Chapter 7: Thermochemistry

Energy & Thermal Chemistry

Themes: Energy – Fueling our Bodies
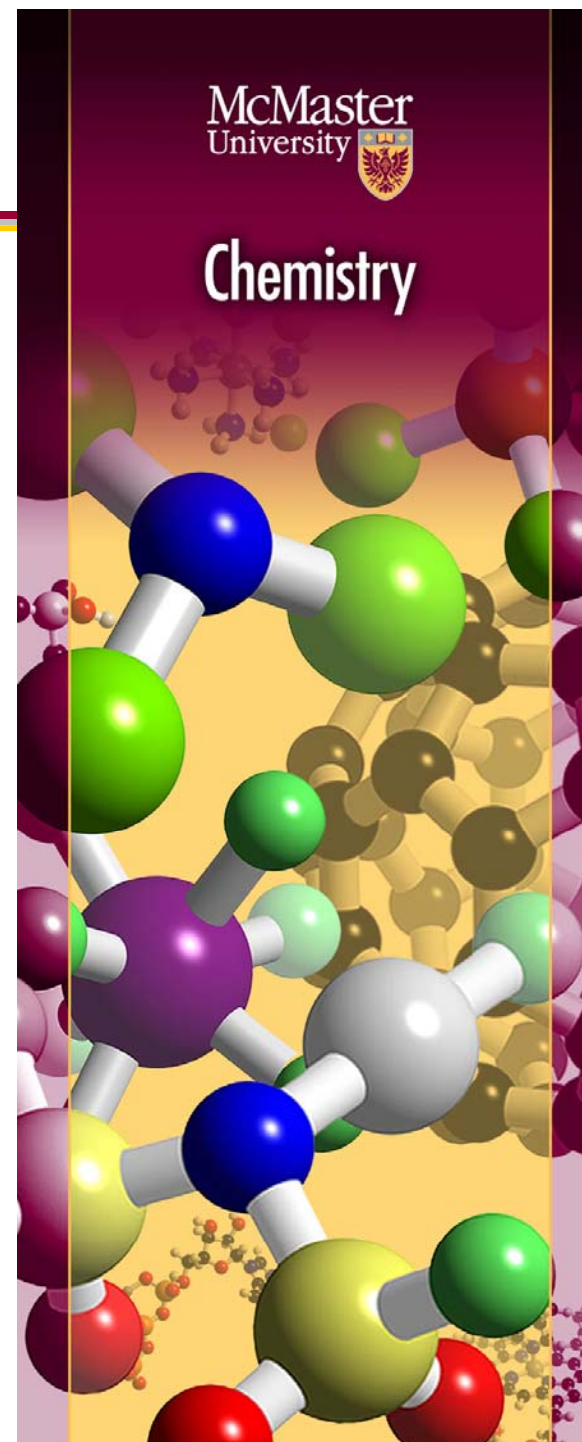
Energy - Fueling our World

en.wikipedia.org/wiki/Image:Leavessnipedale.jpg

en.wikipedia.org/wiki/File:Fries_cooking.jpg

en.wikipedia.org/wiki/File:Grand_Junction_Trip_92007_098.JPG
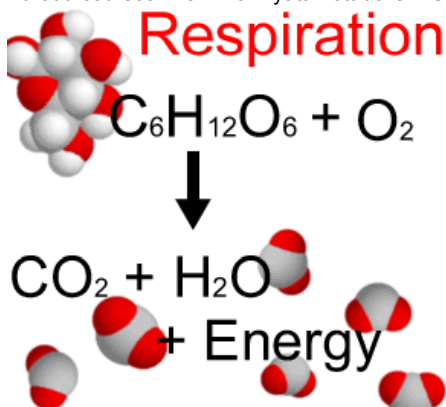
McMaster University

Chemistry

Things We Burn

- **Combustion** or **burning** is a complex sequence of **exothermic** chemical reactions between a **fuel** and an **oxidant**.

  - Rapid Combustion: accompanied by the production of heat or both **heat** and **light** in the form of either a glow or flames.

Respiration

$$C_6H_{12}O_6 + O_2$$

$$\downarrow$$

$$CO_2 + H_2O + Energy$$

Slow Combustion: takes place at low temperatures. **Respiration** is an example of slow combustion.

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Global Energy Sources

Tera-Watts vs Years (1965-2005)

Oil, Coal, Gas — Fossil Fuels

Nuclear
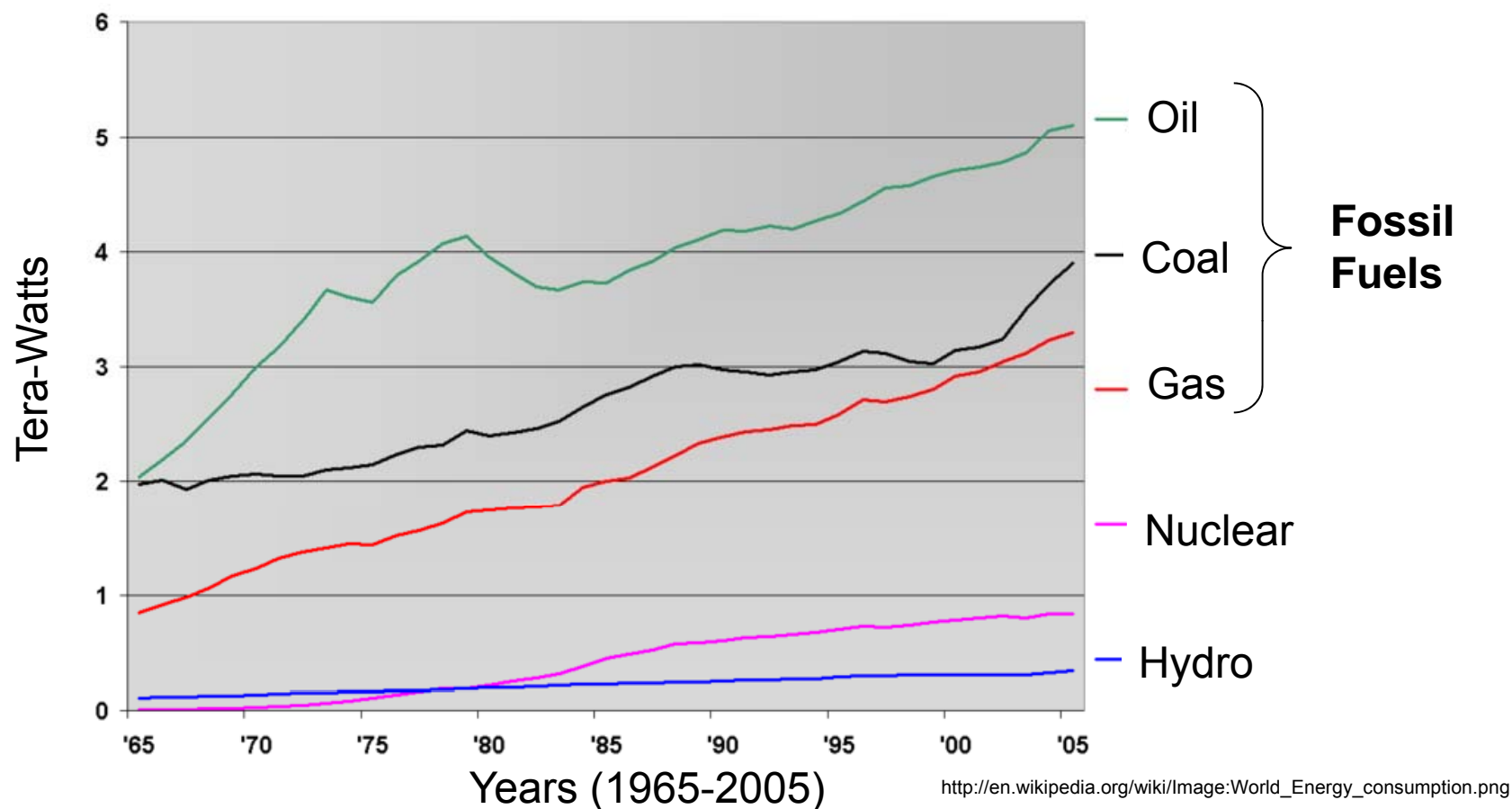
Hydro

- In 2004, the **worldwide energy consumption** of the human race was on average 15 TW (= 1.5×10^{13} W) with 86.5% from burning fossil fuels.

Ch. 7-9, p 275-280 (257-263 9th ed.)

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The Energy We Get from Fuels

- Comparing Heats of Combustion:

Fuel	kJ/g	
Hydrogen	-150.0	
Natural Gas	-49.5	} Fossil Fuels
Gasoline	-47.8	
Coal	-28.3	
Methanol	-22.7	
Cellulose	-17.5	
Municipal waste	-12.7	

- The higher the heat of combustion, the better the fuel!

- What is Heat of Combustion?

- Where does the energy stored in these fuels come from?

Capturing & Using Energy from the Sun

- Photosynthesis is an ENDOTHERMIC process

"A leaf is an amazingly cheap and efficient solar cell."

- Sunlight (energy) is used to build glucose and other simple sugars

en.wikipedia.org/wiki/Image:Leavessnipedale.jpg

- $6CO_2 + 6H_2O \xrightarrow[Sunlight]{Chlorophyll} C_6H_{12}O_6(s) + 6O_2(g)$

$$\Delta H^o = +2.8 \times 10^3 \, kJ/mol$$

- Energy is extracted by *combustion* of the plant material

- As the forward process is **ENDOTHERMIC**, $\Delta H > 0$ the reverse reaction is **EXOTHERMIC**, $\Delta H < 0$
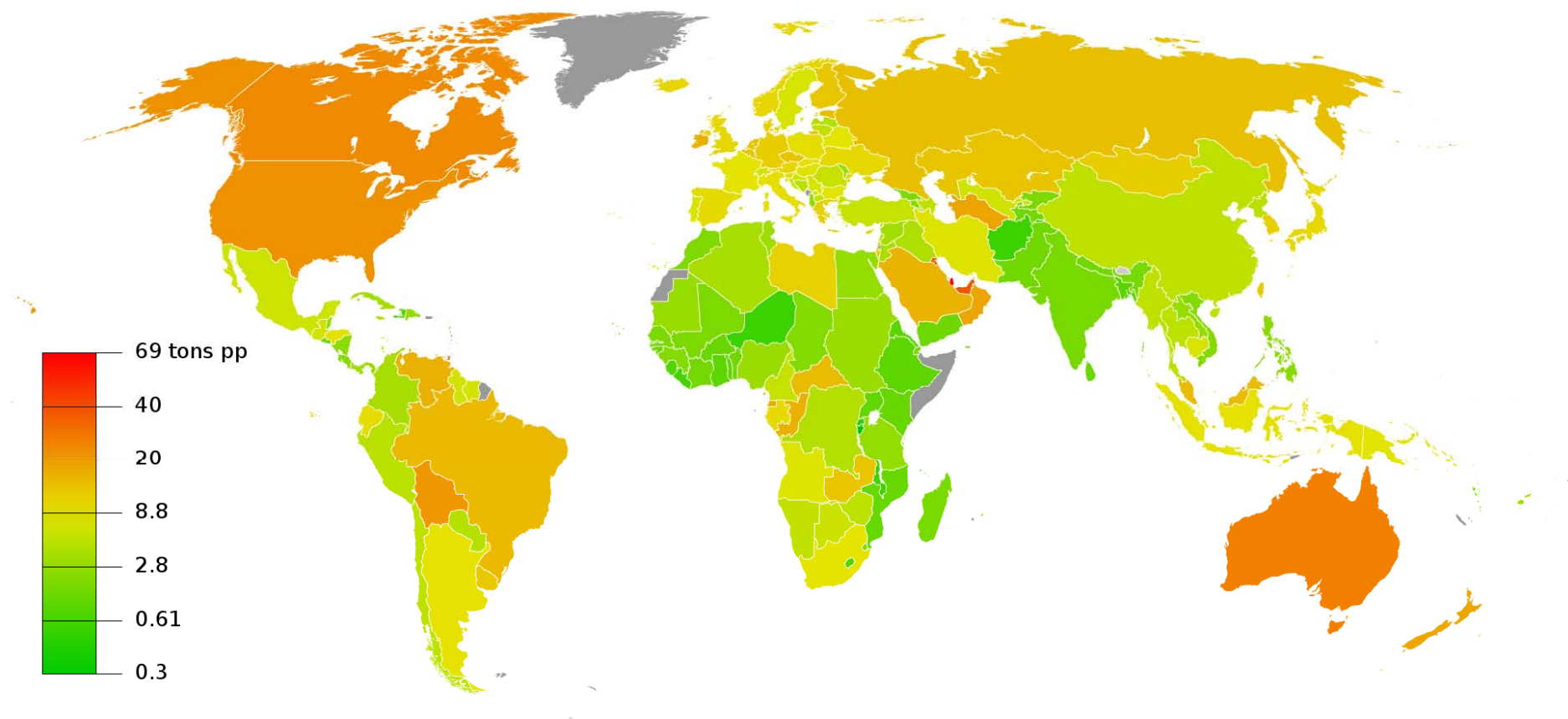
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Issues with Burning Fossil Fuels

- **Non-renewable**
  - Plant Matter, aged >300 million years!
- **Contributions to Global Warming**
  - Net CO_2 increase in atmosphere

en.wikipedia.org/wiki/File:Grand_Junction_Trip_92007_098.JPG

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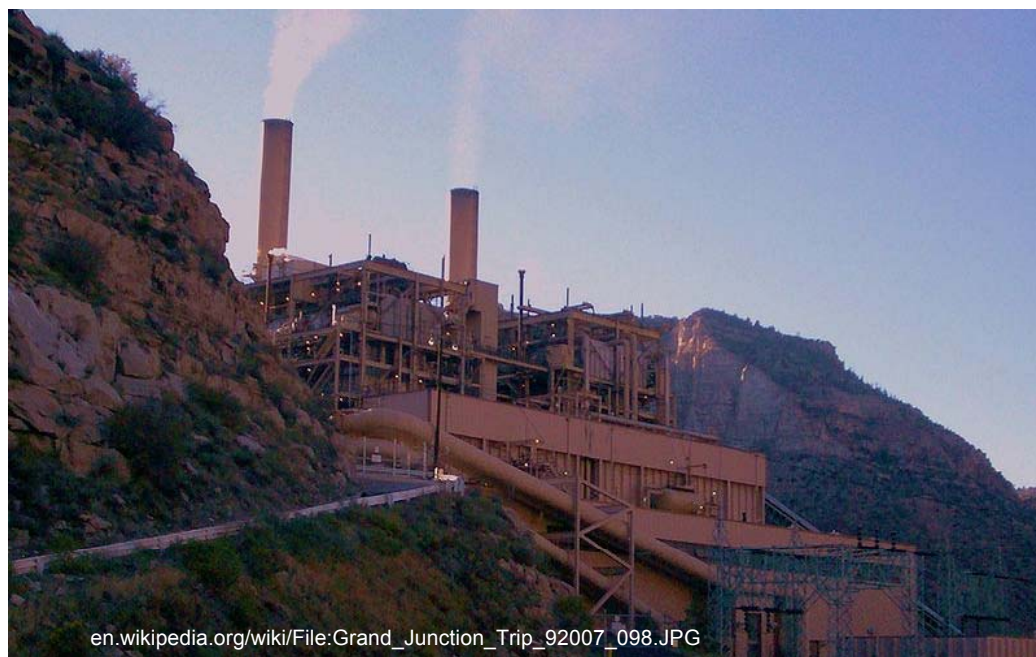
Burning Fossil Fuels – CO_2 Emissions

69 tons pp
40
20
8.8
2.8
0.61
0.3

http://en.wikipedia.org/wiki/File:GHG_per_capita_2005.png

System versus Surroundings

- **Open System:**

  material & energy exchange

- **Closed System:**

  only energy exchange

- **Isolated system:**

  Neither material

  nor energy exchange

Figure 7-1, p 242 (226 9th ed.)

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Energy

- Energy = the capacity to do work

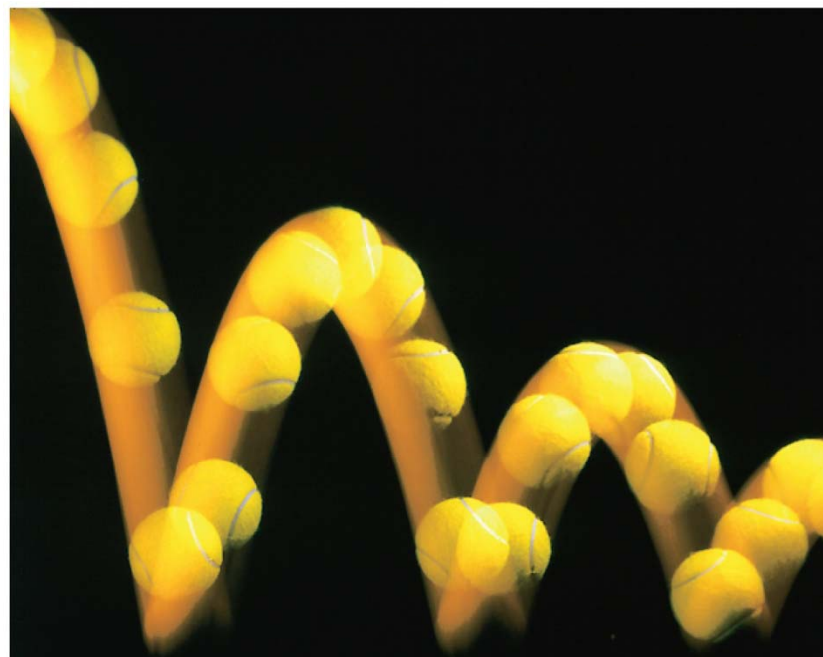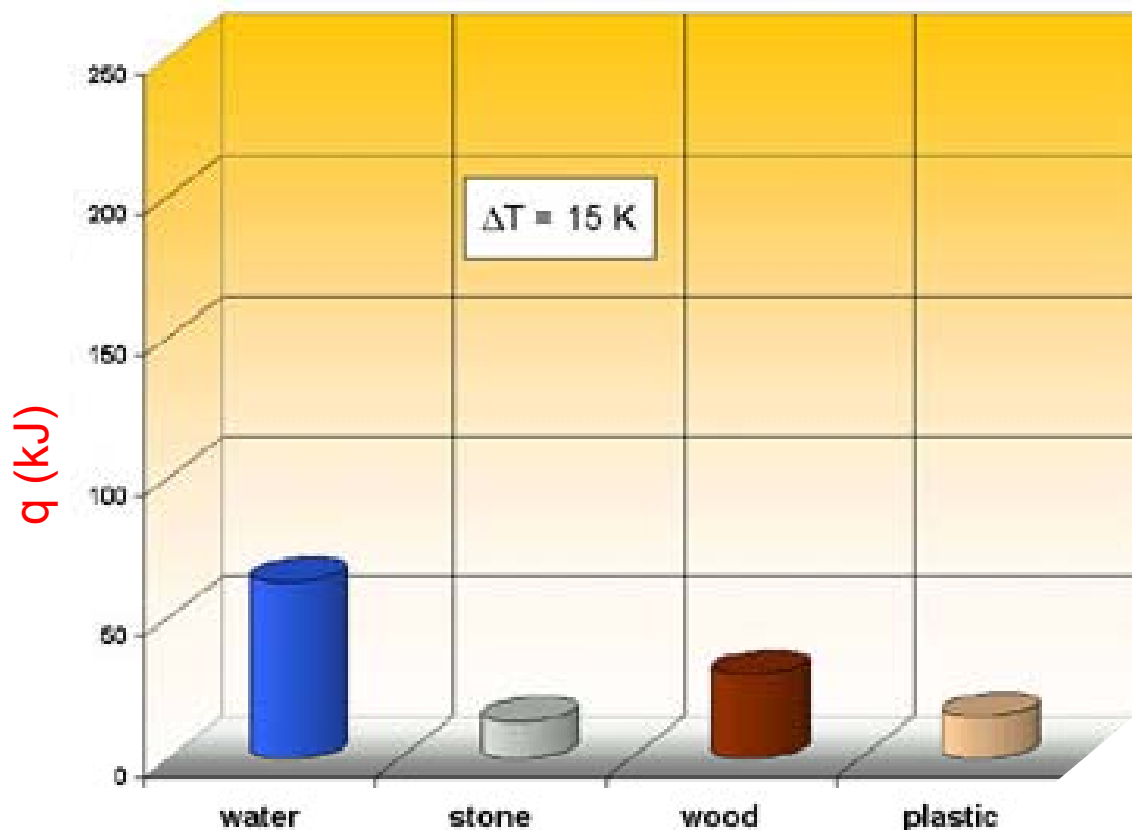- Potential Energy

- Kinetic Energy

- Thermal Energy?

Figure 7-2, p 243 (227 9th ed.)

- Heat (q): energy *transferred* between a system and its surroundings as a result of a temperature gradient
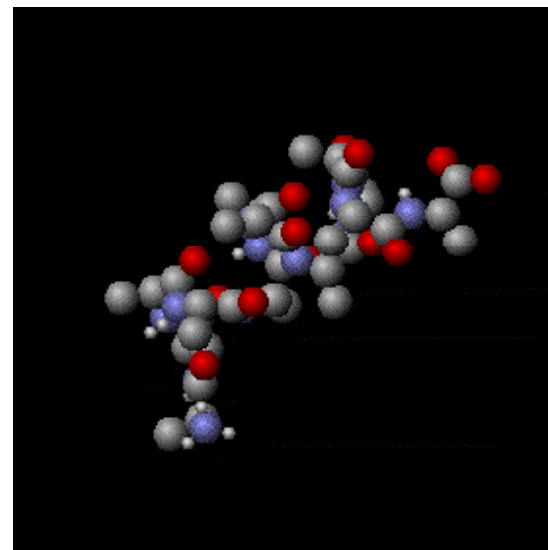
Heat Capacity

- Heat Capacity (C): the amount of heat required to change the temperature of a system by one degree ($J \, °C^{-1}$) or ($J \, K^{-1}$)

Origin of Heat Capacity

- http://en.wikipedia.org/wiki/Image:Thermally_Agitated_Molecule.gif

- Thermal energy is expressed as a molecule's internal motions.

- Molecular-level complexity correlated to heat capacity

- Energy available from these *internal degrees of freedom* contributes to a substance's specific heat capacity.

Defining a System's Capacity to Store Heat

$$q = m \times \text{specific heat} \times \Delta T = C \times \Delta T$$

- Heat Capacity (C) = the quantity of heat (q) required to change the temperature of a "system" by one degree

- Specific Heat Capacity = "system" is 1 g of material

- Molar Heat Capacity = "system" is 1 mol of material

Sample Problem

- A 100.0 g copper sample (specific heat = $0.385 J.g^{-1}.^{0}C^{-1}$) at 100.0 ^{o}C is added to 50.0 g water, at 26.5^{o}C.

- What is the final temperature of the copper-water mixture?

$q_{(water)} = -q_{(copper)}$ ← **Heat lost by copper = Heat gained by water!**

Solution

$$m_{water} \times C_{water} \times (T_{final}-T_{initial(water)}) =$$
$$-m_{copper} \times C_{copper} \times (T_{final}-T_{initial(copper)})$$

$$50.0g \times \frac{4.18J}{g.^oC} \times \left(T_f - 26.5^oC\right) = -\left(100.0g \times \frac{0.385J}{g.^oC} \times \left(T_f - 100.0^oC\right)\right)$$

$$209\frac{J}{^oC}\left(T_f - 26.5^oC\right) = -\left(38.5\frac{J}{^oC} \times \left(T_f - 100.0^oC\right)\right)$$

$$\left(209T_f - 5538.5\right)J = -\left(38.5T_f - 3850\right)J$$

$$5538.5 + 3850 = \left(209 + 38.5\right)T_f$$

$$T_f = \frac{9389J}{247.5J\,^oC^{-1}} = 37.9^oC$$

iClicker Question #1

Which of the following substances has the highest specific heat capacity?

a.Al

b.H_2O

c.CH_4

Heat of Reaction - q_{rxn}

- q_{rxn} = the quantity of heat exchanged between a system & its surroundings when a chemical reaction occurs within the system at *constant temperature*.

$q_{rxn} < 0$ exothermic reaction (Heat Produced)

$q_{rxn} > 0$ endothermic reaction (Heat Required)

$q_{system} = 0$ Isolated system: thermal energy transferred between components of the system

Example: $q_{rxn} + q_{calorim} = 0$ (see Calorimetry slides)

Exothermic & Endothermic Demos

- Demo: Thermite + Liquid Nitrogen
  http://www.youtube.com/watch?v=Yex063_Fblk

- Demo: Beaker + Water + Salts

Bomb Calorimetry (Constant Volume):
q_{rxn} for Combustion of Sucrose

Combustion of 1.010g sucrose

$C_{12}H_{22}O_{11}$ = 342.3 g/mol

$T_{initial}$ =24.92°C, T_{final} = 28.33°C

Heat capacity of cal. = 4.90 kJ/°C

$$\boxed{q_{calorim} = C_{calorimeter} \times \Delta T}$$

$$q_{system} = 0$$

$q_{calorim}$ = 4.90 kJ/°C x (28.33-24.92)°C

$\quad$ = 16.71 kJ

q_{sys} = q_{rxn} + $q_{calorim}$ = 0

q_{rxn} = -$q_{calorim}$ = -16.71 kJ

$$q_{rxn} = \frac{-16.7 kJ}{1.010 g} \times \frac{342.3 g}{mol} = -5.65 \times 10^3 kJ / mol$$

Thermometer

Wire for ignition

Stirrer

Water

Reactants

Steel bomb
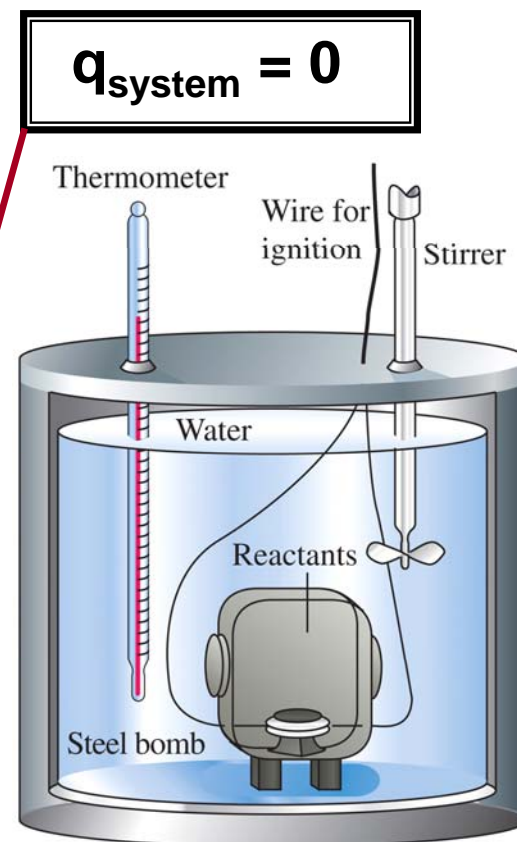
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Figure 7-5

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Calorimeters at Constant Pressure

- You will use an ice-calorimeter in Lab #5 to measure the enthalpy change in a redox or acid base reaction.
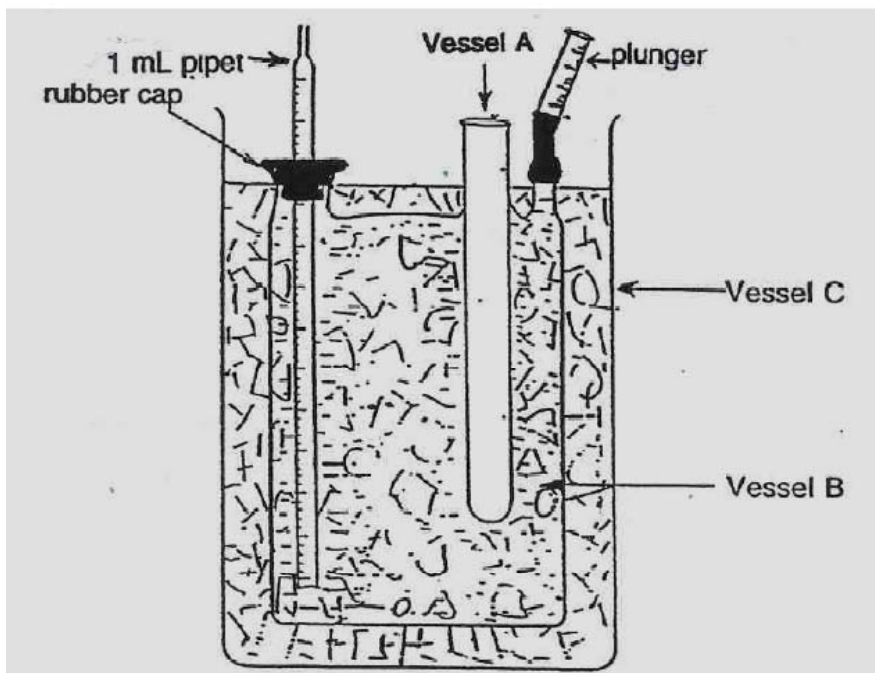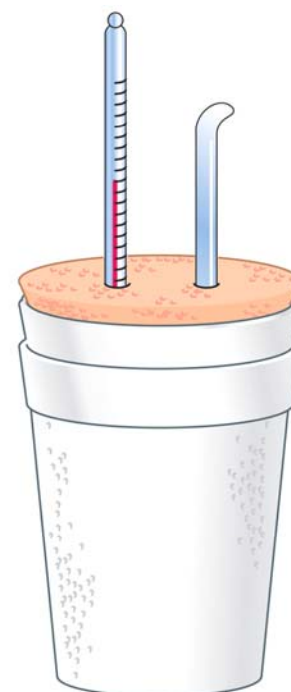

Figure 4.2 The Ice Calorimeter

Figure 7-6

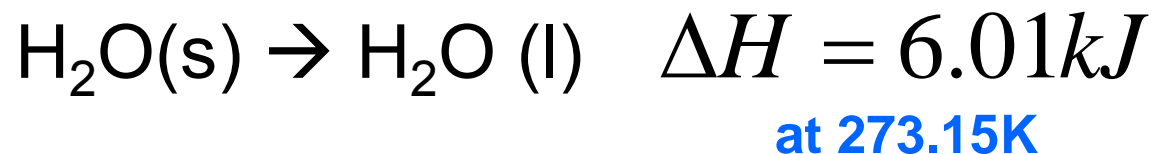Copyright © 2007 Pearson Prentice Hall, Inc.

Coffee Cup calorimeter – like Ice-Calorimeter → constant pressure device

$$q_{system} = 0$$
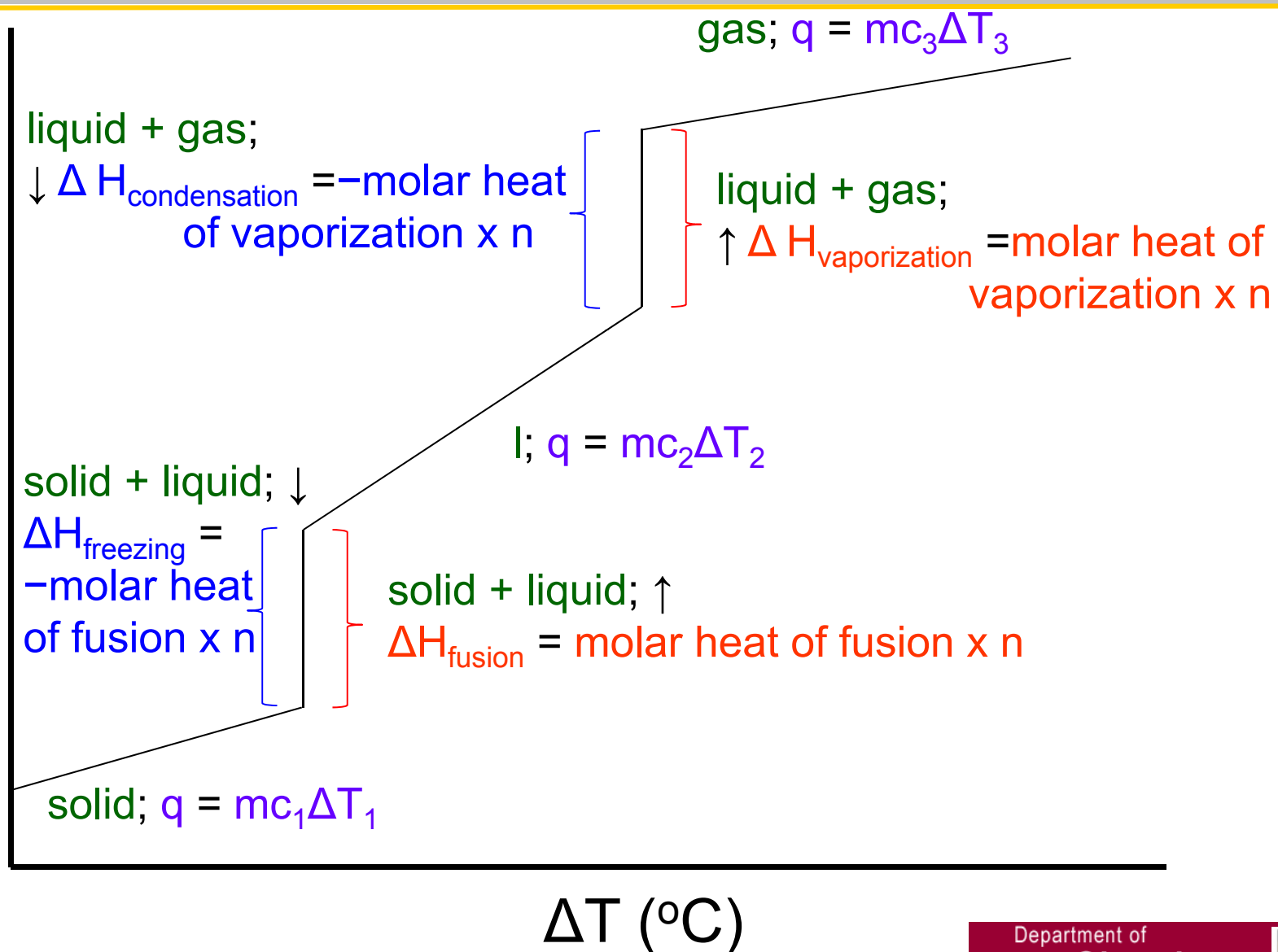
Enthalpy Change, ΔH, & Phase Change

- When water boils or Ice melts,
  what is the temperature of the
  water during the phase transition?

- Heat is required for

  phase transitions (which occur at constant T!)
  → latent (hidden) heat of fusion

- Molar Enthalpy of Fusion (Lab 5):

$$H_2O(s) \rightarrow H_2O \ (l) \quad \Delta H = 6.01 kJ$$

  at 273.15K

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gas; $q = mc_3\Delta T_3$

liquid + gas;
$\downarrow \Delta H_{condensation} = -$molar heat
of vaporization x n

liquid + gas;
$\uparrow \Delta H_{vaporization} = $molar heat of
vaporization x n

l; $q = mc_2\Delta T_2$

solid + liquid; $\downarrow$
$\Delta H_{freezing} = $
$-$molar heat
of fusion x n

solid + liquid; $\uparrow$
$\Delta H_{fusion} = $ molar heat of fusion x n

solid; $q = mc_1\Delta T_1$

ΔH (J)

ΔT (^{o}C)

Take Home – NH_4NO_3 in Coffee Cup Calorimeter

- NH_4NO_3 (MM = 80.05g/mol) is used in cold packs. When 20.0g of this compound dissolves in 125g of water, in a coffee-cup calorimeter, the temperature falls from 23.5°C to 13.4°C. Determine q for the dissolution process. Is it exothermic or endothermic?

$$\Delta T = T_f - T_i = (13.4-23.5)°C = -10.1°C$$

$$q_{calorim} = C_{calorim} \times \Delta T$$

We assume $C_{calorim} = mass_{water} \times C_{water}$

Solution: NH_4NO_3 in Coffee Cup Calorimeter

$$q_{calorim} = m_{H_2O} \times C_{H_2O} \times \Delta T$$

$$= 145 \text{ g} \times \frac{4.184 \text{ J}}{g \cdot {}^oC} \times (13.4 - 23.5)\, {}^oC$$

$$= -6.13 \text{ kJ}$$

$$q_{rxn} = -q_{calorim}$$

$$\therefore q_{dissolving} = +6.13 \text{ kJ}$$

- The temperature of the calorimeter falls during the process, meaning the calorimeter loses heat as the ammonium nitrate dissolves.

- The **ions** gain energy, so the dissolving process is **endothermic**

Take-Home Question: Constant P Calorimeter

- A coffee-cup calorimeter contains 100.0 mL of 0.300M HCl at 20.3 °C. Whan 1.82g Zn(s) is added, the temperature rises to 30.5°C. What is the heat of reaction per mol Zn?

$$Zn(s) \; + \; 2H^+(aq) \rightarrow \; Zn^{2+}(aq) \; + H_2(g)$$

Make the same assumptions as in example 7-4,
and also assume that there is no heat lost with the Hydrogen gas that escapes.

Solution – Constant P Calorimeter

- 0.100L x 0.300M = 0.0300mol HCl,
- 1.82g/65.39g/mol = 0.0278 mol Zn.

- Stoichiometry requires 2 moles of HCl for every 1 mole of Zn. Therefore, HCl is the limiting reactant.

- The reaction is exothermic. We neglect the excess Zn, and assume the volume of the solution is constant, at 100.0ml, with specific heat of 4.18J/G/^{o}C. Enthalpy change, in kJ/mol Zn is:

$$\Delta H = -\frac{100.0g \times \frac{4.18J}{g.^oC} \times (30.5 - 20.3)\,^oC}{0.0300molHCl \times \frac{1molZn}{2molHCl}} \times \frac{1kJ}{1000J} = -280kJ/mol$$

Differentiating Work and Heat

- Familiar with ΔH → **endothermic** or **exothermic**, indicating energy required, or given off during a chemical reaction.

- Energy can also be input or output from a system via "**work**"

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Pressure-Volume Work, w

- Explosives

- Gases formed on combustion of gasoline

- How much work is done by an expanding gas?

http://www.jupiterimages.com/Image/royaltyFree/88008147#Header

> work = force x distance

$$w = -\frac{m \times g}{A} \times \Delta h \times A = -P_{ext}\Delta V$$

Ch. 7-4, p 252-255 (235-238 9ᵗʰ ed.)

Calculating Pressure-Volume Work

- Suppose that in a paint ball pistol, the gas is pressurized using a hand pump, which takes the total pressure of air (assume 0.100mol of 100% N_2), to 50.00atm. The pistol is then fired, releasing the air to 1.00atm. What is the amount of work done by the pistol in firing the paintball?

$$V_{initial} = \frac{nRT}{P_{initial}} = \frac{0.100mol \times 0.0821 L \cdot atm \cdot mol^{-1} K^{-1} \cdot 298K}{50.00atm} = 0.0489_3 L$$

$$V_{final} = \frac{nRT}{P_{final}} = \frac{0.100mol \times 0.0821 L \cdot atm \cdot mol^{-1} K^{-1} \cdot 298K}{1.00atm} = 2.44_7 L$$

$$\Delta V = V_{final} - V_{initial} = 2.446 - 0.04893 = 2.39_7 L$$

$$w = -P_{ext}\Delta V = -1.00atm \times 2.39_7 L \times \frac{101.325J}{1Latm} = -2.42 \times 10^2 J$$

The First Law of Thermodynamics
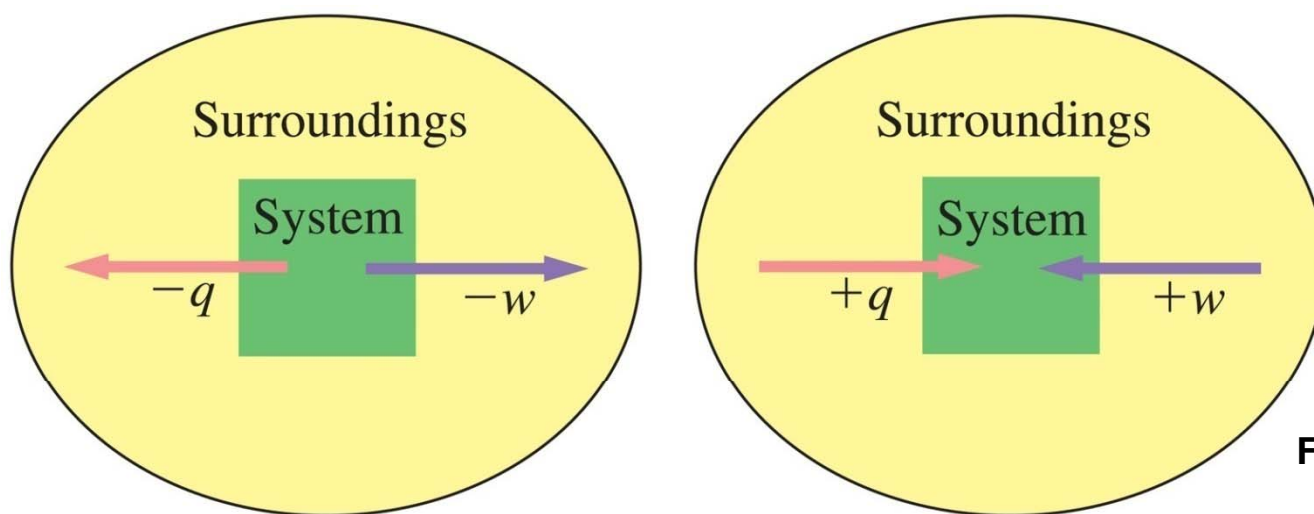
- ## Internal Energy, U

$$\Delta U = q + w$$

Figure 7-10

Law of Conservation of Energy

$$\Delta U_{system} + \Delta U_{surroundings} = \Delta U_{universe} = 0$$

$$\Delta U_{system} = -\Delta U_{surroundings}$$

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iClicker Question #2

Which one of the expressions below is true for a system which undergoes an adiabatic change (i.e., with no heat transfer) and has work done on it by the surroundings?

a. $w > \Delta U$

b. $w < 0$ and $\Delta U > 0$

c. $w > 0$ and $\Delta U < 0$

d. $w = \Delta U$

e. $w = -\Delta U$

Flanders & Swan Lyrics

After me...

The First Law of Thermodymamics:
Heat is work and work is heat

Very good!

The Second Law of Thermodymamics:
Heat cannot of itself pass from one body to a hotter body

Heat won't pass from a cooler to a hotter

You can try it if you like but you far better notter
'Cos the cold in the cooler with get hotter as a ruler
'Cos the hotter body's heat will pass to the cooler

Heat is work and work is heat and work is heat and heat is work

Heat will pass by conduction
Heat will pass by convection
Heat will pass by radiation

And that's a physical law

Heat is work and work's a curse
And all the heat in the Universe
Is gonna cooool down 'cos it can't increase
Then there'll be no more work and there'll be perfect peace

Really?
Yeah - that's entropy, man!

And all because of the Second Law of Thermodynamics, which lays down:

That you can't pass heat from the cooler to the hotter
Try it if you like but you far better notter
'Cos the cold in the cooler will get hotter as a ruler
'Cos the hotter body's heat will pass to the cooler
Oh, you can't pass heat from the cooler to the hotter
You can try it if you like but you'll only look a fooler
'Cos the cold in the cooler will get hotter as a ruler
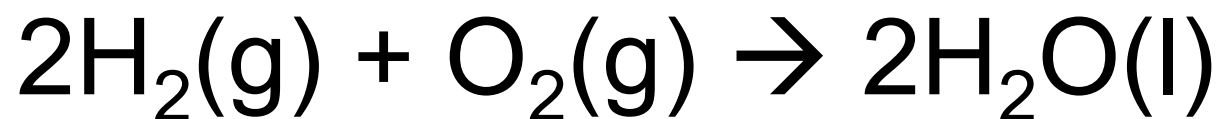That's a physical Law!

Implications of 1st Law

- Energy entering the system carries a "+" sign

  – heat absorbed q>0,   work done ON system **w**>0

- Energy leaving the system carries a "-" sign

  – heat released q<0,   work done BY system **w**<0

iClicker Question #3

Consider the following reaction:

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

Which statement is correct?

a. Work is being done on the system
b. Work is being done by the system

State Functions vs Path Functions - Skit

- **State Function:** a property that has a unique value for a specified state of a system
    - Eg: Density, Pressure, Volume, Temperature, Internal Energy, Enthalpy

- **Path Function:** depends on the process or mechanism that takes the system from one set of conditions to another.
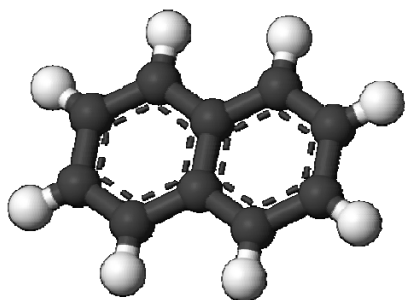   - Eg: Heat & Work

- Change
    - Reversible change → system at eq'm with surrounding throughout infinitesimal changes.
    - Irreversible → system not at eq'm with surrounding.
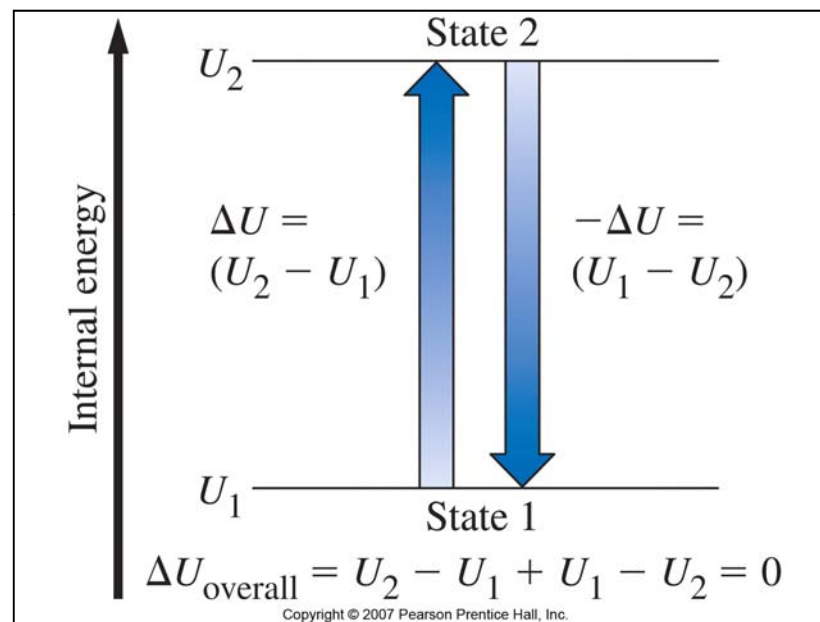
Fats & Carbohydrates

- House Clip
- List some observations, relating the diagnosis to basic chemistry

en.wikipedia.org/wiki/File:Naphthalene-from-xtal-3D-balls.png
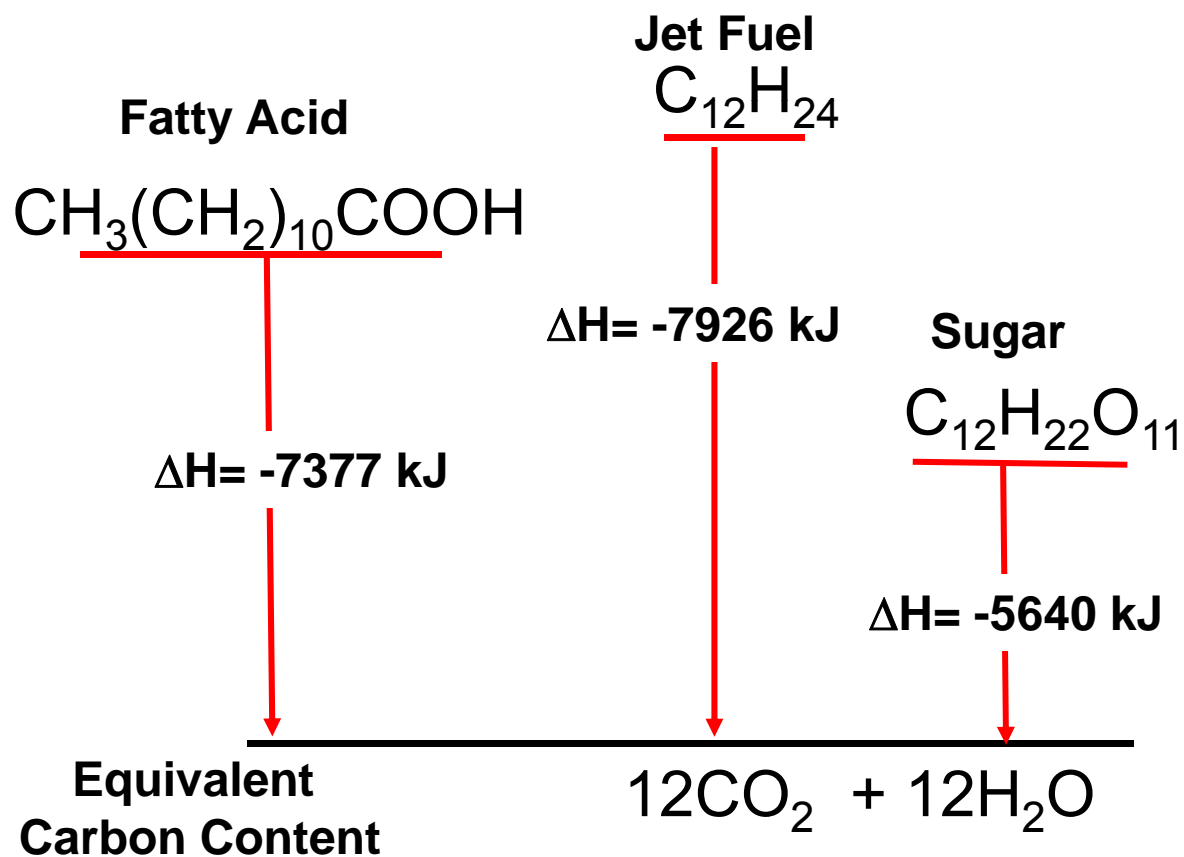
Napthalene (mothballs)

en.wikipedia.org/wiki/File:Hugh_Laurie_2009_crop.jpg

Enthalpy Diagrams

- Why does the body store energy as fat, rather than sugar?

Jet Fuel

$C_{12}H_{24}$

Fatty Acid

$CH_3(CH_2)_{10}COOH$

$\Delta H= -7926$ kJ

Sugar

$C_{12}H_{22}O_{11}$

$\Delta H= -7377$ kJ

$\Delta H= -5640$ kJ

Equivalent Carbon Content

$12CO_2 + 12H_2O$

ΔU from Calorimetry Experiments

- Bomb Calorimeter – Constant Volume Experiment

$$\Delta U = q_V + w = q_V - P\Delta V \quad = 0$$

No work done at constant volume!
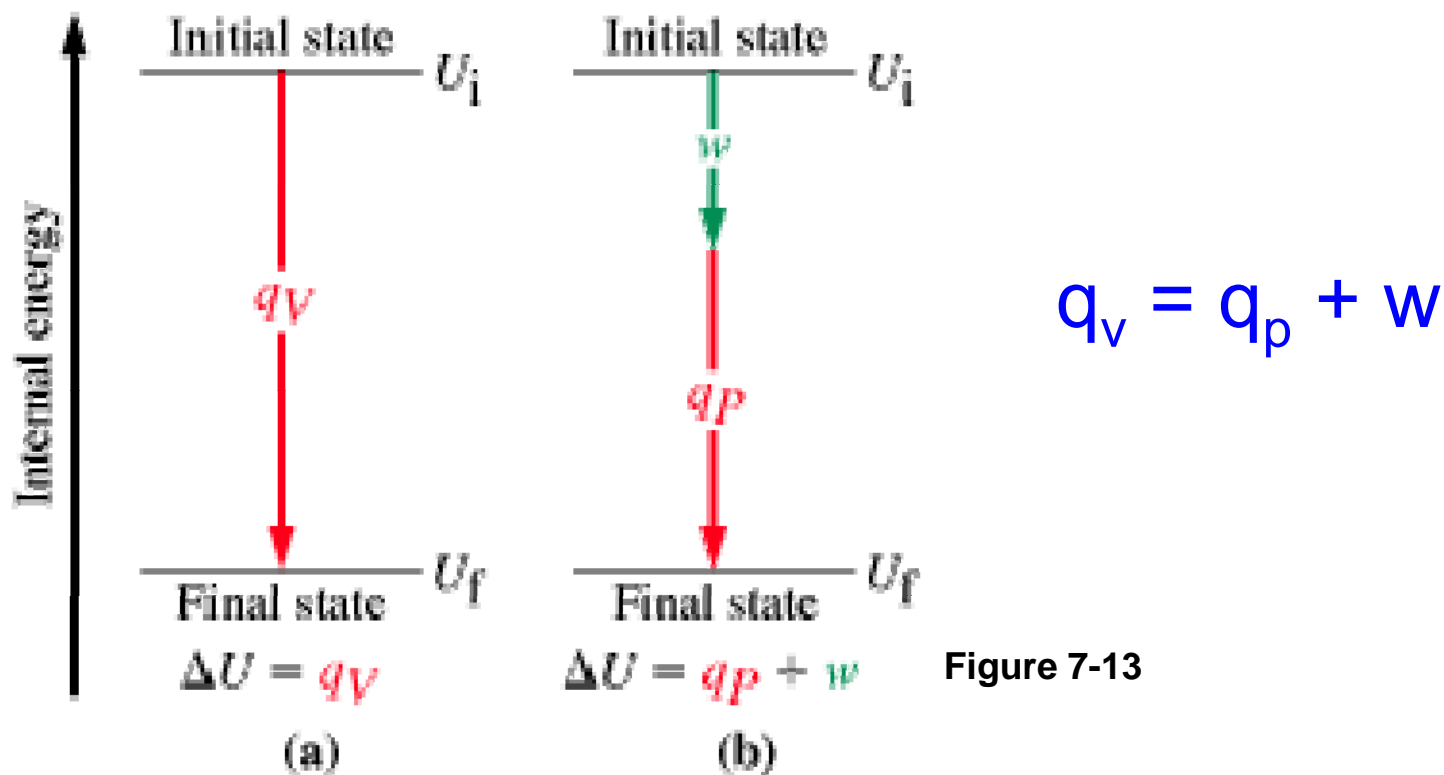
$$\therefore \Delta U = q_V$$

- Other Calorimetry Experiments: Constant Pressure

$$\Delta U = q_P + w = q_P - P\Delta V$$

– Only when w = 0, $q_P = q_V$

Relating Bomb Calorimeters to Real Life

$$q_v = q_p + w$$

Figure 7-13

- Since ΔU is a state function, reactions that take place in a bomb calorimeter or in real life are related by their change in internal energy

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Enthalpy, ΔH

- **Internal Energy & Enthalpy Closely Related:**

$$\Delta U = q + w = q_P - P\Delta V$$

$\leftarrow$ solve for q_P

$$q_P = \Delta U + P\Delta V$$

- **Definition of Enthalpy:** $H = U + PV$

$$\Delta H = H_f - H_i = (U_f + P_f V_f) - (U_i + P_i V_i)$$

$$\Delta H = \Delta U + \Delta PV$$

- **If T & P are constant,** $\quad \Delta H = \Delta U + P\Delta V$

$$\boxed{\Delta H_P = q_P}$$

- $q_P = q_V$ where there is no change in volume

From Bomb Calorimetry to ΔH

$$\Delta U = q_V + w \qquad \leftarrow \text{w = 0 at constant volume} \qquad \therefore \Delta U = q_V$$

If we know ΔU from a bomb calorimetry experiment, how can we find ΔH?

$$w = -P_{ext}\Delta V \qquad \textbf{Assuming Ideal Gases} \rightarrow \quad \Delta V = \Delta n \frac{RT}{P}$$

$$\therefore w = -P\Delta V = -\Delta n_{gases} RT$$

$$\text{and} \quad \Delta H = \Delta U + P\Delta V$$

$$= \Delta U + \Delta n_{gases} RT$$
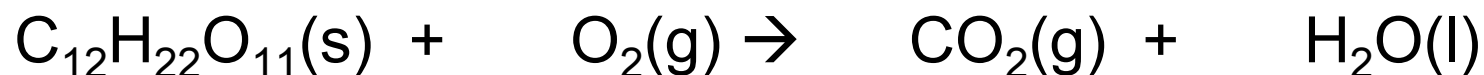
Thus, from the balance chemical equation, we can find Δn, (change in # moles of gases) and solve for work, w at a given temperature. (see Tutorial)

iClicker Question #4

For the complete combustion of sucrose, does $q_V = q_P$?

Unbalanced reaction (balance before answering):

$$C_{12}H_{22}O_{11}(s) + \quad O_2(g) \rightarrow \quad CO_2(g) + \quad H_2O(l)$$

(A) $q_P > q_V$

(B) $q_P < q_V$

(C) $q_P = q_V$

\# moles gas (reactants) =
         \# moles gas (products)

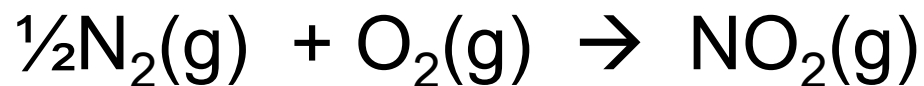http://sciencehack.com/videos/view/MUensqImzXM

Hess's Law

- If a process occurs in stages or steps (even hypothetically), the enthalpy change for the overall process is the sum of the enthalpy changes for the individual steps.

- Recall:
  - ΔH is an extensive property
  - ΔH is a state function

$$\tfrac{1}{2}N_2(g) + O_2(g) \rightarrow NO_2(g)$$

$$\Delta H^o = +33.18 \text{ kJ}$$

$$NO(g) + \tfrac{1}{2}O_2(g)$$

$$\Delta H^\circ = -57.07 \text{ kJ}$$

$$\Delta H^\circ = +90.25 \text{ kJ}$$

$$NO_2(g)$$

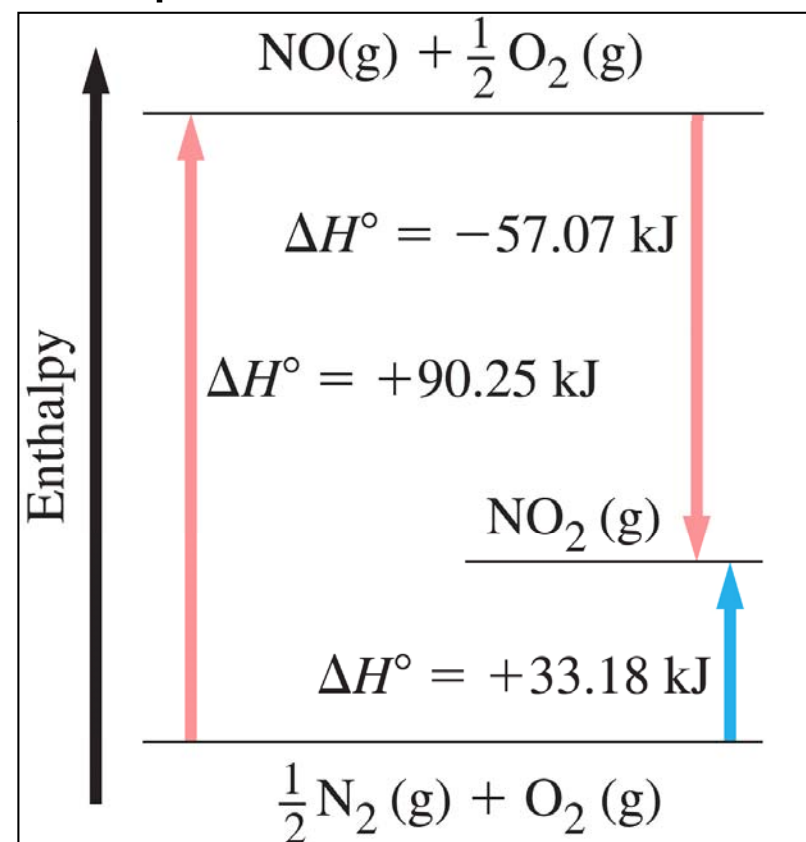$$\Delta H^\circ = +33.18 \text{ kJ}$$

$$\tfrac{1}{2}N_2(g) + O_2(g)$$

Enthalpy

Manipulating Thermochemistry Equations

- Standard enthalpy of formation of a pure element in its reference form is zero.

- Reversing a reaction → reverse sign of ΔH

- Summing reactions → sum ΔH values

- Multiplying a reaction by a factor → multiply ΔH by same factor.

- Include enthalpies of any phase changes.

Take-Home Example: Heat of Formation of Propane

From the data below, determine ΔH^o for the reaction:

$$3C(\text{graphite}) + 4H_2(g) \rightarrow C_3H_8(g)$$

A) $C_3H_8(g) + 5O_2(g) \rightarrow 3CO_2(g) + 4H_2O(l)$ $\Delta H^o = -2219.9kJ$

B) $C(\text{graphite}) + O_2(g) \rightarrow CO_2(g)$ $\Delta H^o = -393.5kJ$

C) $H_2(g) + \frac{1}{2} O_2(g) \rightarrow H_2O(l)$ $\Delta H^o = -285.8kJ$

Steps: 1) Reverse Reaction A), and sign of its ΔH^o

2) Multiply Reaction B) by 3, and its ΔH^o by 3 as well

3) Multiply Reaction C) by 4, and its ΔH^o by 4 as well

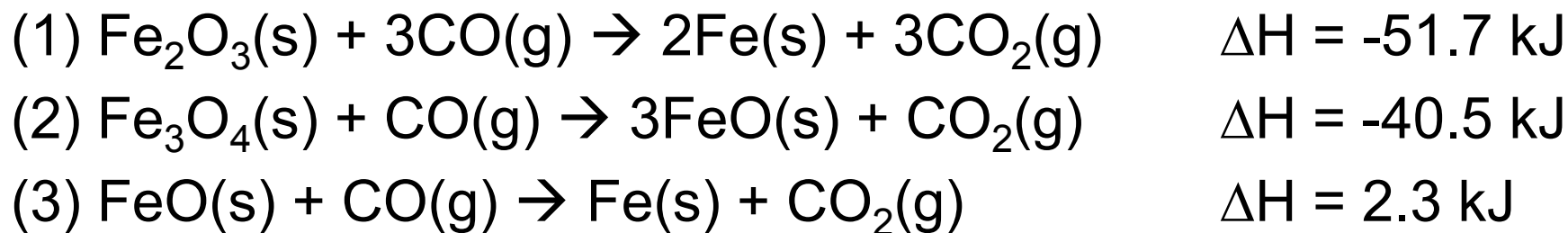# Take-Home Example: Heat of Formation of Propane

Reverse A)

$3CO_2(g) + 4H_2O(l) \rightarrow C_3H_8(g) + 5O_2(g)$ $\Delta H^o = +2219.9kJ$

3x B)

$3C(graphite) + 3O_2(g) \rightarrow 3CO_2(g)$ $\Delta H^o = 3x\ (-393.5kJ)$

4x C)

$4H_2(g) + 4(½)O_2(g) \rightarrow 4H_2O(l)$ $\Delta H^o = 4x\ (-285.8kJ)$

$3C(graphite) + 4H_2(g) \rightarrow C_3H_8(g)$
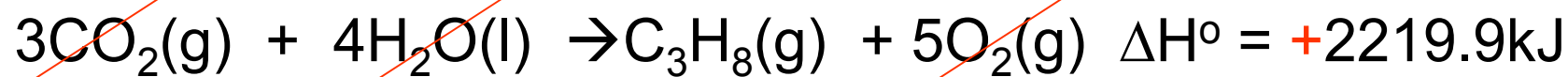
$$\Delta H = \left[2219.9 + 3(-393.5) + 4(-285.8)\right]kJ$$

$$= -104kJ$$

iClicker Question #5

How would the following be used:

(1) $Fe_2O_3(s) + 3CO(g) \rightarrow 2Fe(s) + 3CO_2(g)$ $\Delta H = -51.7$ kJ

(2) $Fe_3O_4(s) + CO(g) \rightarrow 3FeO(s) + CO_2(g)$ $\Delta H = -40.5$ kJ

(3) $FeO(s) + CO(g) \rightarrow Fe(s) + CO_2(g)$ $\Delta H = 2.3$ kJ

to calculate the ΔH_{rxn} for:

$2Fe_3O_4(s) + CO_2(g) \rightarrow 3Fe_2O_3(s) + CO(g)$
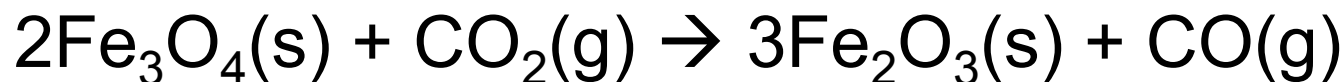
a. (-3)(Rxn 1) + (2)(Rxn 2) + (6)(Rxn 3)

b. (-3)(Rxn 1) + (-2)(Rxn 2) + (3)(Rxn 3)

c. (3)(Rxn 1) + (-2)(Rxn 2) + (-6)(Rxn 3)

Standard Enthalpies of Formation ΔH_f^o

ΔH_f^o = enthalpy change that occurs in the formation of *one mole* of a substance in its standard state from the *reference* forms (most stable forms) of the elements

ΔH_{rxn}^o determined by combining Hess's Law & ΔH_f^o

$$\Delta H_{rxn}^o = \Sigma \, \nu \, \Delta H_f^o \text{ (products) } - \Sigma \, \nu \, \Delta H_f^o \text{ (reactants)}$$

Sum   **Stoichiometric Coefficients**

iClicker Question #6

- Which of the following is in its reference form?

  (A) $Br_2(g)$
  (B) $O_3(g)$
  (C) $Na(s)$
  (D) $C(diamond)$
  (E) $H(g)$

Practice Question: ΔH_f° Glucose

Given that $\quad \Delta H_{rxn}^o = +2.8 \times 10^3 \, kJ/mol \quad$ for

$$6CO_2 + 6H_2O \xrightarrow[\textit{Sunlight}]{\textit{Chlorophyll}} C_6H_{12}O_6(s) + 6O_2(g)$$
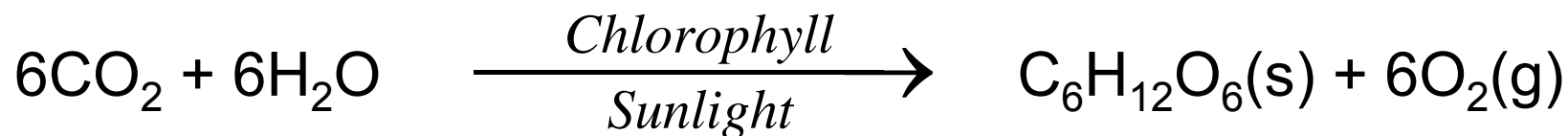
calculate ΔH_f° for glucose, $C_6H_{12}O_6(s)$ at 298 K.

Data: $\Delta H_f^\circ (CO_2(g)) = -393.5$ kJ/mol

$\Delta H_f^\circ (H_2O(l)) = -285.5$ kJ/mol

Bond Energy Calculations

Recall: Enthalpy of Combustion for Propane

$$C_3H_8(g) + 5O_2(g) \rightarrow 3CO_2(g) + 4H_2O(g) \quad \Delta H^o = -2043.9 kJ$$
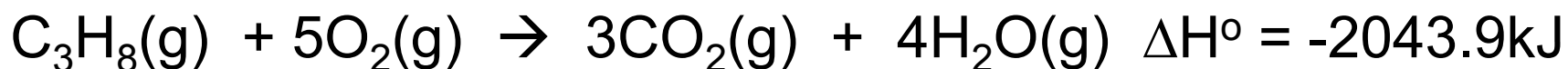
Can we get a comparable value from the Bond
Energies that are broken & formed?
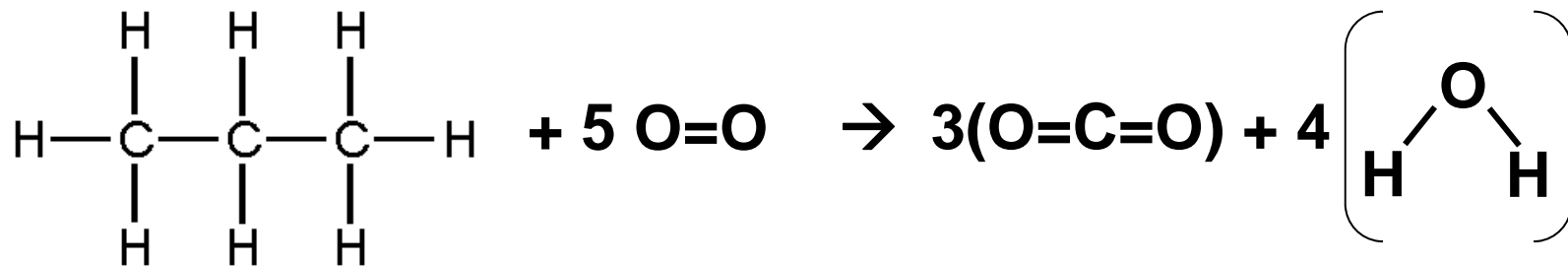
$$\Delta H_{rxn} = \Delta H(bonds \cdot broken) + \Delta H(bonds \cdot formed)$$

$$= \sum BE(reactants) - \sum BE(products)$$

Refer to Ch. 10-9 pgs 408-412

Bond Energy Calculations

ΔH_{Net}
bonds broken:

$8x\ (C\text{-}H) = 8x\ (414)$
$2x\ (C\text{-}C) = 2x\ (347)$
$5x\ (O=O) = 5x\ (498)$

$\left.\right\}$ 6,496 kJ

ΔH_{Net}
bonds formed:

$6x\ (C=O)^* = -\ 6x\ (799)$
$8x\ (O\text{-}H)\ \ = -\ 8x\ (464)$

$\left.\right\}$ - 8506 kJ

$\Delta H_{rxn} = (6,496 - 8,506)\ kJ = -2010\ kJ$
for combustion of propane

Compared to -2043.9 kJ, from enthalpy data.

Recall that most bond energies are an "average" value.