proper
2002 ste chi 0
methyl methacrylate
Sample 1 (cm;fd;99.95m%,glc,99.974m%,co2)
C5H8O2 + 6 O2 = 5 CO2 + 4 H2O (CMO, methyl methacrylate, carbon dioxide, water, oxygen)
^C: UV (1, 0, 0, 0, 1), B
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.**