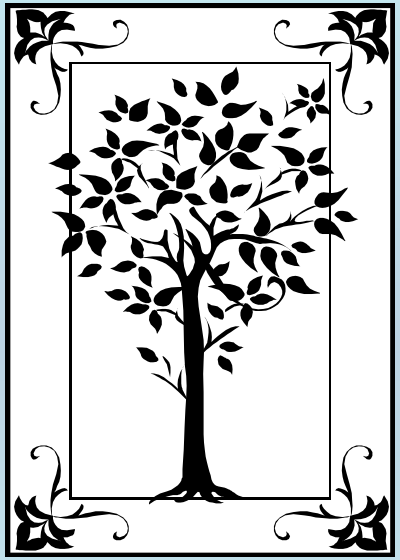
METADATA AND NUMERICAL DATA CAPTURE:
Enthalpy of Formation
$\Delta_f H_m°$ (kJ/mol)

Guided Data Capture (GDC)



This tutorial describes
METADATA AND NUMERICAL DATA CAPTURE:
for **Enthalpy of Formation $\Delta_f H_m°$ (kJ/mol)**
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

W. V. Steele,*,† R. D. Chirico,‡ A. B. Cowell, S. E. Knipmeyer, and A. Nguyen

BDM Petroleum Technologies, P.O. Box 2543, Bartlesville, Oklahoma 74005-2543

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.

Enthalpy of Formation from the elements: **methyl methacrylate** at $T = 298.15$ K and $p = 101.3$ kPa

Table 6. Condensed-Phase Molar Thermochemical Functions at 298.15 K and $p^\circ = 101.325$ kPa[a]

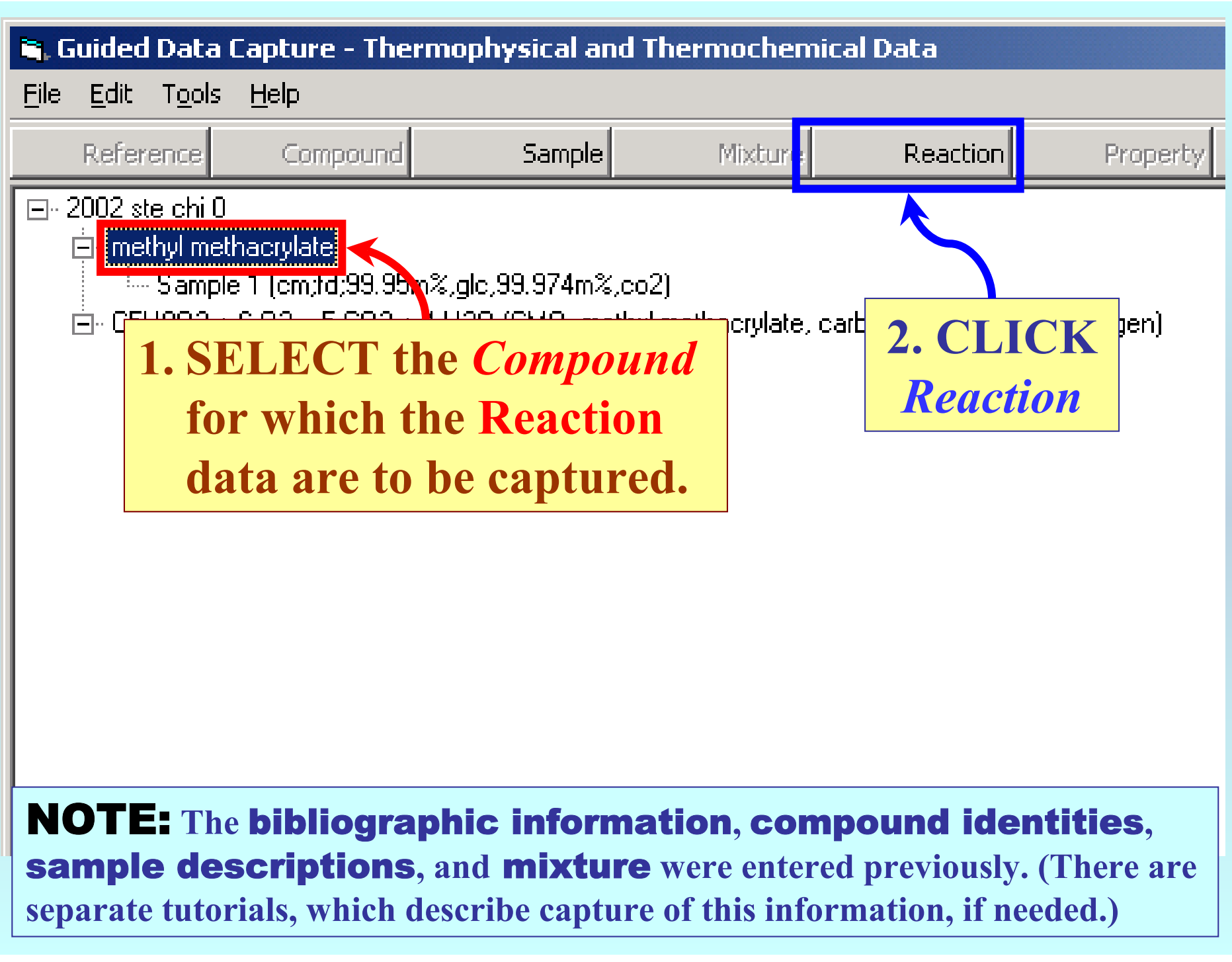
	$\Delta_c U^\circ_m$/kJ·mol^{-1}	$\Delta_c H^\circ_m$/kJ·mol^{-1}	$\Delta_f H^\circ_m$/kJ·mol^{-1}
methyl methacrylate (l)	−2733.33 ± 0.46	−2735.80 ± 0.46	−375.07 ± 0.54
trans-methyl cinnamate (cr)	−5058.32 ± 0.76	−5062.04 ± 0.76	[illegible]
α-methyl cinnamaldehyde (l)	−5286.14 ± 0.96	−5291.09 ± 0.96	−73.1[illegible] ± 1.08
1-nonyne (l)	−5833.98 ± 0.88	−5843.90 ± 0.88	15.6[illegible] ± 1.02
trimethylacetic acid (cr)	−2824.07 ± 0.52	−2827.79 ± 0.52	−568.[illegible]1 ± 0.60
trimethylacetic anhydride (l)	−5713.97 ± 0.90	−5721.41 ± 0.90	−78[illegible].16 ± 1.06
ethyl trimethyl acetate (l)	−4189.16 ± 0.70	−4195.36 ± 0.70	−[illegible]0.02 ± 0.82

[a] The results listed in this table are for the stable [liqui[illegible]e at 298.15 K for each of the compounds.

This data set is considered here.

Experimental Method Info:

Rotating Combustion Bomb Calorimetry

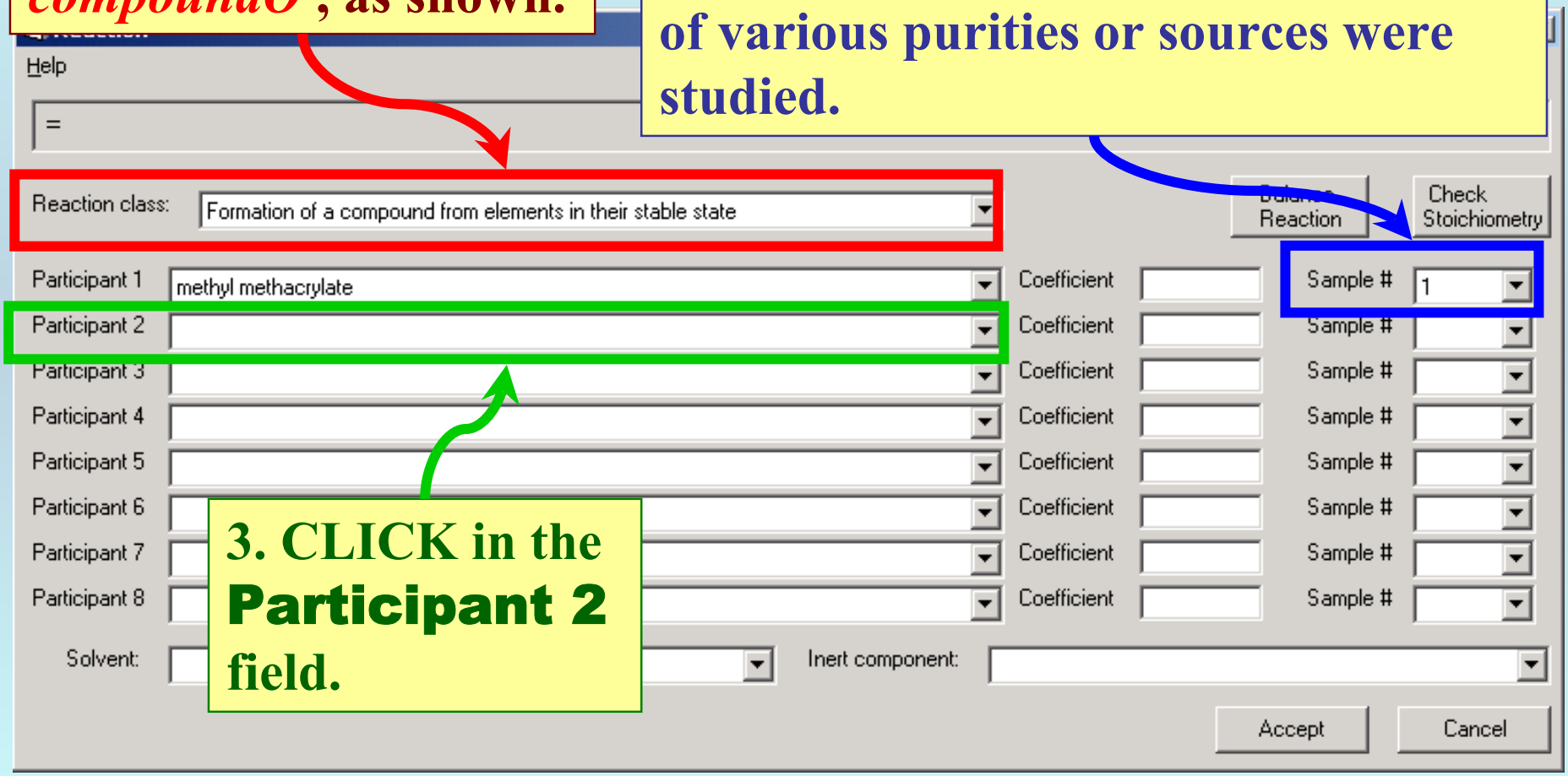


NOTE: The **bibliographic information**, **compound identities**, **sample descriptions**, and **mixture** were entered previously. (There are separate tutorials, which describe capture of this information, if needed.)

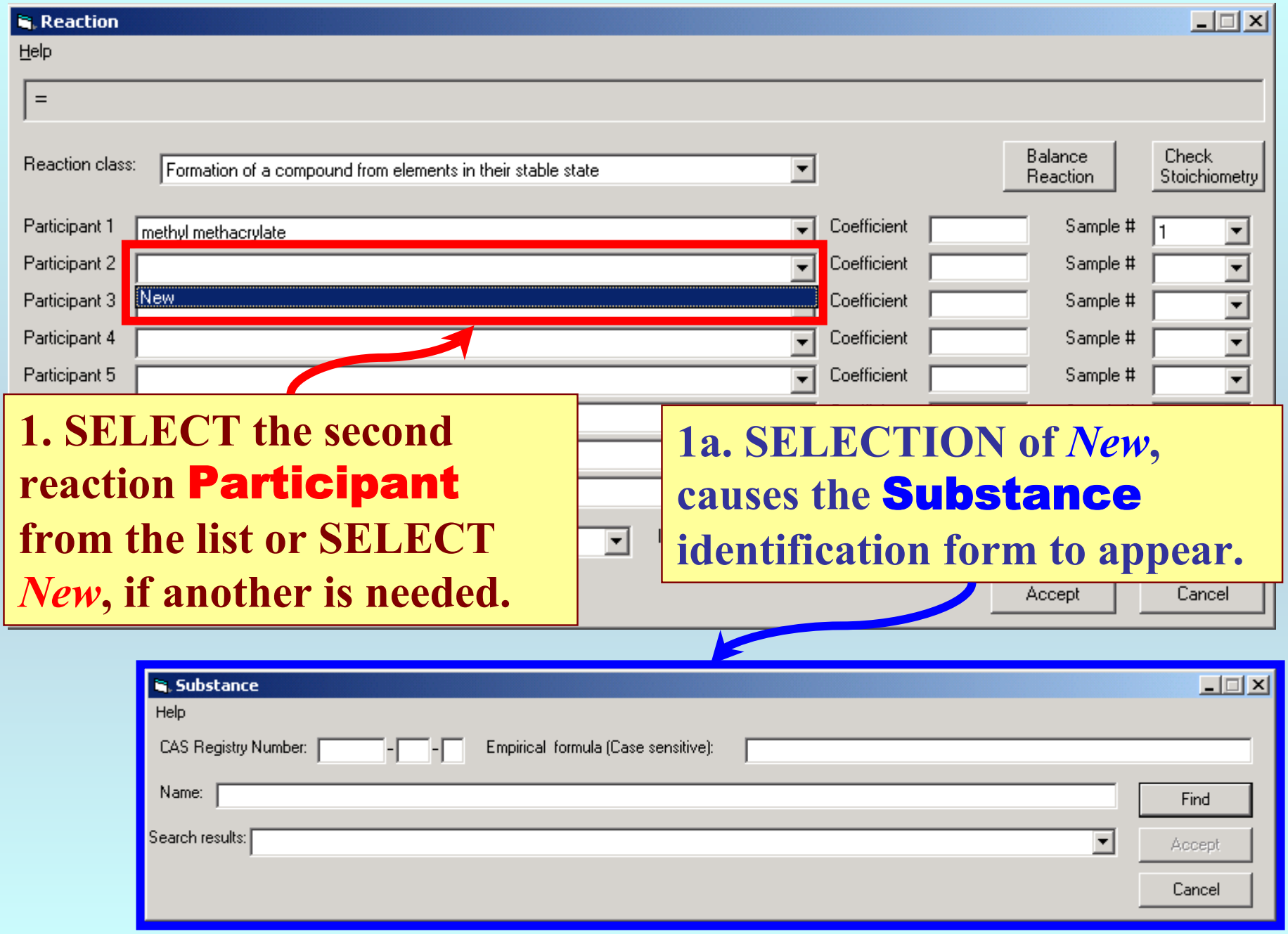
1. SELECT the **Reaction Class**: *Formation of a compoundÖ* , as shown.

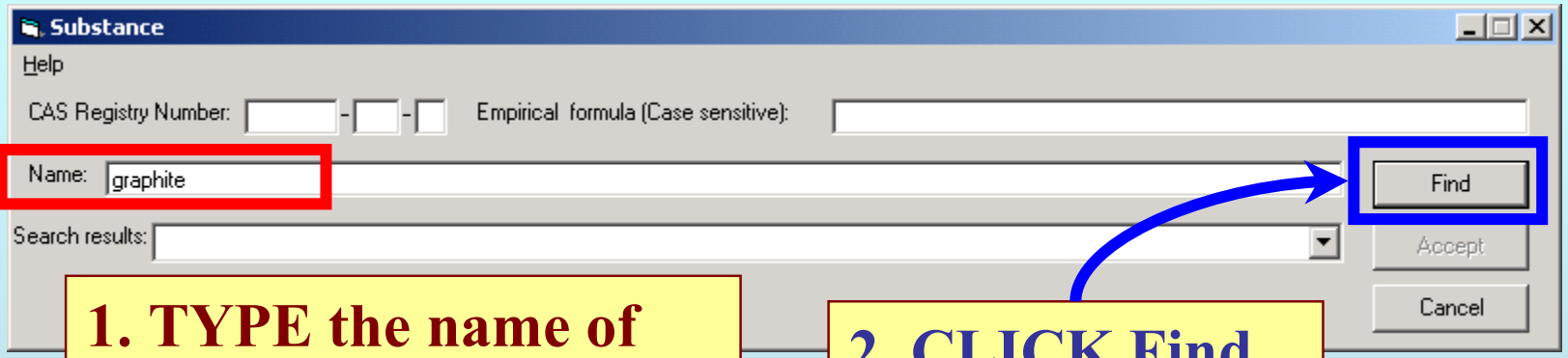
2. SELECT the **Sample #**: *1*, here.

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



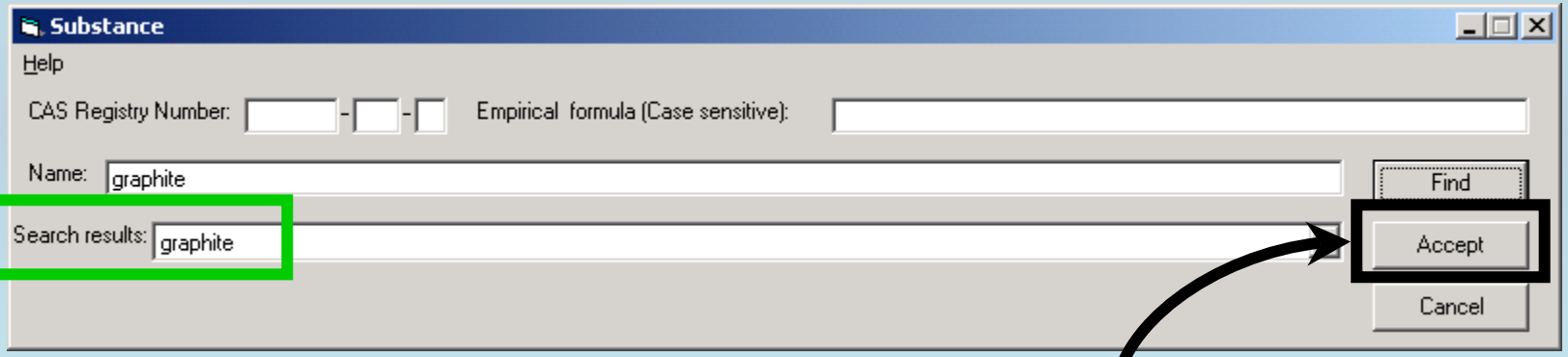
3. CLICK in the **Participant 2** field.


Reaction
Help
=
Reaction class:
Formation of a compound from elements in their stable state
Balance Reaction
Check Stoichiometry
Participant 1
methyl methacrylate
Coefficient
Sample #
1
Participant 2
Participant 3
New
Participant 4
Participant 5
1. SELECT the second reaction Participant from the list or SELECT New, if another is needed.
1a. SELECTION of New, causes the Substance identification form to appear.
Accept
Cancel
Substance
Help
CAS Registry Number:
Empirical formula (Case sensitive):
Name:
Find
Search results:
Accept
Cancel



1. TYPE the name of the required reaction **Participant**

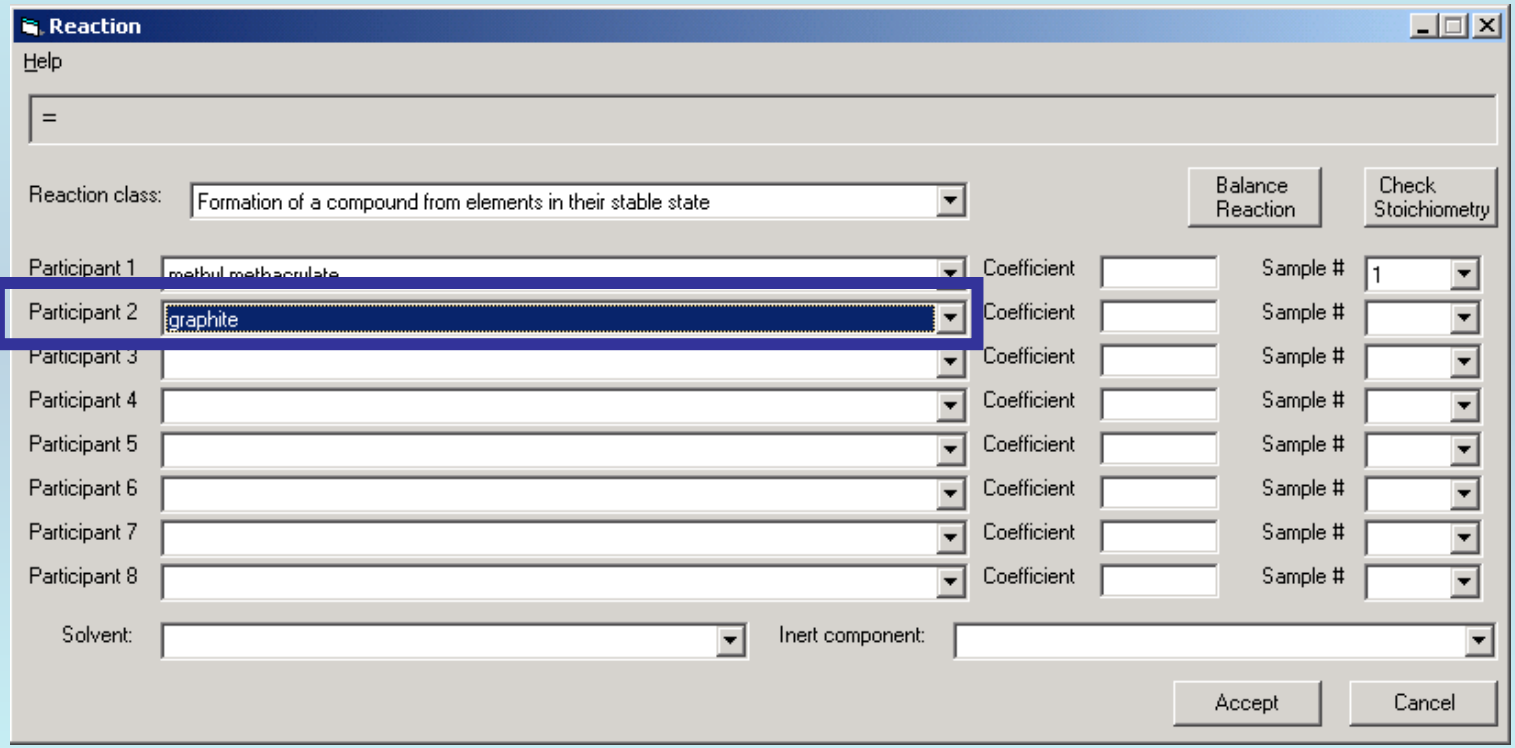
2. CLICK Find



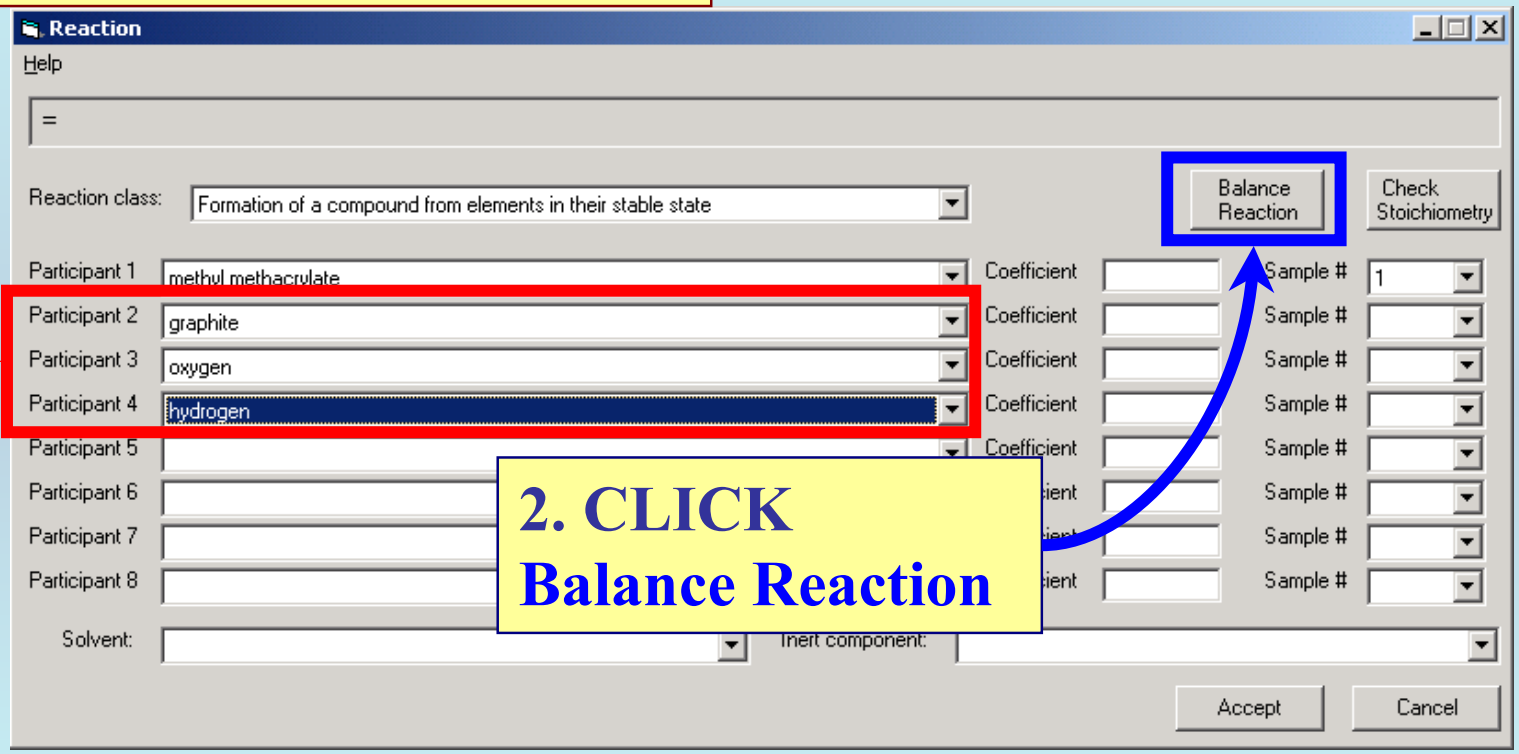
3. The found substance appears in the **Search Results**

4. CLICK *Accept*

NOTE: The substance now appears as **Participant 2**.
ALSO: The *order* in which the participants are added is *NOT* important.

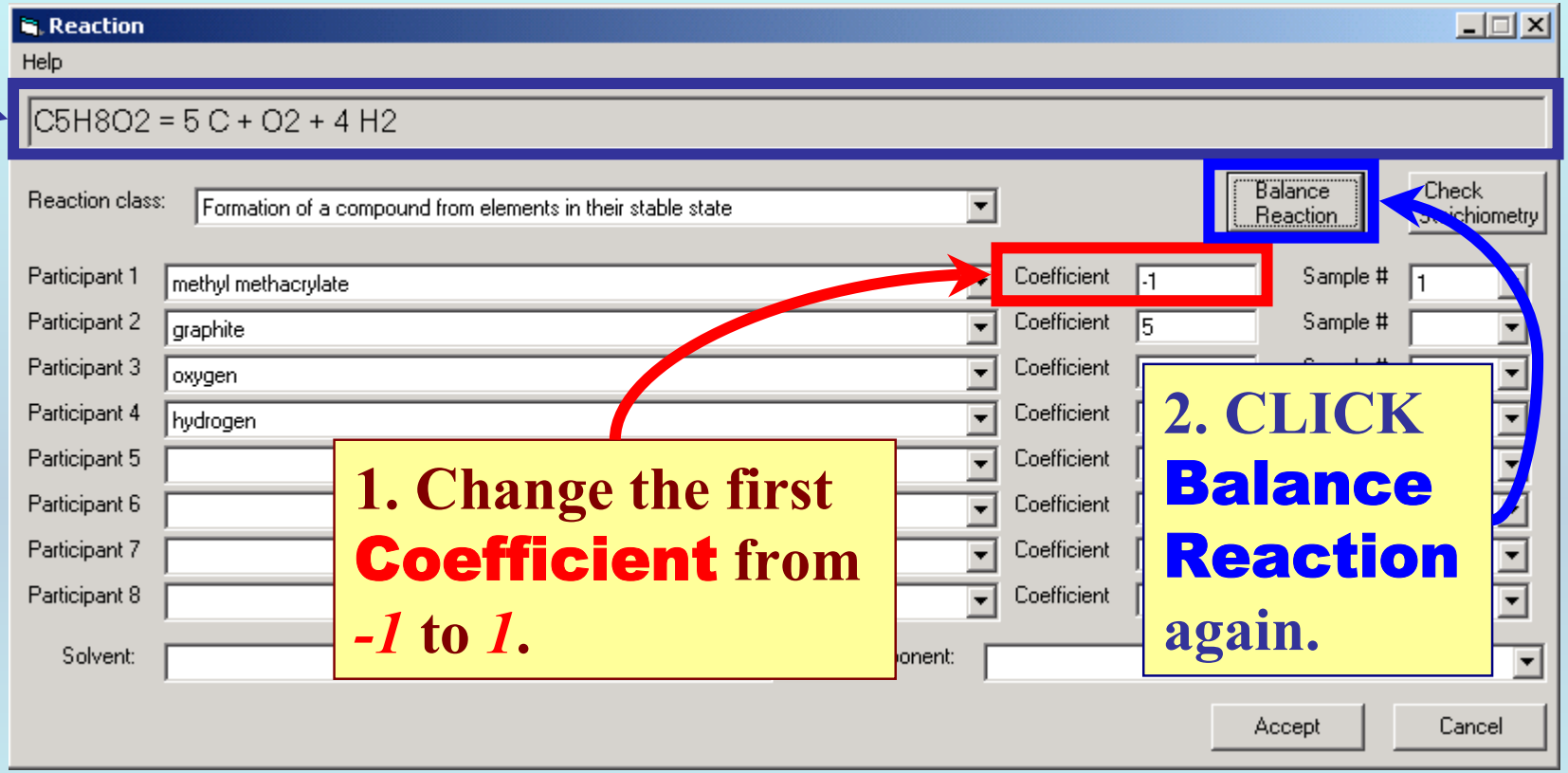


1. Identify all of the reaction Participants

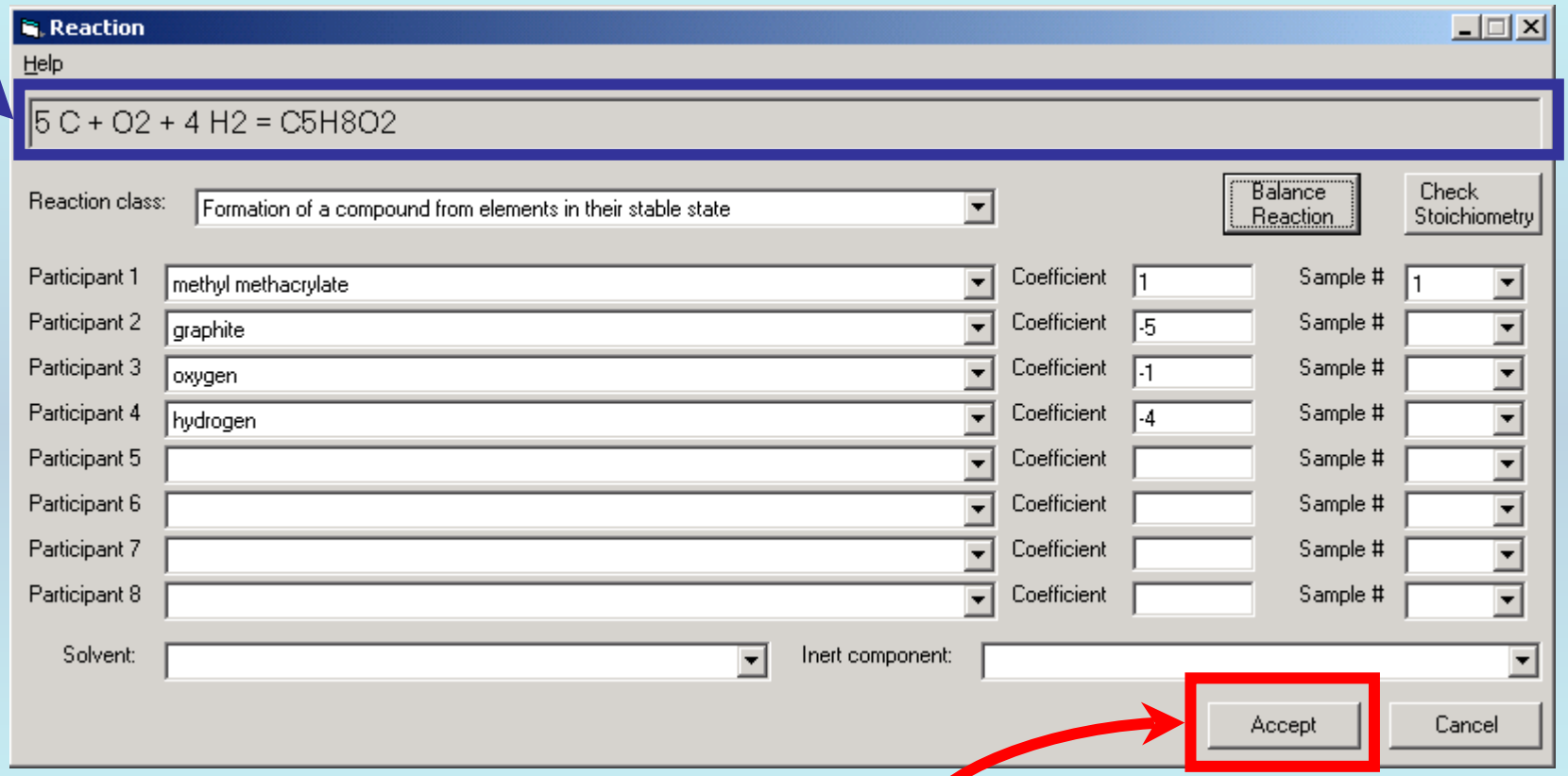


2. CLICK Balance Reaction

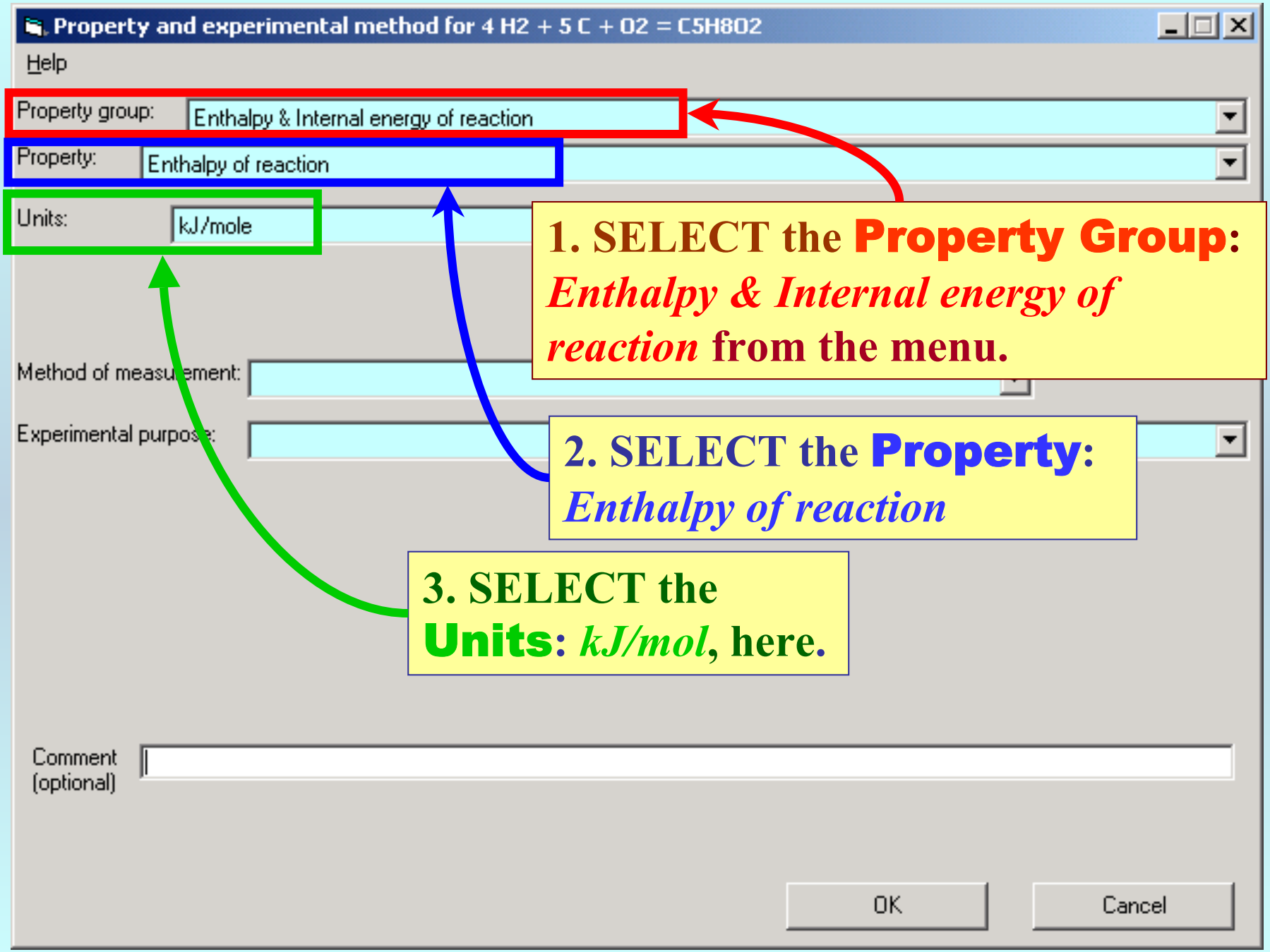
NOTE: The balanced reaction appears in this field.
ALSO NOTE: The reaction is in the **WRONG** direction.

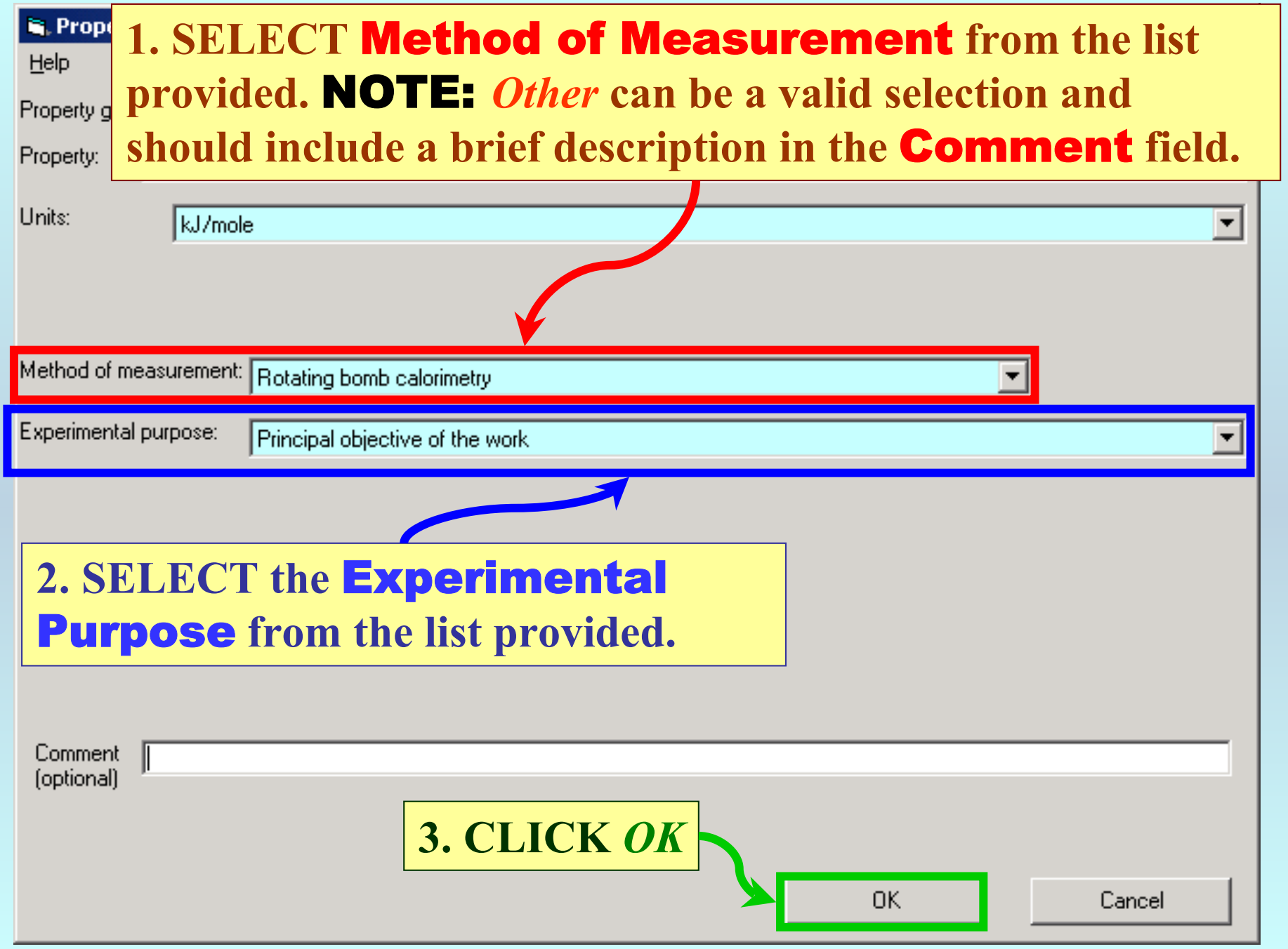


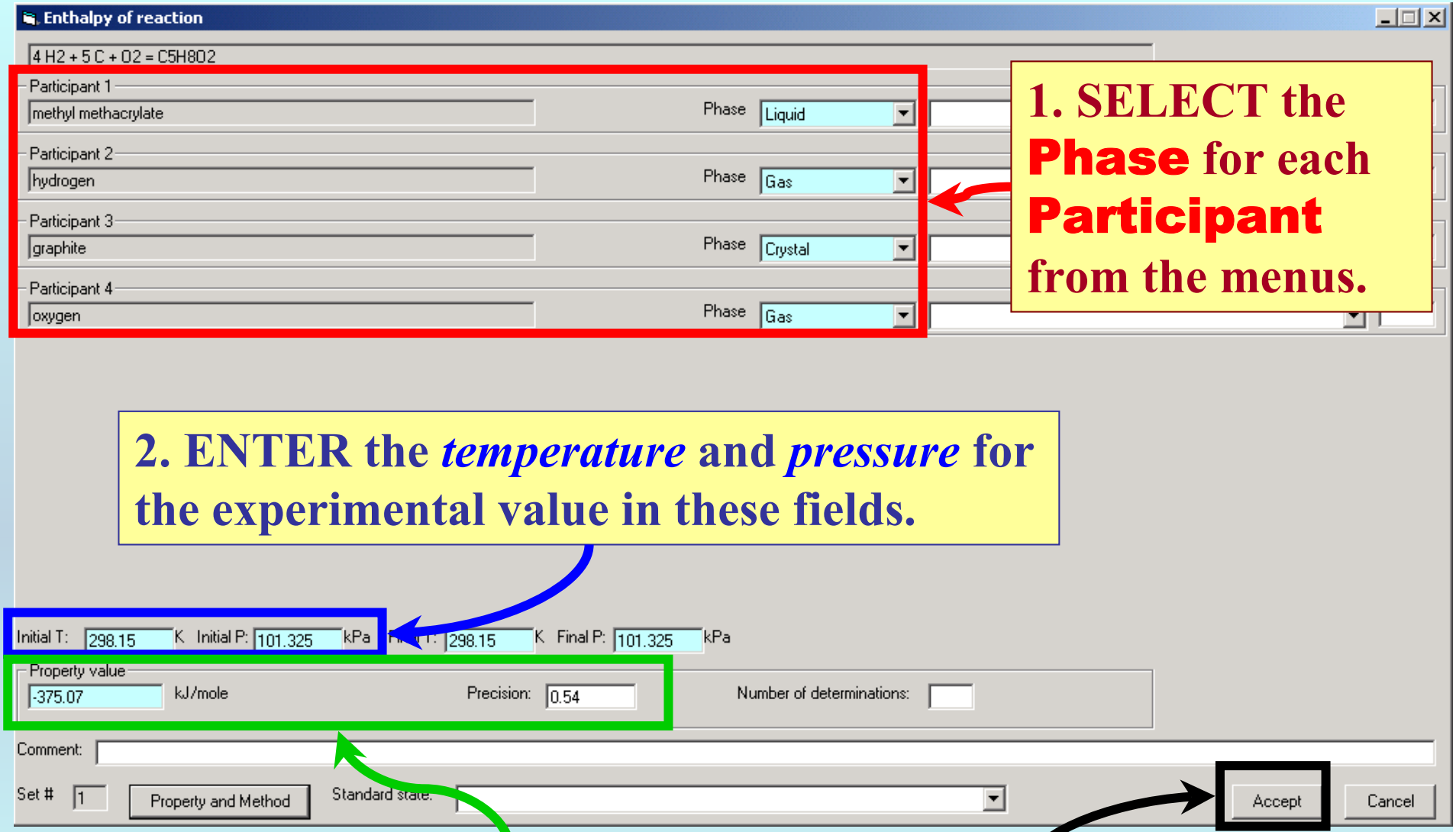
NOTE: The balanced reaction now appears in the **CORRECT** direction.

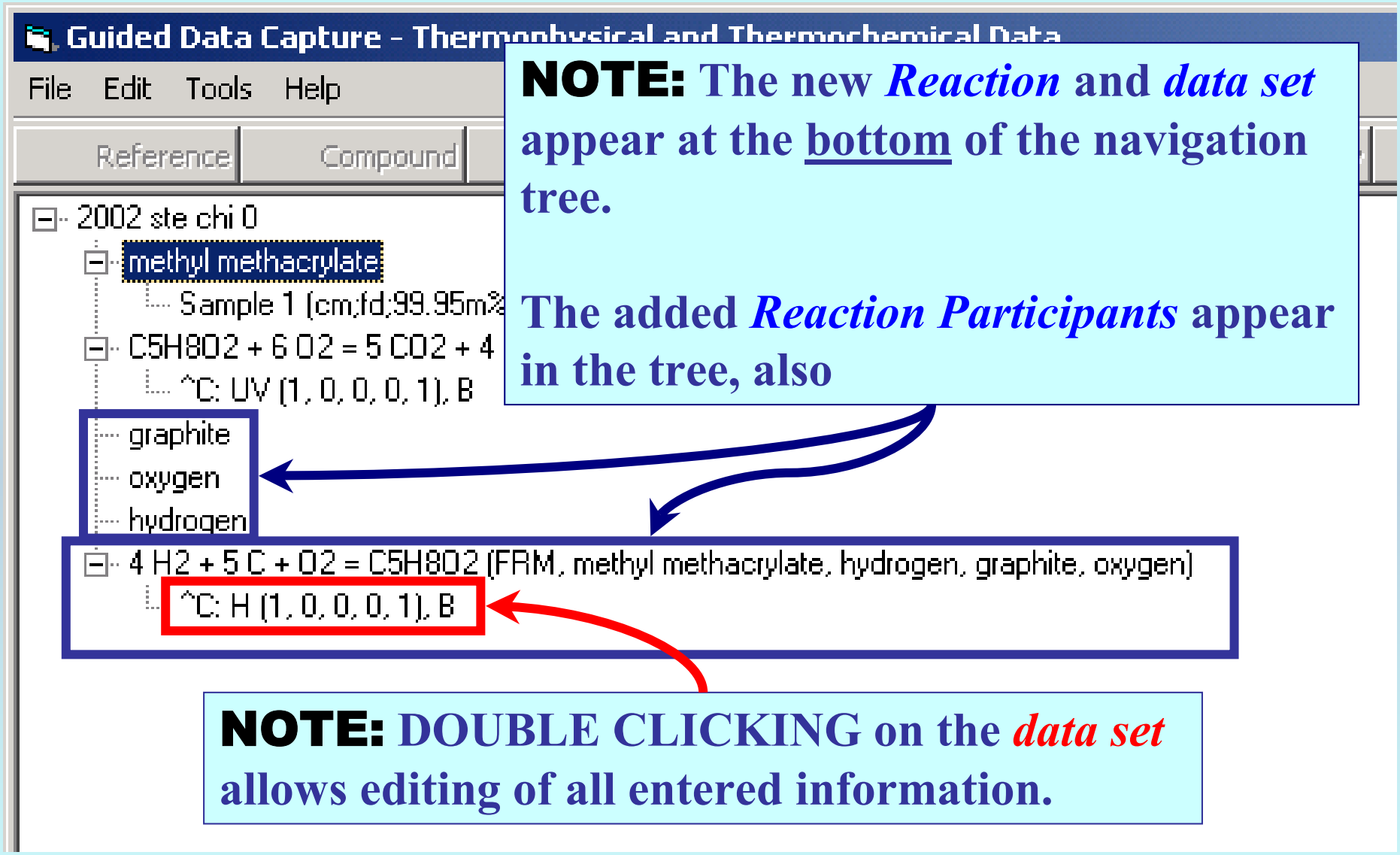


1. CLICK *Accept*


Property and experimental method for 4 H2 + 5 C + O2 = C5H8O2
Help
Property group:
Enthalpy & Internal energy of reaction
Property:
Enthalpy of reaction
Units:
kJ/mole
Method of measurement:
Experimental purpose:
1. SELECT the Property Group: Enthalpy & Internal energy of reaction from the menu.
2. SELECT the Property: Enthalpy of reaction
3. SELECT the Units: kJ/mol, here.
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.
Help
Property g
Property:
Units:
kJ/mole
Method of measurement:
Rotating bomb calorimetry
Experimental purpose:
Principal objective of the work
2. SELECT the Experimental Purpose from the list provided.
Comment (optional)
3. CLICK OK
OK
Cancel


Enthalpy of reaction
4 H2 + 5 C + O2 = C5H8O2
Participant 1
methyl methacrylate
Phase
Liquid
Participant 2
hydrogen
Phase
Gas
Participant 3
graphite
Phase
Crystal
Participant 4
oxygen
Phase
Gas
1. SELECT the Phase for each Participant from the menus.
2. ENTER the temperature and pressure for the experimental value in these fields.
Initial T:
298.15
K
Initial P:
101.325
kPa
Final T:
298.15
K
Final P:
101.325
kPa
Property value
-375.07
kJ/mole
Precision:
0.54
Number of determinations:
Comment:
Set #
1
Property and Method
Standard state:
Accept
Cancel
3. ENTER the Property value and Precision, if known.
4. CLICK Accept


Guided Data Capture - Thermophysical and Thermochemical Data
File Edit Tools Help
Reference Compound
2002 ste chi 0
methyl methacrylate
Sample 1 (cm;fd;99.95m%
C5H8O2 + 6 O2 = 5 CO2 + 4
^C: UV (1, 0, 0, 0, 1), B
graphite
oxygen
hydrogen
4 H2 + 5 C + O2 = C5H8O2 (FRM, methyl methacrylate, hydrogen, graphite, oxygen)
^C: H (1, 0, 0, 0, 1), B
NOTE: The new Reaction and data set appear at the bottom of the navigation tree.
The added Reaction Participants appear in the tree, also
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.**