Chapter 6 - Principles of Reactivity: Energy and Chemical Reactions

- Introduction to thermodynamics - science of heat or energy flows 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? hot
- when thermometer is put into a beaker of water, the atoms of mercury in the thermometer reach thermal equilibrium with water - they start moving faster, the Hg atoms get a little further apart, the Hg(l) expands, & column of Hg rises until thermal energy is the same as that of H2O. At that point, temperature of Hg & temperature of the H2O 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:

heat + H₂O(s) \rightarrow H₂O(l)  
\uparrow  
heat is reactant  

system: water  
surroundings: everything else  
enothermic process

Turn this process around: what happens when H₂O freezes?

H₂O(l) \rightarrow H₂O(s) + heat  
\uparrow  
heat is product  

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 $\rightarrow$ liquid $\rightarrow$ gas.
The process of breaking intermolecular forces is ENDOThERMIC.
Heat is released by system as gas $\rightarrow$ liquid $\rightarrow$ 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 = \( \text{Sp. H.} \times \text{mass} \times \Delta T \)
- **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 x mass
Difference Between Specific Heat \((\frac{J}{g \cdot ^\circ C})\) 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)?

\[
\text{Specific heat } \left( \frac{J}{g \cdot ^\circ C} \right) = \frac{\text{heat (J)}}{\text{mass (g)} \times \Delta T(\circ C)} = \frac{173 \text{ J}}{15.0 \text{ g} \times (35.0 - 9.0) \circ C} = 0.444 \ J/\circ C
\]

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

- Heat of fusion: solid \(\rightarrow\) liquid occurs at freezing/melting point
- Heat of vaporization: liquid \(\rightarrow\) 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 \(\text{CH}_3\text{CH}_2\text{OH}\) at -117°C, what is the heat of fusion of ethanol? The freezing point of ethanol is -117°C.

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

Note: Temperature or temperature change is not involved 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). It 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 H₂O at 50°C to convert it to 500 g of steam at 120°C?

Given:
- Specific heat H₂O(l): 4.18 J/°C
- Specific heat H₂O(g): 2.03 J/°C
- Heat of vaporization H₂O: 2.26 × 10³ J/g
- B.P. H₂O: 100°C

Liquid  → liquid  → gas  → gas

50°C   → 100°C → 100°C → 120°C

where
1. Heat needed to raise T of 500 g H₂O 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

\[
= \left[ \text{Sp. H. H₂O(l) × mass H₂O × ΔT} \right] + \left[ \text{H. of vap. × mass H₂O} \right] + \left[ \text{Sp. H. of H₂O(g) × mass H₂O × ΔT} \right]
\]

\[
= \left[ 4.18 \text{ J/°C } \times 500 \text{ g } \times (100-50 \text{ °C}) \right] + \left[ 2.26 \times 10³ \text{ J/g } \times 500 \text{ g } \right] + \left[ 2.03 \text{ J/°C } \times 500 \text{ g } \times (120-100 \text{ °C}) \right]
\]

\[
= 104 \text{ kJ } + 1130 \text{ kJ } + 20 \text{ kJ}
\]

= 1250 kJ

= 1.25 × 10^6 J

Note that the energy required to break the intermolecular bonds in liquid water is very high, due primarily to hydrogen bonding.
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 \( c \): 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

\[
\text{T} \quad (°C) \\
\begin{array}{c}
120 \\
90 \\
60 \\
5.5 \\
\end{array}
\]

\( \text{heat released} \rightarrow \)

Plan:
- \( C_6H_6(g) \) \( \xrightarrow{\text{cool}} \) \( C_6H_6(g) \) \( \xrightarrow{\text{condenses}} \) \( C_6H_6(l) \) \( \xrightarrow{\text{cool}} \) \( C_6H_6(l) \) \( \xrightarrow{\text{freezes}} \) \( C_6H_6(s) \)

\[
\text{Total heat released} = (1) + (2) + (3) + (4)
\]

1. \[
\text{heat released} = \text{Sp. Ht} \times \text{mass} \times \Delta T = 1.04 \text{ J/g°C} \times 155 \text{ g} \times (120.0 - 80.1)\text{°C} = 64.3 \text{ kJ}
\]

2. \[
\text{heat released} = \text{Ht} \times \text{mass} = 395 \text{ J/g} \times 155 \text{ g} = 61.2 \text{ kJ}
\]

3. \[
\text{heat released} = \text{Sp. Ht} \times \text{mass} \times \Delta T = 1.74 \text{ J/g°C} \times 155 \text{ g} \times (80.1 - 5.48)\text{°C} = 20.1 \text{ kJ}
\]

4. \[
\text{heat released} = \text{Ht} \times \text{mass} = 127 \text{ J/g} \times 155 \text{ g} = 19.7 \text{ kJ}
\]

\[
\therefore \text{total heat released} = (1) + (2) + (3) + (4) = 107.4 \text{ kJ}
\]
Example: If 500 g of lead at 200°C are placed in 100 g 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 H₂O (l) : 4.18 \( \frac{J}{g \cdot ^\circ C} \)
- Specific heat of Pb(s) : 0.159 \( \frac{J}{g \cdot ^\circ C} \)

\[
\begin{align*}
H₂O (l) & \rightarrow H₂O(aq) + Pb (s) \leftarrow Pb(s) \\
20°C & \quad T_f & \quad 200°C \\
100g & \quad & \quad 500g
\end{align*}
\]

\[
\text{heat gained by water} = \text{heat lost by Pb}
\]

\[
4.18 \frac{J}{g \cdot ^\circ C} \times 100g \times (T_f-20) = 0.159 \frac{J}{g \cdot ^\circ C} \times 500g \times (200-T_f)
\]

\[
418 T_f - 8360 J = 15900 J - 79.5 T_f
\]

\[
498 T_f = 24260 J
\]

\[
T_f = 48.7 ^\circ C
\]

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 500 g of H₂O (l) at 62°C what will be its final temperature?

\[
5000 J = 4.18 \frac{J}{g \cdot ^\circ C} \times 500g \times (62-T_f)
\]

\[
5000 J = 130,000 J - 2090 T_f
\]

\[
2090 T_f = 125,000 J
\]

\[
T_f = 59.8 ^\circ C
\]
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 H₂O(ℓ) 4.184 J/g °C

Heat lost by Cu = Heat gained by H₂O

\[ \text{Sp} \text{Ht Cu} \times \text{mass}_{\text{Cu}} \times \Delta T_{\text{Cu}} = \text{Sp} \text{Ht H₂O} \times \text{mass}_{\text{H₂O}} \times \Delta T_{\text{H₂O}} \]

\[ 0.385 \frac{\text{J}}{\text{g} \cdot ^\circ \text{C}} \times 50 \text{g} \times (T-35.0) = 4.184 \frac{\text{J}}{\text{g} \cdot ^\circ \text{C}} \times 250.0 \text{g} \times (35.0-20.4) \]

\[ 19.25 ^\circ \text{C} \times 392.7 = 15272 \] (Ignoring sig figs)

\[ T = 813 ^\circ \text{C} \]

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 (C₂O₇) in it.

\[ \text{CO₂(s)} \rightarrow \text{CO₂(g)} \] (Sublimation)

and the book will rise as bag inflates.

System: \( \text{CO₂(s)} \rightarrow \text{CO₂(g)} \)

Surroundings: book

\[ W = - \text{Pressure} \times \Delta \text{Volume} \]

Change in energy, \( \Delta E \), is sum of the heat added to the system plus the work done on system:

\[ \Delta E = q + w \]

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 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?

\[ \Delta E = q + w \]
\[ = +30 \text{ J} + (-20 \text{ J}) = +10 \text{ J} \]

- heat is absorbed by system
- system does work
- internal energy increases

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?

\[ \Delta E = q + w \]
\[ -50 \text{ J} = q + (+20 \text{ J}) \]

- system loses internal energy
- work done on system

\[ q = -50 \text{ J} - 20 \text{ J} = -70 \text{ J} \]

- system loses heat, \( \Delta E \) exothermic

**Enthalpy** - heat content of a substance at constant pressure
- designated by \( H \)
- \( \Delta H = H_{\text{final}} - H_{\text{initial}} \)
  - change in enthalpy

\[ \Delta H = q_p, \text{ heat transferred at constant pressure} \]
\[ \Delta E = q_v, \text{ heat transferred at constant volume} \]

The values of \( \Delta H \) and \( \Delta E \) are close and sometimes the same.
Sign conventions are same:
- \( \Theta \) 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 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 $\Delta P$: pressure
- $T$ and $\Delta T$: temperature
- $V$ and $\Delta V$: volume

and

- $U$, $\Delta U$, $E$, $\Delta E$

NOT $q$, $w$: work is easy to see that it is dependent on path since $work = force \times distance$

but $q_f$, $q_i$, $q+w$ 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:

$$H_2O(g) \rightarrow H_2(g) + \frac{1}{2}O_2(g) \quad \Delta H_{\text{rxn}} = +241 \text{ kJ}$$

1 mole 1 mole $\frac{1}{2}$ mole heat is absorbed endothermic rxn

$\Rightarrow$ when 1 mol $H_2O$ as a gas breaks down to 1 mol of $H_2(g)$ and $\frac{1}{2}$ mol of $O_2(g)$, 241 kJ of heat at constant pressure is required.

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

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

heat is released exothermic

How much heat is released for this reaction?

$$2H_2(g) + O_2(g) \rightarrow 2H_2O(g) \quad \text{Ans.} +482 \text{ kJ}$$

2 mol 1 mol 2 mol $\Delta H_{\text{rxn}} = -482 \text{ kJ}$
Tricky! If one uses the words “released,” the heat is always +
However, when stating $\Delta H = -482 \text{kJ}$, 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:

$$\text{C}_2\text{H}_6(\text{g}) + \text{O}_2(\text{g}) \rightarrow \text{CO}_2(\text{g}) + \text{H}_2\text{O}(\text{l}) \hspace{1cm} \text{unbalanced}$$

(a) If the $\Delta H_{\text{recl}}$ is $-1561 \text{kJ/mol C}_2\text{H}_6$, how much heat is released
if 20.0 g of CO$_2(\text{g})$ is produced?

(b) If 385 kJ of heat is released, how many grams of C$_2$H$_6$ was
combusted?

Step 1: Balance the reaction.

Note: in thermodynamic problems, it is OK to have fractional coeff.

$$1 \text{C}_2\text{H}_6(\text{g}) + \frac{7}{2} \text{O}_2(\text{g}) \rightarrow 2 \text{CO}_2(\text{g}) + 3 \text{H}_2\text{O}(\text{l}) + 1561 \text{kJ}$$

Since $\Delta H_{\text{recl}} = -1561 \text{kJ/mol C}_2\text{H}_6$, when 1 mole of C$_2$H$_6(\text{g})$
is consumed, 1561 kJ of heat is produced.

Step 2: Plan!!

Plan-fn (a): \[ \text{g CO}_2 \rightarrow \text{mol CO}_2 \rightarrow \text{mol C}_2\text{H}_6 \rightarrow \text{heat} \]

$? \text{heat released} = 20.0 \text{g CO}_2 \times \frac{1 \text{mol CO}_2}{44.0 \text{g}} \times \frac{1 \text{mol C}_2\text{H}_6}{2 \text{mol CO}_2} \times \frac{1561 \text{kJ released}}{1 \text{mol C}_2\text{H}_6} = 385 \text{kJ released}$

Plan-fn (b): \[ \text{heat released} \rightarrow \text{mol C}_2\text{H}_6 \rightarrow \text{g C}_2\text{H}_6 \]

$? \text{g C}_2\text{H}_6 = 385 \text{kJ} \times \frac{1 \text{mol C}_2\text{H}_6}{1561 \text{kJ}} \times \frac{30.1 \text{g}}{1 \text{mol C}_2\text{H}_6} = 7.04 \text{g C}_2\text{H}_6(\text{g})$

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**
- Heat
  - measure at constant pressure (ΔP = 0) gives \( \Delta H = q_p \)
    - "coffee cup" calorimeter
  - measure heat at constant volume (ΔV = 0) gives \( \Delta E = q_v \)
    - "bomb" calorimeter

"Coffee Cup" Calorimetry -
- tends to measure heat evolved in aqueous reactions

**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) \( \Delta H_{ox} \) in kJ/mol Mg.

![Diagram](image)

Reaction: \( \text{Mg}(s) + 2\text{HCl}(aq) \rightarrow \text{MgCl}_2(aq) + \text{H}_2(9) \)

Data:
- Temperature increases from 22.2°C to 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

\[
\text{heat evolved} = \text{heat gained by solution} + \text{heat gained by calorimeter} \\
= \text{SptH of soln} \times \text{mass of soln} \times \Delta T + \text{heat capacity} \times \Delta T \\
= 4.20 \text{ J/}°\text{C} \times 100.0 \text{ g} \times (44.8 - 22.2) + 0.50 \text{ J/}°\text{C} \times (44.8 - 22.2) \\
= 9492 \text{ J} + 11.3 \text{ J} \\
= 9500 \text{ J} \approx 9.50 \times 10^3 \text{ J} \\
\]

\[ q_p = -9.50 \times 10^3 \text{ J} \]

(b) now simply do stochiometry:

\[
\Delta H (\text{kJ/mol Mg}) = -9.50 \times 10^3 \text{ J} \\ 0.500 \text{ g Mg} \
\times \frac{1 \text{ kJ}}{1000 \text{ J}} \times \frac{24.31 \text{ g Mg}}{1 \text{ mol Mg}} = -462 \text{ kJ/mol Mg} 
\]
"Bomb" Calorimetry

- tends to measure combustion reactions

Example: Consider reacting a 2.00g sample of octane, C₈H₁₈(l), with oxygen in a complete combustion. Find (a) qᵥ (b) ΔE kJ/g octane (c) ΔE (kJ/mol)

Reaction: C₈H₁₈(l) + \frac{25}{2} O₂(g) → 8CO₂(g) + 9H₂O(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/°C

heat evolved = heat gained by water + heat gained by the bomb
= specific Ht of water \times mass H₂O \times ΔT + heat capacity \times ΔT
= 4.184 J/°C \times 1.20 \times 10^3 g \times (41.40-25.00) + 837 J/°C \times (41.40-25.00)
= 82,300 J + 13,700 J
= 96,100 J or 96.1 kJ

qᵥ = -96.1 kJ

(b) \[ \frac{ΔE}{g \text{ C}_8\text{H}_{18}} = \frac{-96.1 \text{ kJ}}{2.00 \text{ g C}_8\text{H}_{18}} = -48.0 \text{ kJ/g C}_8\text{H}_{18} \]

(c) \[ \frac{ΔE}{\text{mol C}_8\text{H}_{18}} = \frac{-48.0 \text{ kJ}}{1 \text{ g C}_8\text{H}_{18}} \times \frac{114.2 \text{ g}}{1 \text{ mol C}_8\text{H}_{18}} = -5480 \text{ kJ/mol C}_8\text{H}_{18} \]

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 $\Delta H_{rxn}$ for $A \rightarrow D$
We do know $\Delta H_{rxn}$'s for $A \rightarrow B$, $B \rightarrow C$, and $C \rightarrow D$
We can calculate $\Delta H$ for $A \rightarrow D$.

\[
\begin{array}{c|c}
\text{reaction} & \Delta H_{rxn} \\
\hline
A \rightarrow B & -10 \text{ kJ} \\
B \rightarrow C & -20 \text{ kJ} \\
+ C \rightarrow D & + 5 \text{ kJ} \\
A \rightarrow D & (-10 -20 +5) \\
 & -25 \text{ kJ}
\end{array}
\]

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

In other words

\[
\begin{array}{c|c}
\text{B} & -20 \text{ kJ} \rightarrow \text{C} \\
\hline
-10 \text{ kJ} \uparrow & +5 \text{ kJ} \\
\text{A} & -25 \text{ kJ} \rightarrow \text{D} \\
\text{Path 1} & \text{Path 2}
\end{array}
\]

This is called Hess' Law of Heat Summation.
Here's a real example:

Example: Calculate $\Delta H^\circ$ for the reaction: $\text{Na}_2\text{O}(s) + \text{SO}_3(g) \rightarrow \text{Na}_2\text{SO}_4(s)$
given the following information:
\[
\begin{align*}
(1) & \quad \text{Na}(s) + \text{H}_2\text{O}(l) \rightarrow \text{NaOH}(s) + \frac{1}{2} \text{H}_2(g) & -418 \text{ kJ} \\
(2) & \quad \text{Na}_2\text{SO}_4(s) + \text{H}_2\text{O}(l) \rightarrow 2\text{NaOH}(s) + \text{SO}_3(g) & +129.5 \text{ kJ} \\
(3) & \quad 2\text{Na}_2\text{O}(s) + 2\text{H}_2(g) \rightarrow 4\text{Na}(s) + 2\text{H}_2\text{O}(l) & +259 \text{ kJ}
\end{align*}
\]

Hint: Look for a compound in $\text{rxn}$ that only appears once in equations given.
In this case (2) has $\text{Na}_2\text{SO}_4$, but on wrong side - flip equation

- change sign of $\Delta H$

(a) reverse (2) \quad 2\text{NaOH} + \text{SO}_3 \rightarrow \text{Na}_2\text{SO}_4 + \text{H}_2\text{O} \quad \Delta H_{rxn} = -418 \text{ kJ}

(b) \quad \frac{1}{2} \times \text{(3)} \quad 2\text{Na}_2\text{O} + \text{H}_2 \rightarrow 2\text{Na} + \text{H}_2\text{O} \quad \Delta H_{rxn} = +129.5 \text{ kJ}

(c) we use (1) to "mop up" compounds we don't want
\[
\begin{align*}
\times(1) \times 2 & \quad 2\text{Na} + 2\text{H}_2\text{O} \rightarrow 2\text{NaOH} + \text{H}_2 \\
\text{add together, cancel terms} & \quad \text{Na}_2\text{O} + \text{SO}_3 \rightarrow \text{Na}_2\text{SO}_4
\end{align*}
\]

\[
\begin{align*}
\Delta H_{rxn} & = -259 \times 2 = -518 \text{ kJ} \\
\Delta H_{rxn} & = -146 \times 2 = -292 \text{ kJ}
\end{align*}
\]

$\Delta H_{rxn} = -580 \text{ kJ}$ ans.
Hess' Law can be restated in mathematical terms:

$$
\Delta H_{\text{rxn}}^0 = \sum n \Delta H_f^0 \text{ products} - \sum n \Delta H_f^0 \text{ reactants}
$$

where $\Delta H_f^0$ is "naught" - at 1 atm pressure

- $n$ stoichiometric coefficient
- $\Delta H_f^0$ standard molar enthalpy of formation (kJ/mol)

(data is available in table)

Notes: Standard molar enthalpy of formation, $\Delta H_f^0$, is amount of heat absorbed in a reaction where 1 mole of a substance in a specific state is made from elements in their standard state.

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

- Hydrogen: $\text{H}_2(\text{g})$
- Mercury: $\text{Hg}(\ell)$
- Helium: $\text{He}(\text{g})$
- Iron: $\text{Fe}(\text{s})$
- Chlorine: $\text{Cl}(\text{g})$
- Carbon: $\text{C}(\text{s, graphite})$
- Bromine: $\text{Br}_2(\ell)$
- Iodine: $\text{I}_2(\ell)$

$$
\begin{align*}
\Delta H_f^0 \text{ H}_2\text{O}(\text{g}) &= -241.8 \text{ kJ/mol} \\
\Delta H_f^0 \text{ H}_2\text{O}(\ell) &= -285.8 \text{ kJ/mol}
\end{align*}
$$

Example: What is the reaction whose $\Delta H_{\text{rxn}}^0$ is equal to $\Delta H_f^0$ for

(a) $\text{Ca(OH)}_2(\text{s})$:

$$
\text{Ca(s)} + \frac{1}{2} \text{O}_2(\text{g}) + \text{H}_2(\text{g}) \rightarrow \text{Ca(OH)}_2(\text{s})
$$

(b) $\text{NaHCO}_3(\text{s})$:

$$
\text{Na(s)} + \frac{1}{2} \text{H}_2(\text{g}) + \text{C}_(\text{s, graphite}) + \frac{3}{2} \text{O}_2(\text{g}) \rightarrow \text{NaHCO}_3(\text{s})
$$

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

$$
\begin{align*}
2 \text{C}_3\text{H}_5(\text{NO}_3)_3(\ell) &\rightarrow 3 \text{N}_2(\text{g}) + \frac{1}{2} \text{O}_2(\text{g}) + 6 \text{CO}_2(\text{g}) + 5 \text{H}_2\text{O}(\text{g}) \\
\Delta H_f^0(\text{kJ/mol}) &= -364 \quad 0 \quad 0 \quad -393.5 \quad -241.8
\end{align*}
$$

Plan: Find $\Delta H_{\text{rxn}}^0$ first, then do stoichiometry
\[ \Delta H^\circ_{rxn} = \sum n \Delta H^\circ_f \text{products} - \sum n \Delta H^\circ_f \text{reactants} \]

\[ = \left( 3 \Delta H^\circ_f \text{Na}_2(q) + \frac{1}{2} \Delta H^\circ_f \text{O}_2(g) + 6 \Delta H^\circ_f \text{CO}_2(g) + 5 \Delta H^\circ_f \text{H}_2(g) \right) - \left( 2 \times \Delta H^\circ_f \text{nitro} \right) \]

\[ = \left( 3 \times 0 + \frac{1}{2} \times 0 + 6 \times (-393.5) + 5 \times (-241.8) \right) - \left( 2 \times (-364) \right) \]

\[ = -3570 \text{ kJ} - (-728 \text{ kJ}) \]

\[ = -2842 \text{ kJ} \]

so 2842 kJ of heat are released when 2 moles of nitroglycerine decompose.

What is \( \Delta H^\circ_{rxn} \) when 5.00 g of nitro decompose?

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

\[ = -31.3 \text{ kJ} \]

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 \( \Delta H^\circ \)?

**No**

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

if \( \Delta H > 0 \), 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.