

Calculation of Heat During a Phase Change or Reaction

During a phase change, a physical process or chemical reaction, the temperature of the system does not change. Therefore the formula $q = mc\Delta T$ would be useless. To correctly calculate the change in heat in a system not undergoing a temperature change, use this formula:

$$q = n \Delta H \quad \text{where } H \text{ is the change in molar potential energy}$$

Example: Calculate the energy required to melt a 2.9 kg block of ice.

Answer: Melting is a phase change - there is no change in temperature

Given: $m = 2.9 \times 10^3 \text{ g}$

$\Delta H = 6.02 \text{ kJ/mol}$ (taken from table or provided)

Determine $M = 18.02 \text{ g/mol}$

$$\begin{aligned} q &= n \Delta H \\ &= (m/M) (\Delta H) \\ &= \frac{2.9 \times 10^3 \text{ g}}{18.02 \text{ g/mol}} \times 6.02 \text{ kJ/mol} \\ &= 9.7 \times 10^2 \text{ kJ} \end{aligned}$$

Example: 27615.2 kJ of energy was released when 345 g of propane was combusted. Calculate the molar enthalpy of combustion of propane (ΔH_{comb})

Given:

$m = 345 \text{ g}$

$q = -27615.2 \text{ kJ}$

$M = 44.11 \text{ g/mol}$

$$q = n \Delta H$$

$$q = m/M \Delta H$$

$$\frac{q}{m/M} = \Delta H$$

$$\begin{aligned} q \times M/m &= \Delta H \\ (-27615.2 \text{ kJ}) \times \frac{44.11 \text{ g/mol}}{345 \text{ g}} &= \Delta H \\ -3.53 \times 10^3 \text{ kJ/mol} &= \Delta H \end{aligned}$$

Example: The molar enthalpy of vaporization of ethene (C₂H₄) is measured at 16.7 kJ/ mol. An unknown sample of ethene released 79.6 kJ of heat when it condensed. Calculate the mass of the sample.

Given:

$$-\Delta H_{\text{cond}} = \Delta H_{\text{vap}}$$

$$\Delta H_{\text{cond}} = -16.7 \text{ kJ/mol}$$

$$q = -79.6 \text{ kJ}$$

$$M \text{ of C}_2\text{H}_4 = 28.06 \text{ g/mol}$$

$$q = n \Delta H$$

$$q = m/M \Delta H$$

$$m = \frac{q M}{\Delta H}$$

$$= \frac{(-79.6 \text{ kJ})(28.06 \text{ g/mol})}{-16.7 \text{ kJ/mol}}$$

$$= 1.34 \times 10^2 \text{ g}$$

IMPORTANT THINGS TO REMEMBER:

1. ΔH is always provided unless
 - A) it is for water - in your data table
 - B) it is what you're trying to find
2. Phase changes can be given as endothermic, but may need to be reversed to exothermic or vice versa (the molar enthalpy of vaporization may be given, but you need condensation, so reverse the sign)
3. These are generally multiple choice questions

BACK TO CALORIMETRY

Previously in our notes, the first calorimetry problem- type, ones with temperature change, were covered. There are other types of systems that involve physical changes and chemical reactions. These do not have a change in temperature. Energy in those systems was calculated using $n \Delta H$. Now we can include this in our calorimetry problems.

Bomb Calorimetry Problems

In a bomb calorimeter, the system is always combusted and the calorimeter changes temperature, the following formula will probably be used:

$$q_{\text{sys}} = -q_{\text{surr}}$$

$$q_{\text{sys}} = -q_{\text{cal}}$$

$$n \Delta H = -C\Delta T \text{ (always use the } C\Delta T \text{ for bomb calorimetry, not } mc\Delta T)$$

Example : 27.6 g of butyne (C_4H_6) completely combusted in a bomb calorimeter whose heat capacity is $13.4 \text{ kJ/}^\circ\text{C}$. The calorimeter increased in temperature 1.5°C . Calculate the enthalpy of combustion of butyne.

Given:

$$m = 27.6 \text{ g}$$

$$M \text{ of } C_4H_6 = 54.10 \text{ g/mol}$$

$$C = 13.4 \text{ kJ/}^\circ\text{C}$$

$$\Delta T = 1.5^\circ\text{C}$$

$$q_{\text{sys}} = -q_{\text{surr}}$$

$$q_{\text{sys}} = -q_{\text{cal}}$$

$$n \Delta H = -C\Delta T$$

$$\Delta H = \frac{-C\Delta T}{n}$$

$$\Delta H = \frac{-C\Delta T M}{m}$$

$$= \frac{(-13.4 \text{ kJ/}^\circ\text{C})(1.5^\circ\text{C})(54.10 \text{ g/mol})}{27.6 \text{ g}}$$

$$= -39 \text{ kJ/mol}$$

Solution Calorimetry (also in coffee cup calorimetry)

A. Acids and Bases

- When acids and bases are mixed in a coffee cup calorimeter they neutralize each other creating a salt and water
- Both the acid and the base have a molar enthalpy of neutralization (ΔH_{neut})
- The mass of water in this problem type is calculated using the TOTAL VOLUME OF THE ACID AND THE BASE, then convert mL of water to g of water
- The concentration of the salt is assumed to be negligible
- Remember $n = Cv$, to substitute for the n in “ $n \Delta H$ ”

$$q_{\text{sys}} = -q_{\text{surr}}$$

$$q_{\text{sys}} = -q_{\text{cal}}$$

$$n \Delta H = -mc \Delta T$$

Example: 12.6 mL of 0.10 M HCl (aq) completely neutralized 6.3 mL of 0.20 M NaOH (aq) in a coffee-cup calorimeter. The molar enthalpy of neutralization is - 8.9 kJ/mol. Calculate the temperature change in the calorimeter.

Given:

$$V_{\text{HCl}} = 12.6 \text{ mL}$$

$$C_{\text{HCl}} = 0.10 \text{ M}$$

$$V_{\text{NaOH}} = 6.3 \text{ mL}$$

$$C_{\text{NaOH}} = 0.20 \text{ M}$$

$$\Delta H_{\text{neut}} = - 8.9 \text{ kJ/mol} = -8.9 \times 10^3 \text{ J}$$

$$V_{\text{total}} = 18.9 \text{ mL} = 18.9 \text{ g}$$

$$\Delta T = ?$$

$$c \text{ of water} = 4.184 \text{ J/g}^\circ\text{C}$$

Note : since this is neutralization of a 1:1 acid - base, we can just calculate the number of moles for either the acid or the base

$$q_{\text{sys}} = - q_{\text{surr}}$$

$$q_{\text{sys}} = -q_{\text{cal}}$$

$$n \Delta H_{\text{neut}} = - mc \Delta T$$

$$Cv \Delta H_{\text{neut}} = -mc \Delta T$$

$$\Delta T = \frac{Cv \Delta H_{\text{neut}}}{(- mc)_{\text{water}}}$$

$$\Delta T = \frac{(0.10 \text{ mol/L})(12.6 \times 10^{-2} \text{ L})(-8.9 \times 10^3 \text{ J/mol})}{-(18.9 \text{ g})(4.184 \text{ J/g}^\circ\text{C})}$$

$$\Delta T = 0.14 \text{ }^\circ\text{C}$$

B. Dissolving solids

- Another important type of solution calorimetry is when a solid is dissolved in the water of the calorimeter. WHEN YOU HAVE THIS TYPE OF PROBLEM TO YOU NEED TO ADD THE MASS OF THE SOLID TO THE MASS OF THE WATER TO GET THE TOTAL MASS FOR THE $mc\Delta T$ PART

Example: 29.6 g of ammonium nitrate was dissolved in 745.3 mL of water. The water's temperature rose from 18.4 °C to 21.3 °C. Calculate the molar enthalpy of solution formation of NH_4NO_3 .

Given:

$$m \text{ of } \text{NH}_4\text{NO}_3 = 29.6 \text{ g}$$

$$v \text{ of water} = 745.3 \text{ mL}$$

$$m \text{ of water} = (745.3 + 29.6 \text{ g}) \\ = 774.9 \text{ g}$$

$$\Delta T = (21.3 - 18.4)^\circ \text{C}$$

$$M \text{ of } \text{NH}_4\text{NO}_3 = 80.06 \text{ g/mol}$$

$$\Delta H_{\text{soln}} = ?$$

$$q_{\text{sys}} = -q_{\text{surr}}$$

$$q_{\text{sys}} = -q_{\text{cal}}$$

$$n\Delta H_{\text{soln}} = -mc\Delta T$$

$$\Delta H_{\text{soln}} = -\frac{mc\Delta T}{M}$$

$$\Delta H_{\text{soln}} = -\frac{(774.5 \text{ g})(4.184 \text{ J/g}^\circ\text{C})(2.9^\circ\text{C})(80.06 \text{ g/mol})}{29.6 \text{ g}}$$

$$= -2.5 \times 10^4 \text{ J/mol}$$