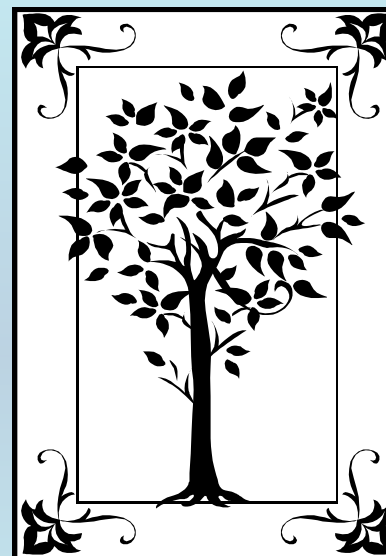


METADATA AND NUMERICAL DATA CAPTURE:

Enthalpy of Formation

$\Delta_f H_m^\circ$ (kJ/mol)

Guided Data Capture (GDC)



This tutorial describes
METADATA AND NUMERICAL DATA CAPTURE:
for **Enthalpy of Formation $\Delta_f H_m^\circ$ (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

	$\Delta_c U_m^\circ / \text{kJ} \cdot \text{mol}^{-1}$	$\Delta_c H_m^\circ / \text{kJ} \cdot \text{mol}^{-1}$	$\Delta_f H_m^\circ / \text{kJ} \cdot \text{mol}^{-1}$
methyl methacrylate (l)	-2733.33 ± 0.46	-2735.80 ± 0.46	-375.07 ± 0.54
<i>trans</i> -methyl cinnamate (cr)	-5058.32 ± 0.76	-5062.04 ± 0.76	-362.71 ± 0.88
α -methyl cinnamaldehyde (l)	-5286.14 ± 0.96	-5291.09 ± 0.96	-73.15 ± 1.08
1-nonyne (l)	-5833.98 ± 0.88	-5843.90 ± 0.88	15.61 ± 1.02
trimethylacetic acid (cr)	-2824.07 ± 0.52	-2827.79 ± 0.52	-568.51 ± 0.60
trimethylacetic anhydride (l)	-5713.97 ± 0.90	-5721.41 ± 0.90	-789.16 ± 1.06
ethyl trimethyl acetate (l)	-4189.16 ± 0.70	-4195.36 ± 0.70	-550.02 ± 0.82

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

**This data set is
considered here.**

Experimental Method Info:

Rotating Combustion Bomb Calorimetry

Guided Data Capture - Thermophysical and Thermochemical Data

File Edit Tools Help

Reference Compound Sample Mixture **Reaction** Property

2002 ste chi 0

methyl methacrylate

Sample 1 (cm;td;99.95m%,glc,99.974m%,co2)

054000 0.00 5.000 1.420 (CH₂=C(CH₃)COOCH₃, carb (gen)

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:** *Formation of a compound*, 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.

The screenshot shows a software interface for setting up a reaction. A red box highlights the 'Reaction class' dropdown menu, which is set to 'Formation of a compound from elements in their stable state'. A blue box highlights the 'Sample #' dropdown menu for the first participant, which is set to '1'. A green box highlights the 'Participant 2' dropdown menu, which is currently empty. A green callout box with an arrow points to the 'Participant 2' field, containing the text '3. CLICK in the Participant 2 field.' The interface includes fields for 'Participant 1' (methyl methacrylate), 'Participant 2' through 'Participant 8', 'Solvent', and 'Inert component'. There are also buttons for 'Balance Reaction', 'Check Stoichiometry', 'Accept', and 'Cancel'.

Participant	Participant 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:

Buttons: Balance Reaction, Check Stoichiometry, Accept, Cancel

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		Coefficient		Sample #	
Participant 3	New	Coefficient		Sample #	
Participant 4		Coefficient		Sample #	
Participant 5		Coefficient		Sample #	

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:

Search results:

Find

Accept

Cancel

The screenshot shows a dialog box titled "Substance" with a "Help" button. It contains three input fields: "CAS Registry Number" (with three small boxes), "Empirical formula (Case sensitive)", and "Name: graphite". The "Name" field is highlighted with a red box. To the right, the "Find" button is highlighted with a blue box. Below the "Name" field is a "Search results:" dropdown menu. At the bottom right are "Accept" and "Cancel" buttons.

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

2. CLICK Find

The screenshot shows the same "Substance" dialog box. The "Name" field still contains "graphite". The "Search results:" dropdown menu now displays "graphite" and is highlighted with a green box. The "Find" button is now disabled (greyed out). The "Accept" button is highlighted with a black box.

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.

Reaction

Help

=

Reaction class: Formation of a compound from elements in their stable state

Balance Reaction

Check Stoichiometry

Participant	Substance	Coefficient	Sample #
Participant 1	methyl methacrylate		1
Participant 2	graphite		
Participant 3			
Participant 4			
Participant 5			
Participant 6			
Participant 7			
Participant 8			

Solvent: Inert component:

Accept Cancel

1. Identify all of the reaction Participants

The screenshot shows a 'Reaction' dialog box with the following fields and controls:

- Reaction class: Formation of a compound from elements in their stable state
- Participant 1: methyl methacrylate
- Participant 2: graphite
- Participant 3: oxygen
- Participant 4: hydrogen
- Participant 5: (empty)
- Participant 6: (empty)
- Participant 7: (empty)
- Participant 8: (empty)
- Solvent: (empty)
- Inert component: (empty)
- Buttons: Balance Reaction, Check Stoichiometry, Accept, Cancel

Annotations:

- A red box highlights the rows for Participant 2, 3, and 4.
- A blue box highlights the 'Balance Reaction' button.
- A red arrow points from the text box to the red box.
- A blue arrow points from the text box to the 'Balance Reaction' button.

**2. CLICK
Balance Reaction**

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

The screenshot shows a software window titled "Reaction" with a "Help" button. The main text area contains the chemical equation: $C_5H_8O_2 = 5 C + O_2 + 4 H_2$. Below this, the "Reaction class" is set to "Formation of a compound from elements in their stable state". There are two buttons: "Balance Reaction" (highlighted with a blue box and a blue arrow) and "Check Stoichiometry".

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

At the bottom, there are "Solvent:" fields and "Accept" and "Cancel" buttons.

1. Change the first Coefficient from -1 to 1.

2. CLICK Balance Reaction again.

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

The screenshot shows a 'Reaction' dialog box with the following details:

- Reaction class: Formation of a compound from elements in their stable state
- Buttons: Balance Reaction, Check Stoichiometry
- Participant 1: methyl methacrylate, Coefficient: 1, Sample #: 1
- Participant 2: graphite, Coefficient: .5
- Participant 3: oxygen, Coefficient: -1
- Participant 4: hydrogen, Coefficient: -4
- Participant 5: (empty), Coefficient: (empty), Sample #: (empty)
- Participant 6: (empty), Coefficient: (empty), Sample #: (empty)
- Participant 7: (empty), Coefficient: (empty), Sample #: (empty)
- Participant 8: (empty), Coefficient: (empty), Sample #: (empty)
- Solvent: (empty)
- Inert component: (empty)
- Buttons: Accept, Cancel

The chemical equation displayed in the text box is: $5 \text{ C} + \text{O}_2 + 4 \text{ H}_2 = \text{C}_5\text{H}_8\text{O}_2$

1. CLICK *Accept*

Property and experimental method for $4 \text{ H}_2 + 5 \text{ C} + \text{O}_2 = \text{C}_5\text{H}_8\text{O}_2$

Help

Property group: Enthalpy & Internal energy of reaction

Property: Enthalpy of reaction

Units: kJ/mole

Method of measurement:

Experimental purpose:

Comment (optional)

OK Cancel

The image shows a software dialog box titled "Property and experimental method for 4 H2 + 5 C + O2 = C5H8O2". It contains several input fields and dropdown menus. Three numbered instructions are overlaid on the dialog, each with a colored arrow pointing to a specific field: 1. A red arrow points to the "Property group" dropdown menu, which is highlighted with a red box. 2. A blue arrow points to the "Property" dropdown menu, which is highlighted with a blue box. 3. A green arrow points to the "Units" text box, which is highlighted with a green box. The dialog also includes fields for "Method of measurement", "Experimental purpose", and "Comment (optional)", along with "OK" and "Cancel" buttons at the bottom.

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.

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:

Method of measurement:

Experimental purpose:

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%

$C_5H_8O_2 + 6 O_2 = 5 CO_2 + 4$

$\hat{C}: UV (1, 0, 0, 0, 1), B$

graphite

oxygen

hydrogen

$4 H_2 + 5 C + O_2 = C_5H_8O_2$ (FRM, methyl methacrylate, hydrogen, graphite, oxygen)

$\hat{C}: H (1, 0, 0, 0, 1), B$

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.