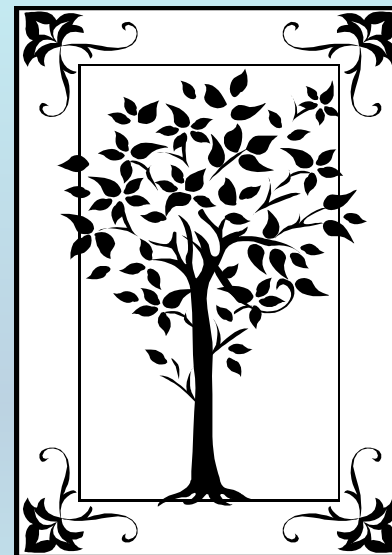


**METADATA AND NUMERICAL DATA CAPTURE:
Energy of Combustion $\Delta_c u^\circ$ (J/g)**

**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 O₂(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	{($\Delta_c U_m^\circ/M$)(compd)}/(J·g ⁻¹)	⟨{($\Delta_c U_m^\circ/M$)(compd)}⟩/(J·g ⁻¹)
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
<i>trans</i> -methyl cinnamate	-31 187.3, -31 187.3, -31 186.3, -31 185.2, -31 188.3, -31 187.7, -31 189.3, -31 190.0	-31 187.9 ± 0.5
α -methyl cinnamaldehyde	-36 168.7, -36 157.5, -36 171.0, -36 152.7, -36 155.5, -36 156.3, -36 178.9, -36 159.8, -36 155.0	-36 159.5 ± 2.1
1-nonyne	-46 956.3, -46 971.0, -46 960.4, -46 967.2, -46 959.3, -46 968.4, -46 960.7	-46 962.3 ± 1.7
trimethyl	-27 655.8, -27 654.7, -27 645.0, -27 651.3	-27 650.7 ± 1.7
trimethyl	-30 680.8, -30 681.4, -30 675.2, -30 677.0	-30 678.7 ± 1.1
ethyl trim	-32 176.0, -32 180.9, -32 169.5, -32 179.4, -32 175.4	-32 177.9 ± 1.7

This data set is
considered here.

^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.

Experimental Method Info:

Rotating Combustion Bomb Calorimetry

The screenshot shows a software window titled "Guided Data Capture - Thermophysical and Thermochemical Data". The menu bar includes "File", "Edit", "Tools", and "Help". Below the menu bar is a tabbed interface with tabs for "Reference", "Compound", "Sample", "Mixture", "Reaction", "Property", and "Data Tables". The "Reaction" tab is highlighted with a blue box. In the main area, a tree view shows a folder "2002 ste.chi.0" containing a sub-entry "methyl methacrylate:", which is highlighted with a red box. Below this entry, a sample description is visible: "Sample 1 (cm,rd;99.95m%,cl,99.974m%,co2)". A red arrow points from the "methyl methacrylate:" entry to a yellow callout box. A blue arrow points from the "Reaction" tab to another yellow callout box.

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

2. **CLICK** *Reaction*

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.

Reaction

Help

=

Reaction class: Combustion with oxygen

Auto-complete Reaction

Balance Reaction

Check Stoichiometry

Participant	Chemical Name	Coefficient	Sample #
Participant 1	methyl methacrylate		1
Participant 2			
Participant 3			
Participant 4			
Participant 5			
Participant 6			
Participant 7			
Participant 8			

Solvent: Inert component:

Accept Cancel

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.

Reaction

Help

$C_5H_8O_2 + 6 O_2 = 5 CO_2 + 4 H_2O$

Reaction class:

Participant	Chemical Name	Coefficient	Sample #
Participant 1	methyl methacrylate	-1	1
Participant 2	oxygen	-6	
Participant 3	carbon dioxide	5	
Participant 4	water	4	
Participant 5			
Participant 6			
Participant 7			
Participant 8			

Solvent: Inert component:

CLICK *Accept*

Property and experimental method for $C_5H_8O_2 + 6 O_2 = 5 CO_2 + 4 H_2O$

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.

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/g

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

Internal energy of reaction (mass basis)

$C_5H_8O_2 + 6 O_2 = 5 CO_2 + 4 H_2O$

Participant 1 methyl methacrylate	Phase Liquid
Participant 2 carbon dioxide	Phase Gas
Participant 3 water	Phase Liquid
Participant 4 oxygen	Phase Gas

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

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 -27301.1 J/g	Precision: 1.3	Number of determinations: 7
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Comment:

Set # 1 Property and Method Standard state:

Accept Cancel

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.

The screenshot shows a software window titled "Guided Data Capture - Thermophysical a". The menu bar includes "File", "Edit", "Tools", and "Help". Below the menu bar are tabs for "Reference", "Compound", "Sample", "Mixture", "Reaction", and "Property". The navigation tree on the left shows a folder "2002 ste chi 0" containing "methyl methacrylate", "Sample 1 (cm;fd;99.95m%,glc,99.974m%,co2)", and a reaction: "C5H8O2 + 6 O2 = 5 CO2 + 4 H2O (CMO, methyl methacrylate, carbon dioxide, water, oxygen)". Below the reaction is a data set: "^C: UV (1, 0, 0, 0, 1), B". A blue arrow points from the "Reaction" tab to the reaction entry in the tree. A red arrow points from the "data set" entry to the note below.

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.