Chapter 6 - Principles of Reactivity: Energy and Chemical Reactions

- Introduction to thermodynamics - science of heat or energy flow in chemical reactions or processes.

What is Energy? the capacity to do work
  Kinetic energy - associated with motion
    e.g. thermal, mechanical, electrical, sound
  potential energy - results from an object's position - stored energy
    e.g. gravitational, chemical potential energy, electrostatic (separation of charge)

First Law of Thermodynamics: energy can neither be created or destroyed. The total energy of the universe is constant.

Temperature vs. Heat - Be careful of misconceptions!
- heat is not the same as temperature.
- the more thermal energy a substance has, the greater is the motion of its atoms & molecules.
- the total thermal energy in an object is sum of all the individual energies of all the atoms, molecules, ions in object.

How do you explain how a thermometer works?
- when thermometer is put into a beaker of hot water, the atoms of mercury in the thermometer try to reach <u>thermal equilibrium</u> with water - they start moving faster, the Hg atoms get a little farther apart, the Hg(ℓ) expands, + column of Hg rises until thermal energy is the same as that of H_2O. At that point, temperature of Hg + temperature of the H_2O are the same!

- heat transfer always occurs from an object at higher T to an object at lower T.

System vs. Surroundings
- in thermodynamics, they have precise definitions
- system - object or group of objects being studied
- surroundings - everything else.

exothermic - system loses heat to the surroundings
endothermic - system gains heat from the surroundings

Consider the melting of an ice cube of water:

$$\underset{\substack{\uparrow \\ \text{heat is reactant}}}{\text{heat}} + H_2O(s) \longrightarrow H_2O(\ell)$$

system: water
surroundings: everything else
endothermic process

Turn this process around: what happens when H_2O freezes?

$$H_2O(\ell) \longrightarrow H_2O(s) + \underset{\substack{\uparrow \\ \text{heat is product}}}{\text{heat}} \qquad \text{exothermic}$$

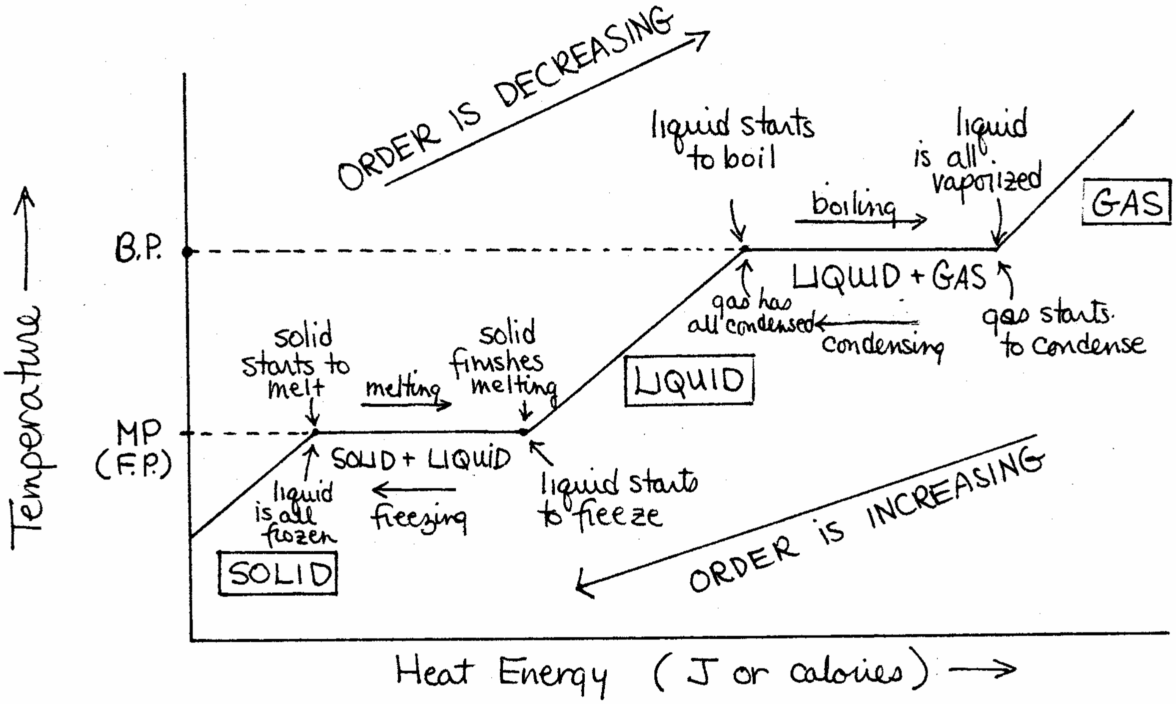
- this is somewhat counterintuitive. When farmers spray their orchards with water during a freeze, the ice does insulate the fruit, but the process also releases heat, protecting the crop.

Units of energy: 1 calorie (cal) = 4.184 joules (J)

Note: the dietary Calorie = 1000 calories

The quantity of heat that can be transferred is a function of
- the amount of material
- the size of the temperature change
- the identity of the material gaining or losing heat
- if a phase change occurs

Let's see what happens!



Heat is absorbed by system as solid ⟶ liquid ⟶ gas.
This process of breaking intermolecular forces is ENDOTHERMIC.
Heat is released by system as gas → liquid → solid
This process is EXOTHERMIC.

The amount of heat absorbed or released by a system during phase changes can be accurately calculated.

Terminology:

Joule and calorie are units of heat. 1 calorie = 4.184 J

Specific heat of a substance in a certain phase (gas, liquid, solid) is the amount of heat required to raise the temperature of 1 g of the substance by 1 °C. with no change in state.

Specific heat has units of (J/g °C). Heat = Sp. H. × mass × ΔT

Heat of fusion: the amount of heat required to melt 1 g of a solid at its melting point. Units: (J/g). It is also the amount of heat released when 1 g of a liquid freezes at its freezing point.

Amount of Heat = heat of fusion × mass

Extra

Difference Between Specific Heat ($\frac{J}{g\cdot °C}$) and Heat of Fusion/Vaporization ($\frac{J}{g}$)

Specific heat is a constant particular to a certain substance in a specific phase which relates how much heat in joules is necessary to change the temperature of a certain amount of the substance (without changing its phase).

Example: If 15.0 g of iron(s) cools from 35.0°C to 9.0°C, thereby releasing 173 J of heat, what is the specific heat of iron(s)?

$$\text{Specific heat } \left(\frac{J}{g\cdot °C}\right) = \frac{\text{heat (J)}}{\text{mass(g)} \times \Delta T(°C)} = \frac{173\ J}{15.0\ g \times (35.0-9.0)°C}$$

$$= 0.444\ J/g°C$$

Heat of Fusion/Vaporization (J/g) is a constant particular to a certain substance that is changing phase at the temperature where the phase change occurs:

Heat of fusion solid $\rightleftarrows$ liquid occurs at freezing/melting pt
Heat of vaporization liquid $\rightleftarrows$ gas occurs at boiling point

The constant relates how much heat is necessary for the phase change to occur at the phase change temperature for a certain mass of compound

Example: If 327 J of heat are removed from 3.00 g of $CH_3CH_2OH(l)$ at -117°C, what is the heat of fusion of ethanol? The freezing point of ethanol is -117°C.

$$\text{Heat of Fusion } \left(\frac{J}{g}\right) = \frac{\text{heat (J)}}{\text{mass (g)}} = \frac{327\ J}{3.00\ g} = 109\ J/g$$

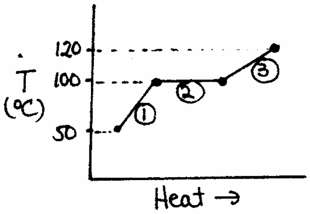
Note: temperature or temperature change is not involved in the calculation for heat of fusion or heat of vaporization because the process is occurring at the phase change temperature.

Heat of vaporization: the amount of heat required to vaporize 1 g of a liquid to a gas at its boiling point. Units: (J/g). H is also the amount of heat released when 1 g of vapor condenses to 1 g of liquid at the boiling point. Amount of heat = heat of vap. × mass

Example: How many joules of energy must be absorbed by 500 g of H_2O at 50°C to convert it to 500 g of steam at 120°C?

Given: Specific heat $H_2O(l)$: 4.18 J/g°C
Specific heat $H_2O(g)$: 2.03 J/g°C
Heat of vaporization H_2O: 2.26×10^3 J/g
B.P. H_2O : 100°C

$$\underset{50^\circ C}{\text{liquid}} \xrightarrow{①} \underset{100^\circ C}{\text{liquid}} \xrightarrow{②} \underset{100^\circ C}{\text{gas}} \xrightarrow{③} \underset{120^\circ C}{\text{gas}}$$



where ① heat needed to raise T of 500 g H_2O to its B.P. at 100°C
② heat needed to change all water into steam at 100°C
③ heat needed to raise T of steam from 100°C to 120°C

Total Heat Absorbed = ① + ② + ③

$$= [\text{Sp. H. } H_2O(l) \times \text{mass } H_2O \times \Delta T] + [\text{H. of vap.} \times \text{mass } H_2O] + [\text{Sp. H. of } H_2O(g) \times \text{mass } H_2O \times \Delta T]$$

$$= [4.18 \tfrac{J}{g\,^\circ C} \times 500\,g \times (100-50\,^\circ C)] + [2.26 \times 10^3 \tfrac{J}{g} \times 500\,g] + [2.03 \tfrac{J}{g\,^\circ C} \times 500\,g \times (120-100\,^\circ C)]$$

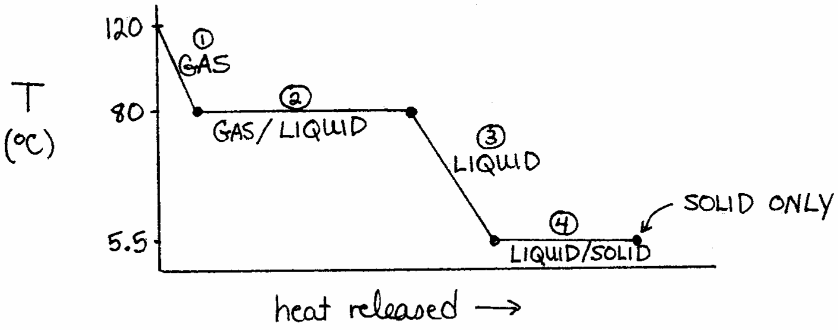
$$= 104 \text{ kJ} + 1130 \text{ kJ} + 20 \text{ kJ}$$
$$= 1250 \text{ kJ}$$
$$= 1.25 \times 10^6 \text{ J}$$

Note that the energy required to break the intermolecular bonds in liquid water is very high due primarily to hydrogen bonding. more later!

Example: How much heat (in kJ) must be removed when cooling 155 g of benzene, C_6H_6, at 120.0°C to solid benzene at 5.48°C?

Given for benzene: b.p. at 1 atm : 80.1 °C
m.p. at 1 atm : 5.48 °C

specific heat (ℓ): 1.74 J/g°C
specific heat (g): 1.04 J/g°C
heat of fusion : 127 J/g
heat of vaporization: 395 J/g



Plan: $\underset{120.0\,^\circ C}{C_6H_6(g)} \xrightarrow[\text{cool}]{①} \underset{80.1\,^\circ C}{C_6H_6(g)} \xrightarrow[\text{condenses}]{②} \underset{80.1\,^\circ C}{C_6H_6(\ell)} \xrightarrow[\text{cool}]{③} \underset{5.48\,^\circ C}{C_6H_6(\ell)} \xrightarrow[\text{freezes}]{④} \underset{5.48\,^\circ C}{C_6H_6(s)}$

Total heat released = ① + ② + ③ + ④

① heat released = Sp. Ht (g) × mass × ΔT = 1.04 J/g°C × 155 g × (120.0 − 80.1°C) = 6.43 kJ

② heat released = Ht vap. × mass = 395 J/g × 155 g = = 61.2 kJ

③ heat released = Sp. Ht (ℓ) × mass × ΔT = 1.74 J/g°C × 155 g × (80.1 − 5.48°C) = 20.1 kJ

④ heat released = Ht fusion × mass = 127 J/g × 155 g = 19.7 kJ

∴ total heat released = ① + ② + ③ + ④ = 107.4 kJ

Example: If 500 g of lead at 200°C are placed in 100g of water at 20°C in an insulated container, what will be the temperature when the lead and water are at the same temperature?

Given: Specific heat of H_2O (l) : $4.18 \frac{J}{g°C}$
Specific heat of Pb(s) : $0.159 \frac{J}{g°C}$

$$\underset{\substack{20°C \\ 100g}}{H_2O\,(l)} \longrightarrow \underset{T_f}{H_2O(l) + Pb\,(s)} \longleftarrow \underset{\substack{200°C \\ 500g}}{Pb(s)}$$

heat gained by water = heat lost by Pb

$$4.18 \frac{J}{g°C} \times 100g \times (T_f - 20) = 0.159 \frac{J}{g°C} \times 500g \times (200 - T_f)$$

$$418\ T_f - 8360\ J = 15900J - 79.5\ T_f$$

$$498\ T_f = 24260\ J$$

$$T_f = 48.7\ °C$$

When substances at different temperatures are mixed, heat is transferred from the warmer substance to the cooler substance and the final temperature of the mixture is intermediate between the original temperatures of the substances.

Example: If 5000 J of heat are removed from 500g of H_2O (l) at 62°C what will be its final temperature?

$$5000\ J = 4.18 \frac{J}{g°C} \times 500g \times (62 - T_f)$$
$$5000\ J = 130{,}000\ J - 2090\ T_f$$
$$2090\ T_f = 125000\ J$$
$$T_f = 59.8\ °C$$

When a 50.0 g bar of copper is placed into 250.0 g of water at 20.4 °C, the temperature of the water rises to 35.00 °C. What was the initial temperature of the copper bar?

Given: specific heat of Cu(s) 0.385 J/g°C
specific heat of $H_2O(l)$ 4.184 J/g°C

heat lost by Cu = heat gained by H_2O

$$\text{Sp Ht Cu} \times \text{mass}_{Cu} \times \Delta T_{Cu} = \text{Sp Ht } H_2O \times \text{mass}_{H_2O} \times \Delta T_{H_2O}$$

$$0.385\ \text{J/g°C} \times 50.0\,\text{g} \times (T - 35.0) = 4.184\ \text{J/g°C} \times 250.0\,\text{g} \times (35.0 - 20.4)$$

$$19.25\,T - 392.7 = 15272\ \text{J} \quad \text{(ignoring sig figs)}$$

$$19.25\,T = 15664$$

$$T = 813\ °\text{C}$$

Note: size of the Kelvin is the same as the °C. Since we are dealing with differences in temperature, we can work in either temperature unit.

Back to the First Law of Thermodynamics:

Consider a book on top of a plastic bag with dry ice ($CO_2(s)$) in it.

$$CO_2(s) \rightarrow CO_2(g) \quad \text{(sublimation)}$$

and the book will rise as bag inflates.

system: $CO_2(s) \rightarrow CO_2(g)$
surroundings: book

system is doing work on the surroundings
w = − Pressure × Δ Volume

change in internal energy, ΔE, is sum of the heat added to the system plus the work done on system.

$$\Delta E = \underset{\text{heat}}{q} + \underset{\text{work}}{w}$$

sign conventions:
- q+ heat is added to system from surroundings.
- q− heat is transferred from system to surroundings
- w+ work done on system by surroundings.
- w− work is done by system on surroundings

Example: What is the change in internal energy of a system which does 20 J of work and absorbs 30 J of heat from its surroundings?

$$\Delta E = q + w$$

$$= \underset{\substack{\uparrow \\ \text{heat is absorbed} \\ \text{by system}}}{+30\,J} + \underset{\substack{\uparrow \\ \text{system does} \\ \text{work}}}{(-20\,J)} = \underset{\substack{\uparrow \\ \text{internal energy} \\ \text{increases}}}{+10\,J}$$

Example: What is the heat involved when a system loses 50 J of internal energy and has 20 J of work done on it by the surroundings? Is the heat change exothermic or endothermic?

$$\Delta E = q + w$$

$$\underset{\substack{\uparrow \\ \text{system loses} \\ \text{internal energy}}}{-50\,J} = q + \underset{\substack{\uparrow \\ \text{work done} \\ \text{on system}}}{(+20\,J)}$$

$$q = -50\,J - 20\,J = \underset{\substack{\uparrow \\ \text{system loses heat} \therefore \text{exothermic}}}{-70\,J}$$

Enthalpy – heat content of a substance at constant pressure

- designated by H
- $\underset{\substack{\uparrow \\ \text{change in} \\ \text{enthalpy}}}{\Delta H} = H_{\text{final state}} - H_{\text{initial state}}$

$\Delta H = q_p$, heat transferred at constant pressure

$\Delta E = q_v$, heat transferred at constant volume

The values of ΔH and ΔE are close and sometimes the same.

Sign conventions are same: $\Delta H = \Delta E - \text{work}$

⊖ heat is released by system

⊕ heat is absorbed by system

State functions: a quantity whose value is determined only by the state of the system. Changes in state functions depend on on the initial and final states, not on how the change occurred, i.e., the path that was taken. They are easy to identify because they are designated by capital letters:

P and ΔP	pressure	$\Delta P = P_{final} - P_{initial}$
T and ΔT	temperature	$\Delta T = T_{final} - T_{initial}$
V and ΔV	volume	$\Delta V = V_{final} - V_{initial}$

and

H, ΔH, E, ΔE

NOT q, w work is easy to see that it is dependent on path since work = force × distance

but, q_V, q_P, $q+w$ are state functions and are independent of path.

Enthalpy Changes for Chemical Reactions

Consider the decomposition of H_2O into hydrogen gas and oxygen gas:

$$H_2O(g) \rightarrow H_2(g) + \tfrac{1}{2}O_2(g) \qquad \Delta H_{rxn} = \underset{\uparrow}{+}241\text{ kJ}$$

1 mole 1 mole ½ mole

heat is absorbed
endothermic rxn

∴ when 1 mol H_2O as a gas breaks down to 1 mol of $H_2(g)$ and ½ mol of $O_2(g)$, 241 kJ of heat at constant pressure is required!

For the reverse reaction, $H_2(g) + \tfrac{1}{2}O_2(g) \rightarrow H_2O(g)$

$$\Delta H_{rxn} = \underset{\uparrow}{-}241\text{ kJ}$$

heat is released
exothermic

How must heat is released for this reaction?

$$2H_2(g) + O_2(g) \rightarrow 2H_2O(g)$$

2 mol 1 mol 2 mol

Ans. +482 kJ

$\Delta H_{rxn} = -482$ kJ

Tricky! If one uses the words "released," the heat is always ⊕
However, when stating $\Delta H = -482$ kJ, one must include the sign convention, so everyone knows which way the heat is moving – into or out of the system.

Consider the following combustion reaction of ethane:

$$C_2H_6(g) + O_2(g) \rightarrow CO_2(g) + H_2O(l) \quad \text{unbalanced}$$

(a) If the ΔH_{rxn} is -1561 kJ/mol C_2H_6; how much heat is released if 20.0 g of $CO_2(g)$ is produced?

(b) If 365 kJ of heat is released, how many grams of C_2H_6 was combusted?

Step 1: Balance the reaction.
Note: in thermodynamic problems, it is OK to have fractional coeff.

$$\underline{\underline{1}}C_2H_6(g) + \frac{7}{2}O_2(g) \longrightarrow 2\,CO_2(g) + 3H_2O(l) + 1561 \text{ kJ}$$

Since $\Delta H_{rxn} = -1561$ kJ/mol C_2H_6, when 1 mole of $C_2H_6(g)$ is consumed, 1561 kJ of heat is produced.

Step 2: Plan!!
Plan for (a): g CO_2 → mol CO_2 → mol C_2H_6 → heat

$$? \text{heat released} = 20.0 \text{ g } CO_2 \times \frac{1 \text{ mol } CO_2}{44.0 \text{ g}} \times \frac{1 \text{ mol } C_2H_6}{2 \text{ mol } CO_2} \times \frac{1561 \text{ kJ released}}{1 \text{ mol } C_2H_6}$$

$$= 355 \text{ kJ released}$$

Plan for (b): heat released → mol C_2H_6 → g C_2H_6

$$? \text{g } C_2H_6 = 365 \text{ kJ} \times \frac{1 \text{ mol } C_2H_6}{1561 \text{ kJ}} \times \frac{30.1 \text{ g}}{1 \text{ mol } C_2H_6} = 7.04 \text{ g } C_2H_6(g)$$

So, heat is handled like any other quantity involved in stoichiometry

How do you experimentally determine the amount of heat evolved or required in a reaction?

Calorimetry –

- measure heat at constant pressure ($\Delta P = 0$) gives $\Delta H = q_P$
  "coffee cup" calorimeter
- measure heat at constant volume ($\Delta V = 0$) gives $\Delta E = q_V$
  "bomb" calorimeter

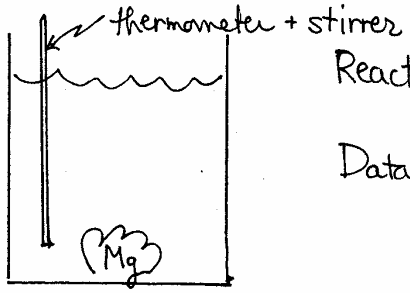
"Coffee Cup" Calorimetry –

- tends to measure heat evolved in aqueous reactions

similar to textbook

Example: Consider adding 0.500 g Mg chips to 100.0 mL of 1.00 M HCl in a coffee cup calorimeter. Find (a) q_P in J (b) ΔH_{rxn} in kJ/mol Mg.

(a)



Reaction: $Mg(s) + 2HCl(aq) \rightarrow MgCl_2(aq) + H_2(g)$

Data: temperature increases from 22.2°C → 44.8°C
specific heat of solution: 4.20 J/g°C
density of solution: 1.00 g/mL
heat capacity of calorimeter: 0.50 J/°C

heat evolved = heat gained by solution + heat gained by calorimeter
= SpHt of soln × mass of soln × ΔT + heat capacity × ΔT
= 4.20 J/g°C × 100.0 g × (44.8 − 22.2) + 0.50 J/°C × (44.8 − 22.2)
= 9492 J + 11.3 J
= 9500 J or 9.50×10^3 J

$\boxed{g\ soln = D \times \#\ mL \qquad D = \frac{g}{mL}}$

$\therefore q_P = -9.50 \times 10^3$ J

(b) now simply do stoichiometry:

$$\Delta H\,(\text{kJ/mol Mg}) = \frac{-9.50 \times 10^3\ J}{0.500\ g\ Mg} \times \frac{1\ kJ}{1000\ J} \times \frac{24.31\ g\ Mg}{1\ mol\ Mg} = -462\ \text{kJ/mol Mg}$$

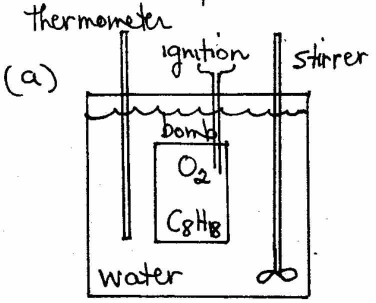
"Bomb" Calorimetry

- tends to measure combustion reactions

similar to book

Example: Consider reacting a 2.00g sample of octane, $C_8H_{18}(l)$, with oxygen in a complete combustion. Find (a) q_v (b) ΔE kJ/g octane (c) ΔE $\left(\frac{kJ}{mol\ octane}\right)$

(a)



Reaction: $C_8H_{18}(l) + \frac{25}{2}O_2(g) \rightarrow 8CO_2(g) + 9H_2O(l)$

Data: mass of water in calorimeter: 1.20 kg
temperature increases from 25.00°C → 41.40°C
heat capacity of bomb = 837 J/°C
Specific heat of water = 4.184 J/g°C

heat evolved = heat gained by water + heat gained by the bomb
= specific Ht of water × $mass_{H_2O}$ × ΔT + heat capacity × ΔT ← 16.4
= 4.184 J/g°C × 1.20×10^3 g × (41.40−25.00) + 837 J/°C × (41.40−25.00
= 82,300 J + 13,700 J
= 96,100 J or 96.1 kJ

$q_v = -96.1$ kJ

(b) $\Delta E\left(\frac{kJ}{g\ C_8H_{18}}\right) = \frac{-96.1\ kJ}{2.00g\ C_8H_{18}} = -48.0$ kJ/g C_8H_{18}

(c) $\Delta E\left(\frac{kJ}{mol\ C_8H_{18}}\right) = \frac{-48.0\ kJ}{1\ g\ C_8H_{18}} \times \frac{114.2\ g}{1\ mol\ C_8H_{18}} = -5480$ kJ/mol C_8H_{18}

What do you do if it isn't possible to use a calorimeter to measure heat involved in a reaction? What happens then?

We use the fact that ΔH and ΔE are state functions and so the path doesn't matter – only the initial reactants and the final products.

Example: Suppose we want to know the ΔH_{rxn} for $A \rightarrow D$
We do know ΔH_{rxn}'s for $A \rightarrow B$, $B \rightarrow C$, and $C \rightarrow D$
We can calculate ΔH for $A \rightarrow D$.

reaction	ΔH_{rxn}
$A \rightarrow B$	-10 kJ
$B \rightarrow C$	-20 kJ
$+ \; C \rightarrow D$	$+5$ kJ
$A \rightarrow D$	$(-10-20+5) = -25$ kJ

If you add up the reactions and cancel out like terms, the desired reaction is the result. The ΔH_{rxn} is the sum of ΔH_{rxn}s of other reactions.

In other words

$$\begin{tikzcd}
B \arrow[r, "-20\text{ kJ}"] & C \arrow[d, "+5\text{ kJ}"] \\
A \arrow[u, "-10\text{ kJ}"] \arrow[r, "-25\text{ kJ}", "\text{Path 1}"'] \arrow[r, bend left=80, "\text{Path 2}"] & D
\end{tikzcd}$$

$$\Delta H_{rxn \text{ Path 1}} = \Delta H_{rxn \text{ Path 2}}$$

since ΔH is state function

This is called <u>Hess' Law of Heat Summation</u>
Here's a real example:

Example: Calculate ΔH° for the reaction: $Na_2O(s) + SO_3(g) \rightarrow Na_2SO_4(s)$
given the following information:

		ΔH°
(1)	$Na(s) + H_2O(l) \rightarrow NaOH(s) + \frac{1}{2} H_2(g)$	-146 kJ
(2)	$Na_2SO_4(s) + H_2O(l) \rightarrow 2NaOH(s) + SO_3(g)$	$+418$ kJ
(3)	$2Na_2O(s) + 2H_2(g) \rightarrow 4Na(s) + 2H_2O(l)$	$+259$ kJ

Hint: Look for a compound in rxn that only appears once in equations given.
In this case (2) has Na_2SO_4, but on wrong side - flip equation
- change sign of ΔH

(a) reverse (2) $\quad 2NaOH + SO_3 \rightarrow Na_2SO_4 + H_2O \qquad \Delta H_{rxn} = \boxed{-418 \text{ kJ}}$

(b) ÷ (3) by 2 $\quad Na_2O + H_2 \rightarrow 2Na + H_2O \qquad \Delta H_{rxn} = +259 \div 2 = \boxed{+129.5 \text{ kJ}}$

(c) we use (1) to "mop up" compounds we don't want
× (1) by 2 $\quad 2Na + 2H_2O \rightarrow 2NaOH + H_2 \qquad \Delta H_{rxn} = -146 \times 2 = \boxed{-292 \text{ kJ}}$

add together, cancel terms

$Na_2O + SO_3 \rightarrow Na_2SO_4 \qquad \Delta H_{rxn} = -580$ kJ ans.

Hess' Law can be restated in mathematical terms:

$$\Delta H^\circ_{rxn} = \sum n \Delta H^\circ_f \text{ products} - \sum n \Delta H^\circ_f \text{ reactants}$$

where ΔH° ← "naught" – at 1atm pressure

n stoichiometric coefficient

ΔH°_f standard molar enthalpy of formation (kJ/mol)
(data is available in tables)

Notes: Standard molar enthalpy of formation, ΔH°_f, is amount of heat absorbed in a reaction where <u>1 mole</u> of a substance in a specific state is made from elements in their standard state.

Examples of elements in their standard states where $\Delta H^\circ_f = 0$.

hydrogen:	$H_2(g)$	mercury	$Hg(l)$
helium:	$He(g)$	iron	$Fe(s)$
chlorine:	$Cl(g)$	carbon	C (s, graphite)
bromine:	$Br_2(l)$		
iodine:	$I_2(s)$		

	Reaction	ΔH_{rxn}
ΔH°_f $H_2O(g) = -241.8$ kJ/mol	$H_2(g) + \frac{1}{2}O_2(g) \rightarrow H_2O(g)$	-241.8 kJ/mol
ΔH°_f $H_2O(l) = -285.8$ kJ/mol	$H_2(g) + \frac{1}{2}O_2(g) \rightarrow H_2O(l)$	-285.8 kJ/mol

Example: What is the reaction whose ΔH°_{rxn} is equal to ΔH°_f for

(a) $Ca(OH)_2(s)$: $Ca(s) + O_2(g) + H_2(g) \rightarrow Ca(OH)_2(s)$

(b) $NaHCO_3(s)$: $Na(s) + \frac{1}{2}H_2(g) + C(s, \text{graphite}) + \frac{3}{2}O_2(g) \rightarrow NaHCO_3(s)$

Example: Calculate the enthalpy change when 5.00g of nitroglycerin is detonated given:

$$\begin{array}{lcccccccccc} & 2\,C_3H_5(NO_3)_3(l) & \rightarrow & 3\,N_2(g) & + & \frac{1}{2}O_2(g) & + & 6\,CO_2(g) & + & 5\,H_2O(g) \\ \Delta H^\circ_f\ (\text{kJ/mol}) & -364 & & 0 & & 0 & & -393.5 & & -241.8 \end{array}$$

Plan: Find ΔH_{rxn} first, then do stoichiometry

$$\Delta H^\circ_{rxn} = \overset{\text{sum}}{\sum} n \Delta H^\circ_f \text{ products} - \sum n \Delta H^\circ \text{reactants}$$

$$= (3 \Delta H^\circ_{f\,N_2(g)} + \tfrac{1}{2} \Delta H^\circ_{f\,O_2(g)} + 6 \Delta H^\circ_{f\,CO_2(g)} + 5 \Delta H^\circ_{f\,H_2O(g)}) - (2 \times \Delta H^\circ_{f\,\text{nitro}}$$

$$= (3 \times 0 + \tfrac{1}{2} \times 0 + 6(-393.5) + 5(-241.8)) - (2 \times (-364))$$

$$= (-3570 \text{ kJ}) - (-728 \text{ kJ})$$

$$= -2842 \text{ kJ}$$

so 2842 kJ of heat are released when <u>2 moles</u> of nitroglycerin decompose.
What is ΔH°_{rxn} when 5.00 g of nitro detonate?

$$\Delta H^\circ_{rxn} = \frac{-2842 \text{ kJ}}{2 \text{ mol nitro}} \times \frac{1 \text{ mol nitro}}{227.1 \text{ g nitro}} \times 5.00 \text{ g nitroglycerin}$$

$$= -31.3 \text{ kJ}$$

Can we tell if a reaction is product-favored (reactants mostly converted to products) or reactant-favored (reactants remain largely unreacted) simply by looking at the sign of ΔH? <u>NO</u>

if $\Delta H < 0$ (exothermic), this helps but is not a guarantee that reaction is product-favored

if $\Delta H > 0$ (endothermic), this helps but does not guarantee that a reaction is reactant favored.

Recall, demos done in class:
exploding H_2 balloons - exothermic - product favored
frozen beaker - endothermic - also product favored.

More in Chem 102.