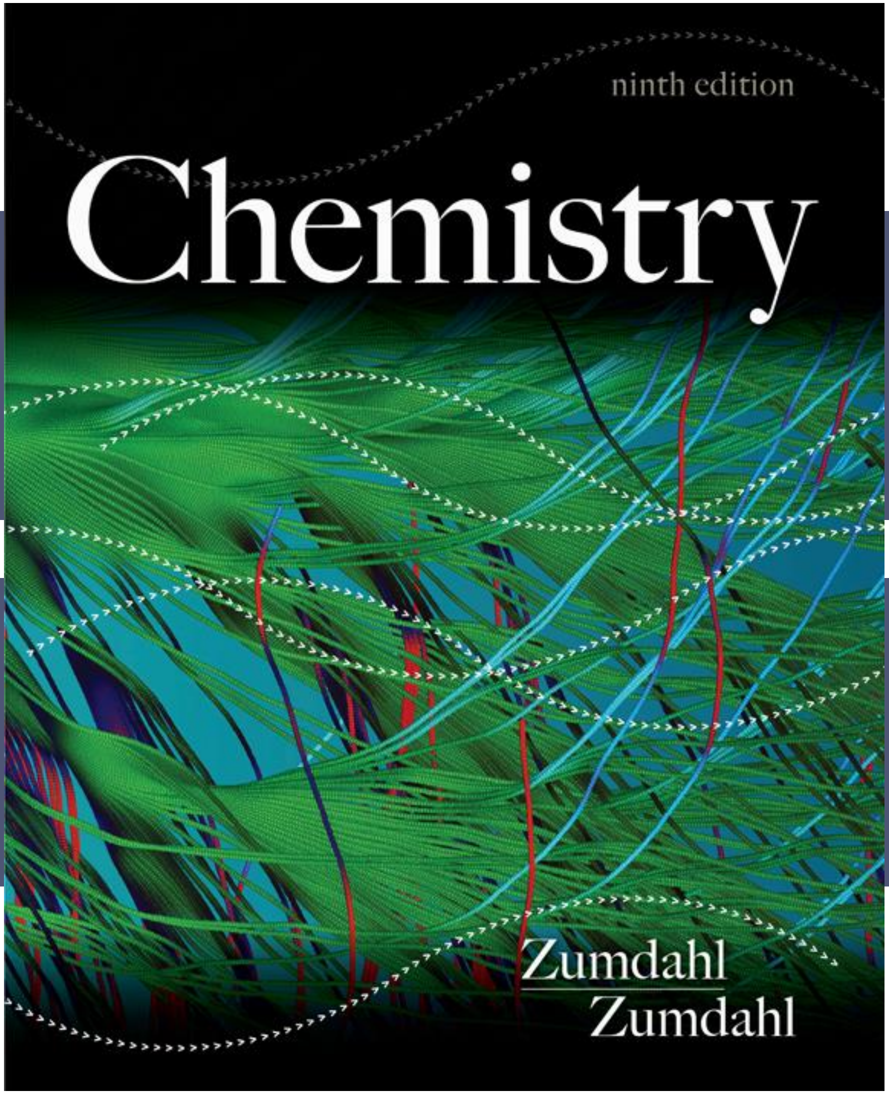


Chapter 6

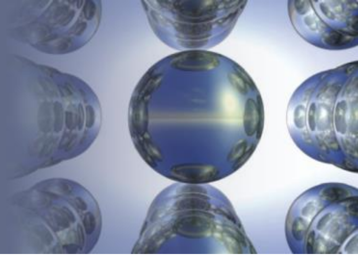
Thermochemistry

Thermochemistry

- This is the study of chemical reactions and the energy changes that involve heat.

Energy

- Capacity to do work or to produce heat.
- Law of conservation of energy – energy can be converted from one form to another but can be neither created nor destroyed.
    - The total energy content of the universe is constant.

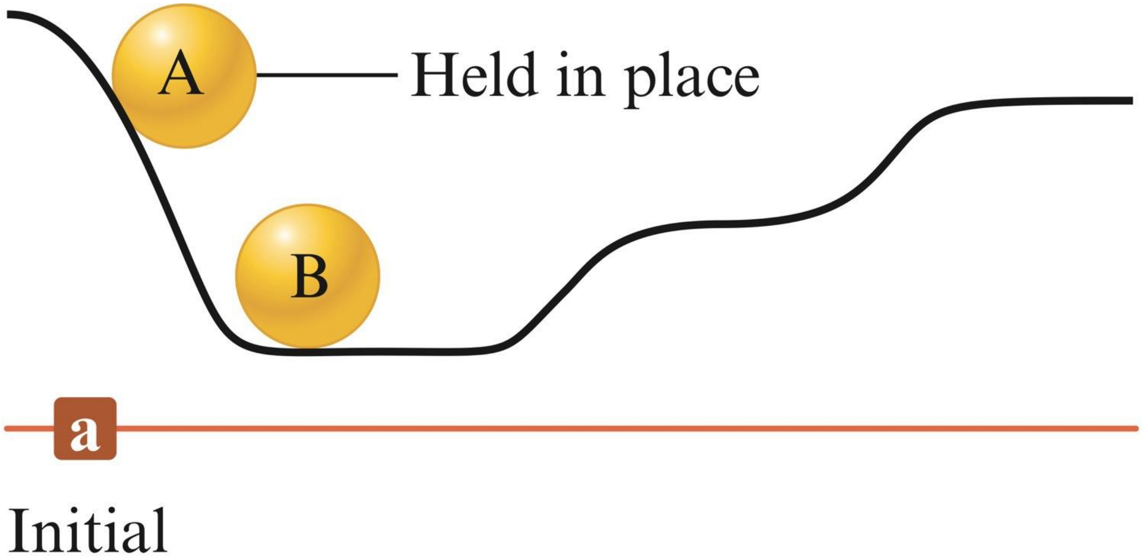


Energy

- Potential energy – energy due to position or composition.
- Kinetic energy – energy due to motion of the object and depends on the mass of the object and its velocity.

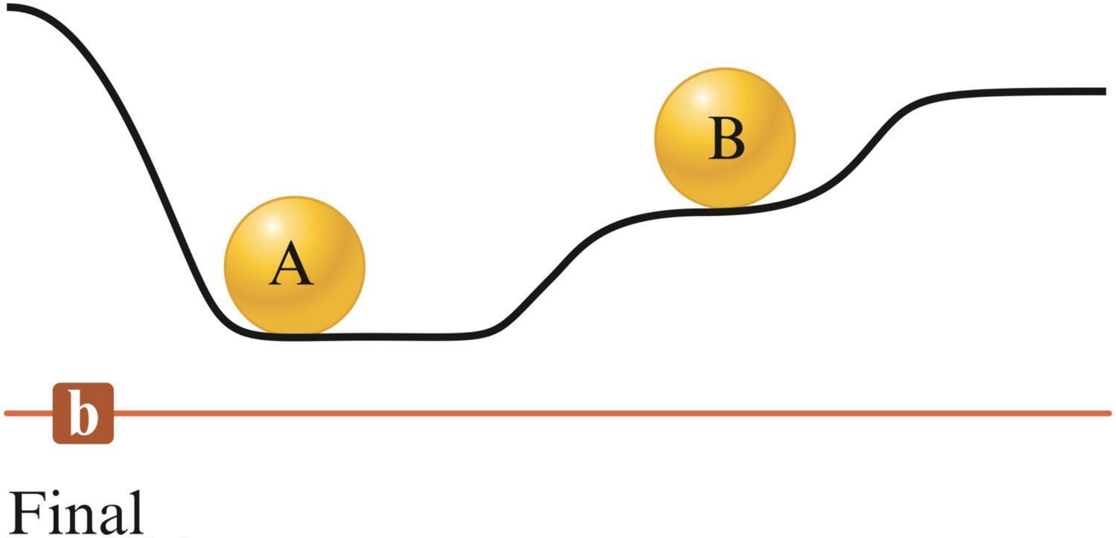
Initial Position

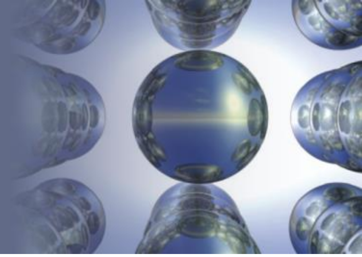
- In the initial position, ball A has a higher potential energy than ball B.



Final Position

- After A has rolled down the hill, the potential energy lost by A has been converted to random motions of the components of the hill (frictional heating) and to the increase in the potential energy of B.





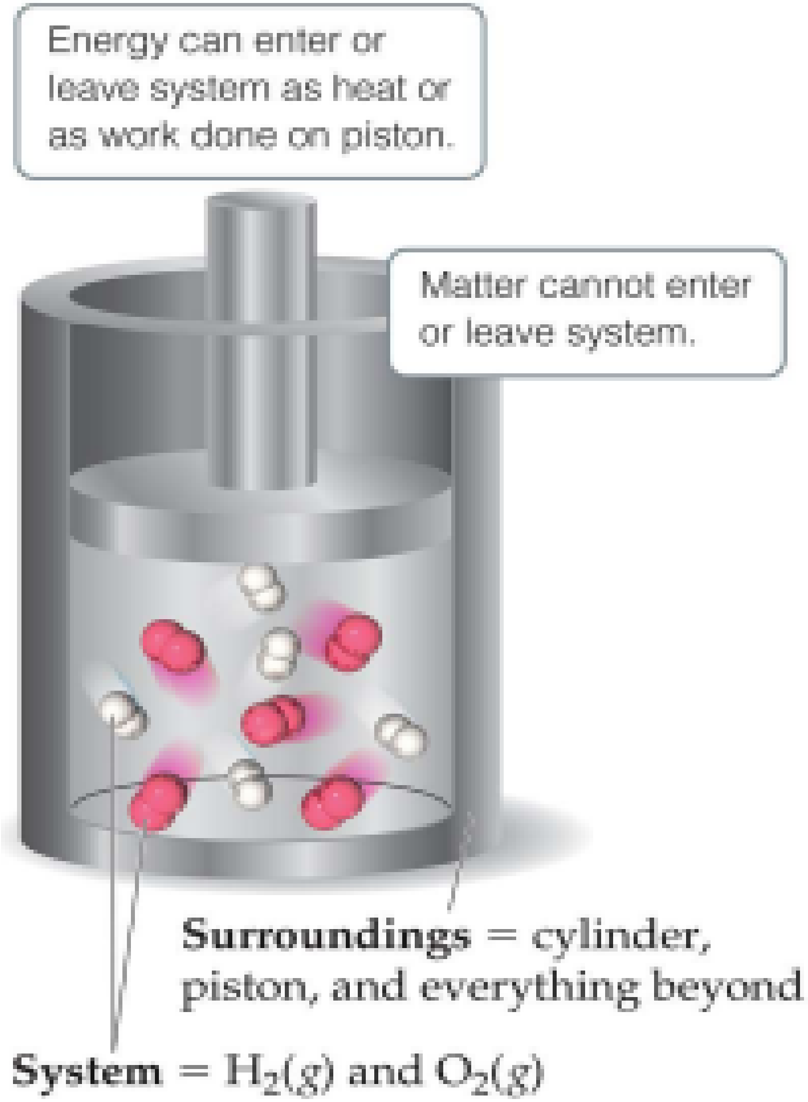
Energy

- Heat involves the transfer of energy between two objects due to a temperature difference.
- Work – force acting over a distance.
- Energy is a state function; work and heat are not
  - State Function – property that does not depend in any way on the system's past or future (only depends on *present* state).
  - state function: A change in this function (property) in going from one state to another state is independent of the particular pathway taken between the two states.

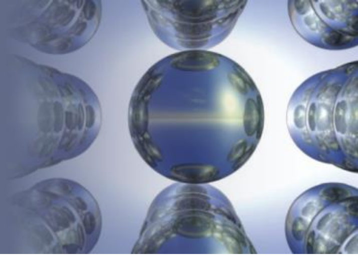
Chemical Energy

- System – part of the universe on which we wish to focus attention.
- Surroundings – include everything else in the universe.
- In a chemical reaction:
  - System - reactants and products of the reaction.
  - Surrounding - anything else other than the reactants and products (e.g rxn container, room).

Section 6.1
The Nature of Energy

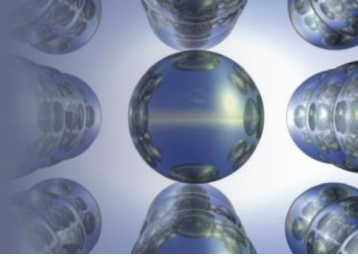


- The **system** includes the molecules of interest.
- The **surroundings** are everything else.
- In thermochemistry we study the exchange of energy between the system and surroundings.
- *open system* – matter and energy can be exchanged with the surroundings
- *closed system* - exchange energy--but not matter--with the surroundings.
- *isolated system* - neither matter nor energy may be exchanged with surroundings.



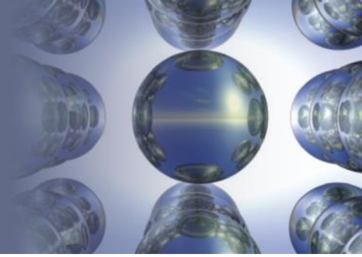
Chemical Energy

- Endothermic Reaction:
    - Heat flow is into a system.
    - Absorb energy from the surroundings.
- Exothermic Reaction:
    - Energy flows out of the system.
- Energy gained by the surroundings must be equal to the energy lost by the system.



CONCEPT CHECK!

Is the freezing of water an endothermic or exothermic process? Explain.



CONCEPT CHECK!

Classify each process as exothermic or endothermic. Explain. The system is underlined in each example.

Exo a) Your hand gets cold when you touch ice.

Endo b) The ice gets warmer when you touch it.

Endo c) Water boils in a kettle being heated on a stove.

Exo d) Water vapor condenses on a cold pipe.

Endo e) Ice cream melts.

CONCEPT CHECK!

For each of the following, define a system and its surroundings and give the direction of energy transfer.

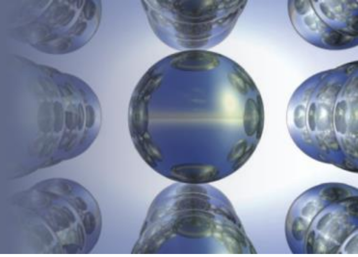
a) Methane is burning in a Bunsen burner in a laboratory.

b) Water drops, sitting on your skin after swimming, evaporate.

CONCEPT CHECK!

Hydrogen gas and oxygen gas react violently to form water. Explain.

- Which is lower in energy: a mixture of hydrogen and oxygen gases, or water?



Thermodynamics

- The study of energy and its interconversions is called thermodynamics.
- Law of conservation of energy is often called the first law of thermodynamics.

Internal Energy

- Internal energy *E* of a system is the sum of the kinetic and potential energies of all the "particles" in the system.
- To change the internal energy of a system:

$$\Delta E = q + w$$

q represents heat

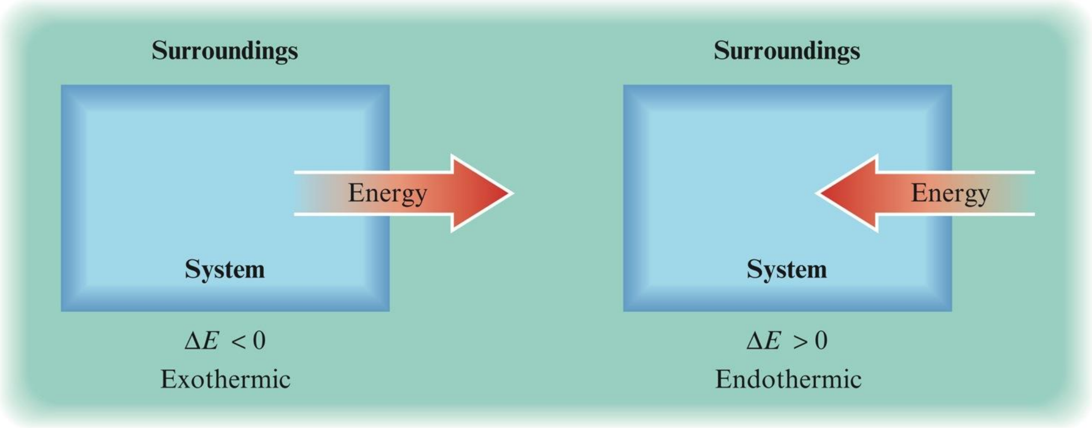
w represents work

Internal Energy

- Thermodynamic quantities consist of two parts:
    - Number gives the magnitude of the change.
    - Sign indicates the direction of the flow.

Internal Energy

- Sign reflects the system's point of view.
- Endothermic Process:
  - *q* is positive
- Exothermic Process:
  - *q* is negative



Internal Energy

- Sign reflects the system’s point of view.
- System does work on surroundings:
    - *w* is negative
- Surroundings do work on the system:
    - *w* is positive

CONCEPT CHECK!

Determine the sign of ΔE for each of the following with the listed conditions:

a) An endothermic process that performs work.
  - $|\text{work}| > |\text{heat}|$ ΔE = negative
  - $|\text{work}| < |\text{heat}|$ ΔE = positive

b) Work is done on a gas and the process is exothermic.
  - $|\text{work}| > |\text{heat}|$ ΔE = positive
  - $|\text{work}| < |\text{heat}|$ ΔE = negative

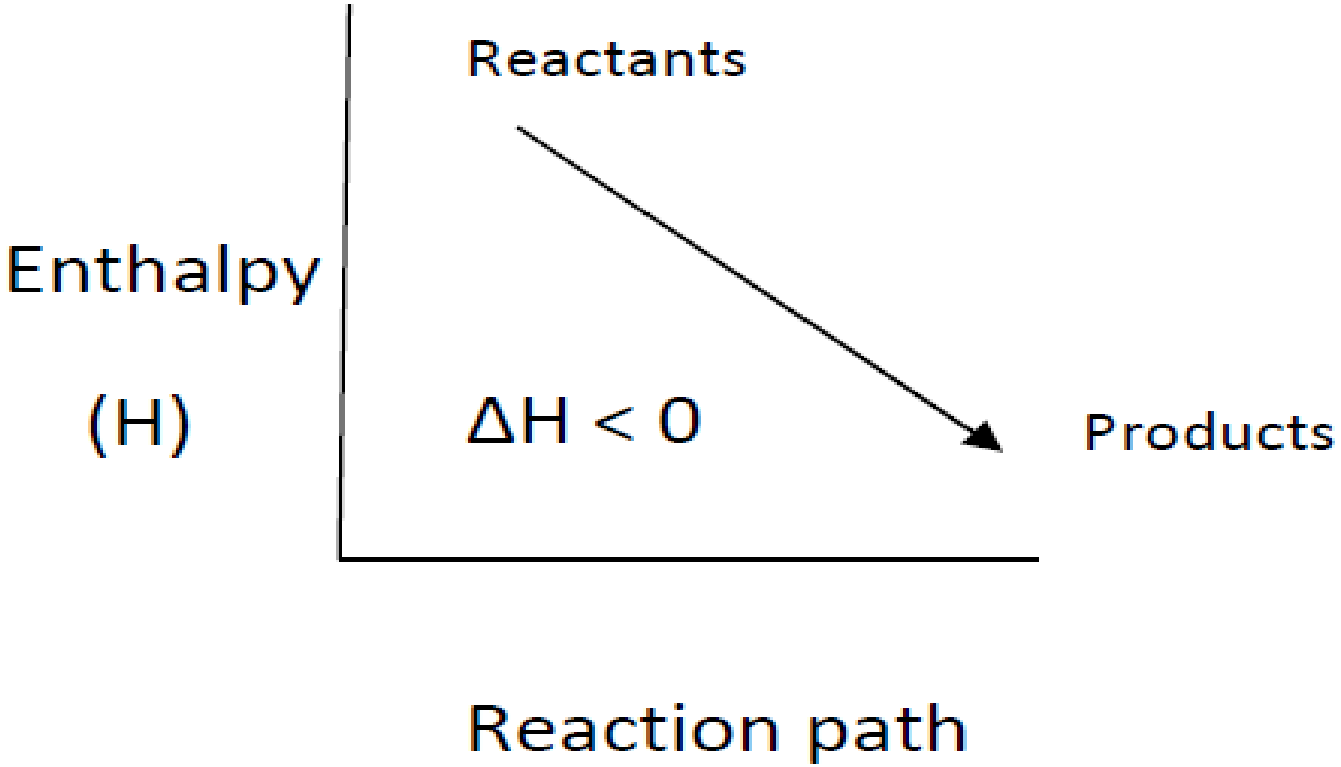
Change in Enthalpy

- Enthalpy – (H) chemical energy sometimes referred to as “heat content”
- It is a State function
- Measures amount of heat flow between system and surroundings under constant pressure.

$$\Delta H = q \text{ at constant pressure}$$

- $\Delta H = H_{\text{products}} - H_{\text{reactants}}$

- If $\Delta H < 0$, the rxn is exothermic
- If $\Delta H > 0$, the rxn is endothermic



Reactants

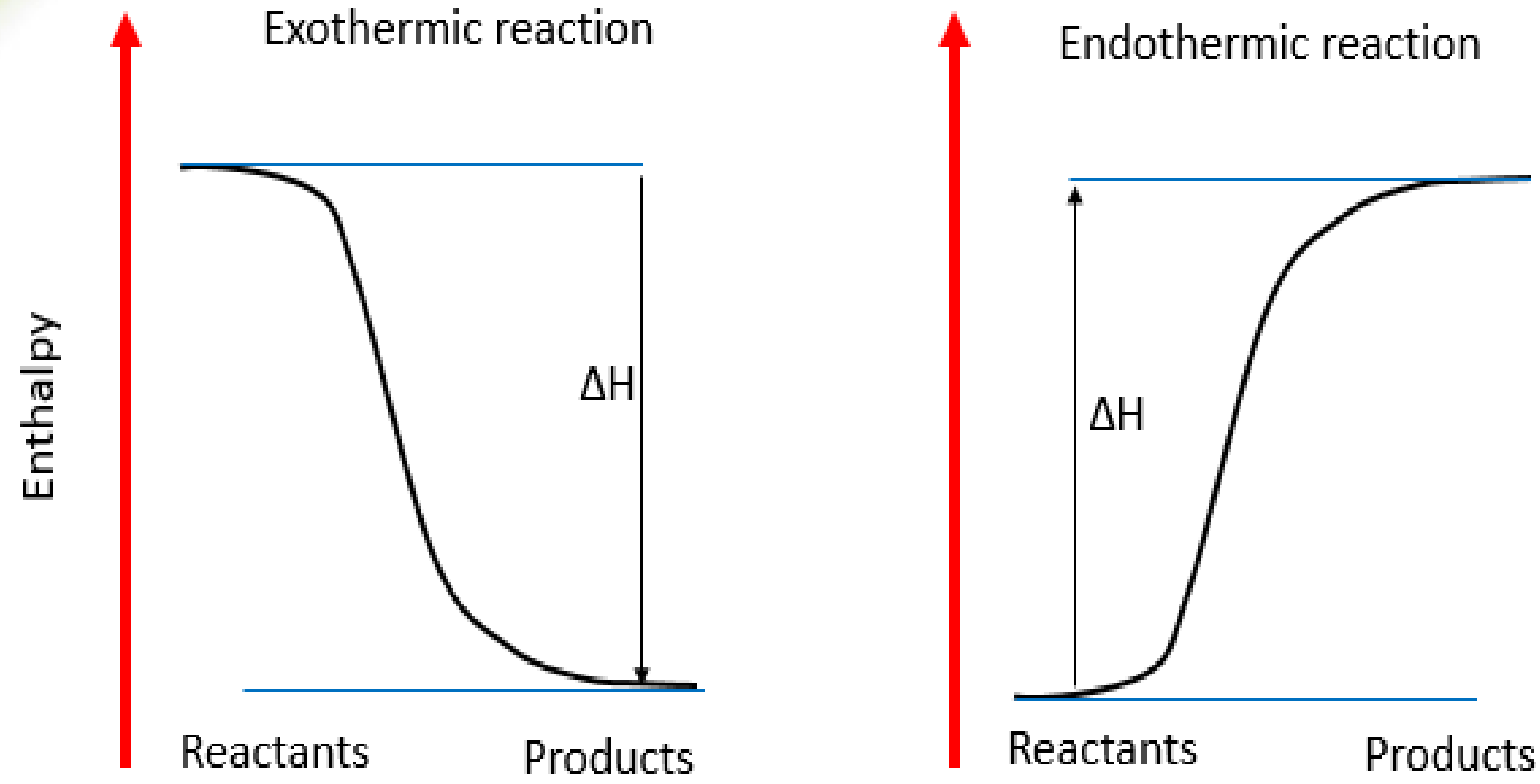
Enthalpy

(H)

$\Delta H < 0$

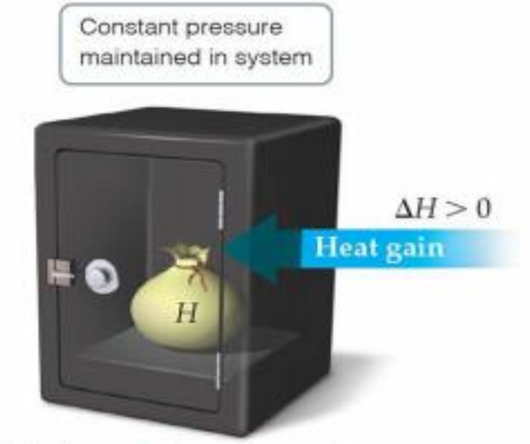
Products

Reaction path



Energy diagram

$$\Delta H = H_{final} - H_{initial} \quad \text{or} \quad \Delta H = H_{products} - H_{reactants}$$



Constant pressure maintained in system

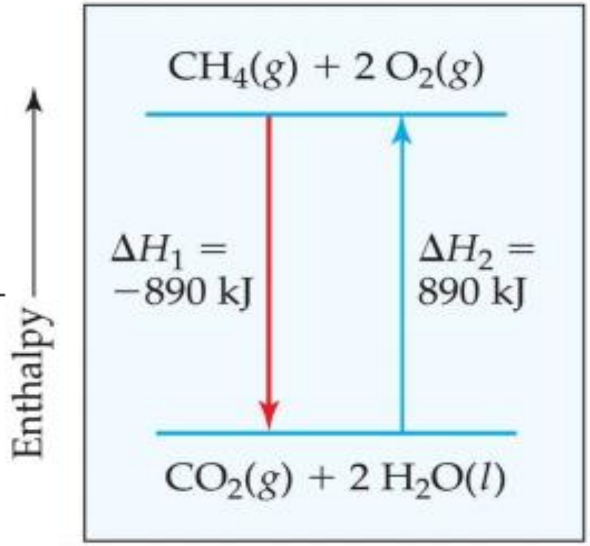
(a) An endothermic reaction

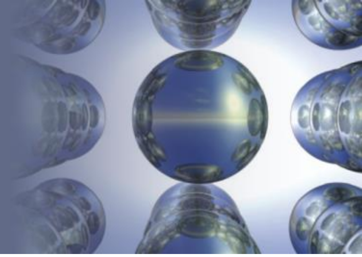
- A process is **endothermic** when ΔH is positive (>0).

(b) An exothermic reaction

ΔH is amount of heat that flows into or out of system under constant pressure.

- A process is **exothermic** when ΔH is negative (<0).



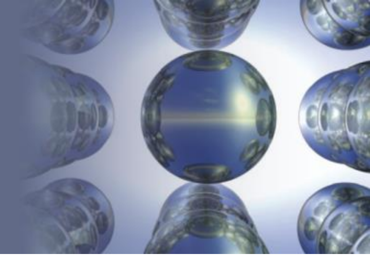


Enthalpies of Reaction

A **thermochemical equation** is an equation for which ΔH is given:

$$2\ H_2(g) + O_2(g) \rightarrow 2\ H_2O(l) \qquad \Delta H = -483.6\ \text{kJ}$$
$$H_2(g) + \tfrac{1}{2}\ O_2(g) \rightarrow H_2O(l) \qquad \Delta H = -241.8\ \text{kJ}$$

The enthalpy changes assume the coefficients are moles of the substances



Thermochemical Equations

- Chemical equation that show enthalpy relation between products and reactants

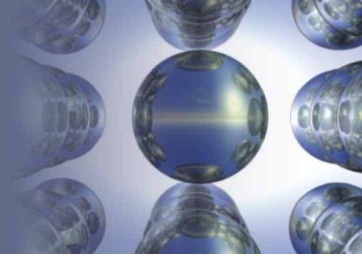
$NH_4NO_{3\,(s)} \rightarrow NH_4^+{}_{(aq)} + NO_3^-{}_{(aq)}$ $\Delta H = 28.1$ kJ

When 1 mole of ammonium nitrate dissociates into ammonium and nitrate ions, 28.1 kJ of energy is absorbed.

If 2 moles of ammonium nitrate dissociate into ammonium and nitrate ions, 56.2 kJ of energy would be absorbed.

$H_{2\,(g)} + Cl_{2\,(g)} \rightarrow 2HCl_{(g)}$ $\Delta H = -185$ kJ

When 2 moles of hydrogen chloride gas are formed from hydrogen and chlorine gas, 185 kJ are evolved.



Rules of Thermochemistry

- The magnitude of ΔH is directly proportional to the amount of reactant or product.
  - If 185 kJ of energy is released when 2 moles of HCl are formed, then 92.5 kJ would be released if 1 mole of HCl was formed.

- ΔH for a rxn is equal in magnitude but opposite in sign to ΔH for the reverse rxn.
  - Since 185 kJ of energy are released when 2 moles of HCl form, that means it takes 185 kJ of energy to break 2 moles of HCl back down.

- The value of ΔH for a reaction is the same whether it occurs in one step or in a series of steps. (state property)
  - $\Delta H_{overall} = \Delta H_1 + \Delta H_2 + ...$ **Hess's Law**

When 1 mole of methane (CH_4) is burned at constant pressure, 890 kJ of energy is released as heat. Calculate ΔH for a process in which a 5.8-g sample of methane is burned at constant pressure.

Solution

At constant pressure, 890 kJ of energy per mole of CH_4 is produced as heat:

$$q_P = \Delta H = -890 \text{ kJ/mol CH}_4$$

Note that the minus sign indicates an exothermic process. In this case, a 5.8-g sample of CH_4 (molar mass = 16.0 g/mol) is burned. Since this amount is smaller than 1 mole, less than 890 kJ will be released as heat. The actual value can be calculated as follows:

$$5.8 \cancel{\text{ g CH}_4} \times \frac{1 \text{ mol CH}_4}{16.0 \cancel{\text{ g CH}_4}} = 0.36 \text{ mol CH}_4$$

and

$$0.36 \cancel{\text{ mol CH}_4} \times \frac{-890 \text{ kJ}}{\cancel{\text{mol CH}_4}} = -320 \text{ kJ}$$

Thus, when a 5.8-g sample of CH_4 is burned at constant pressure,

$$\Delta H = \text{heat flow} = -320 \text{ kJ}$$

EXERCISE!

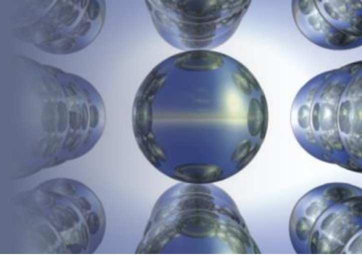
Consider the combustion of propane:

$$C_3H_8(g) + 5O_2(g) \rightarrow 3CO_2(g) + 4H_2O(l)$$

$$\Delta H = -2221 \text{ kJ}$$

Assume that all of the heat comes from the combustion of propane. Calculate ΔH in which 5.00 g of propane is burned in excess oxygen at constant pressure.

–252 kJ



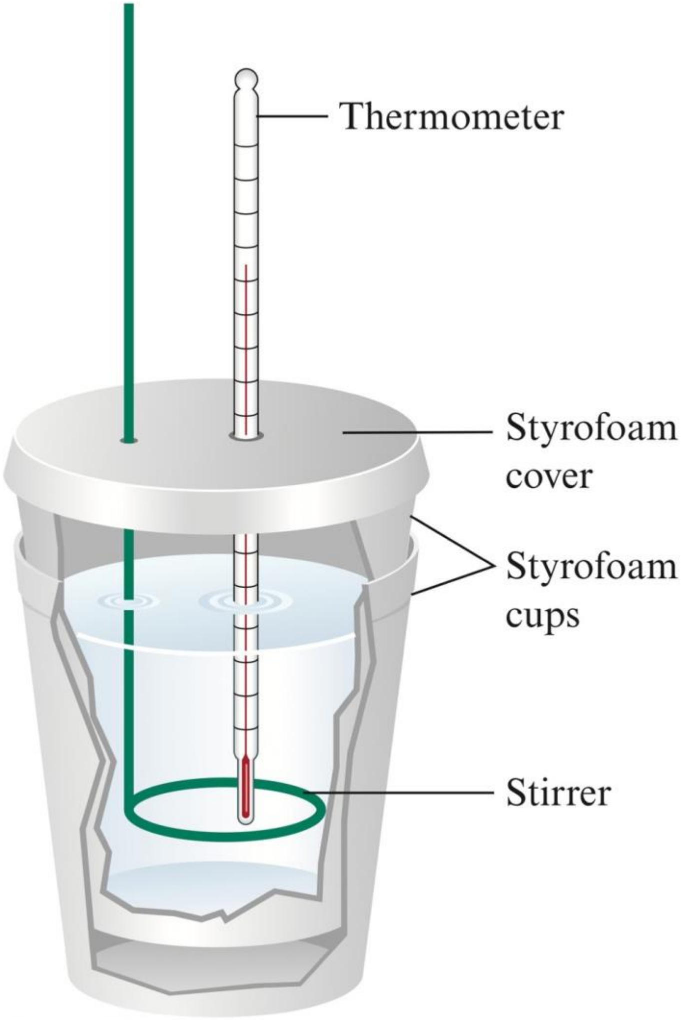
Calorimetry

- Science of measuring heat released or absorbed by a chemical reaction
- The calorimeter is the device used to measure the heat
- Specific heat capacity:
  - The energy required to raise the temperature of one gram of a substance by one degree Celsius.
- Molar heat capacity:
  - The energy required to raise the temperature of one mole of substance by one degree Celsius.

Calorimetry

- If two reactants at the same temperature are mixed and the resulting solution gets warmer, this means the reaction taking place is exothermic.
- An endothermic reaction cools the solution.

A Coffee–Cup Calorimeter Made of Two Styrofoam Cups



Calorimetry

- Energy released (heat) = $s \times m \times \Delta T$

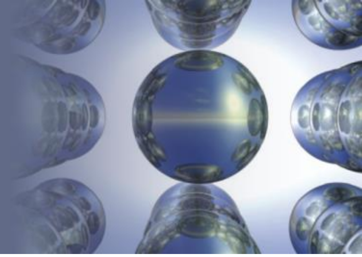
s = specific heat capacity (J/°C·g)

amount of heat required to raise T of 1 gram of substance by 1°C

m = mass of solution (g)

ΔT = change in temperature (°C)

1 cal = 4.184 J



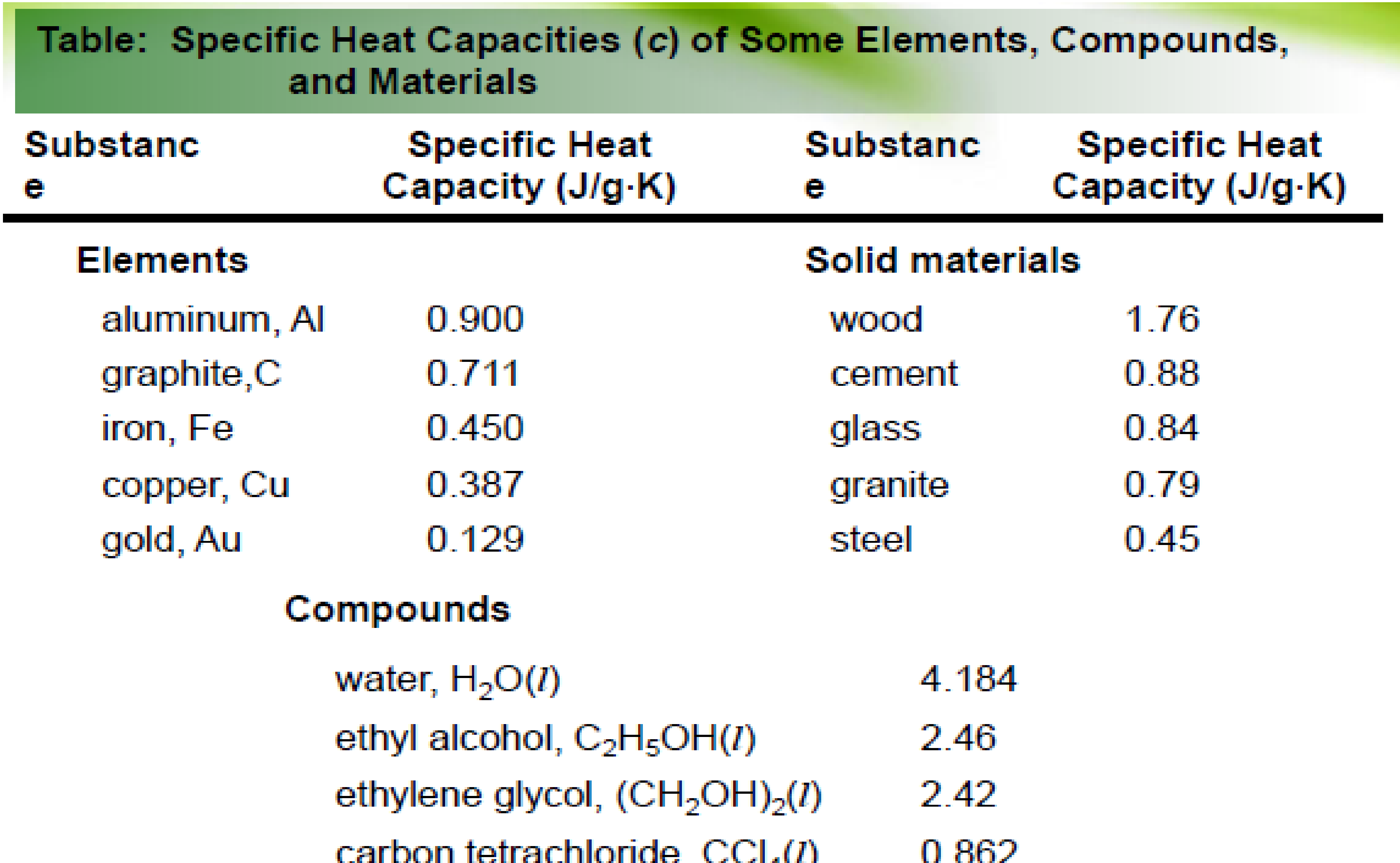


Table: Specific Heat Capacities (c) of Some Elements, Compounds, and Materials

Substance	Specific Heat Capacity (J/g·K)	Substance	Specific Heat Capacity (J/g·K)
Elements		**Solid materials**	
aluminum, Al	0.900	wood	1.76
graphite,C	0.711	cement	0.88
iron, Fe	0.450	glass	0.84
copper, Cu	0.387	granite	0.79
gold, Au	0.129	steel	0.45
Compounds			
water, $H_2O(l)$	4.184		
ethyl alcohol, $C_2H_5OH(l)$	2.46		
ethylene glycol, $(CH_2OH)_2(l)$	2.42		
carbon tetrachloride, $CCl_4(l)$	0.862		

EXAMPLE1

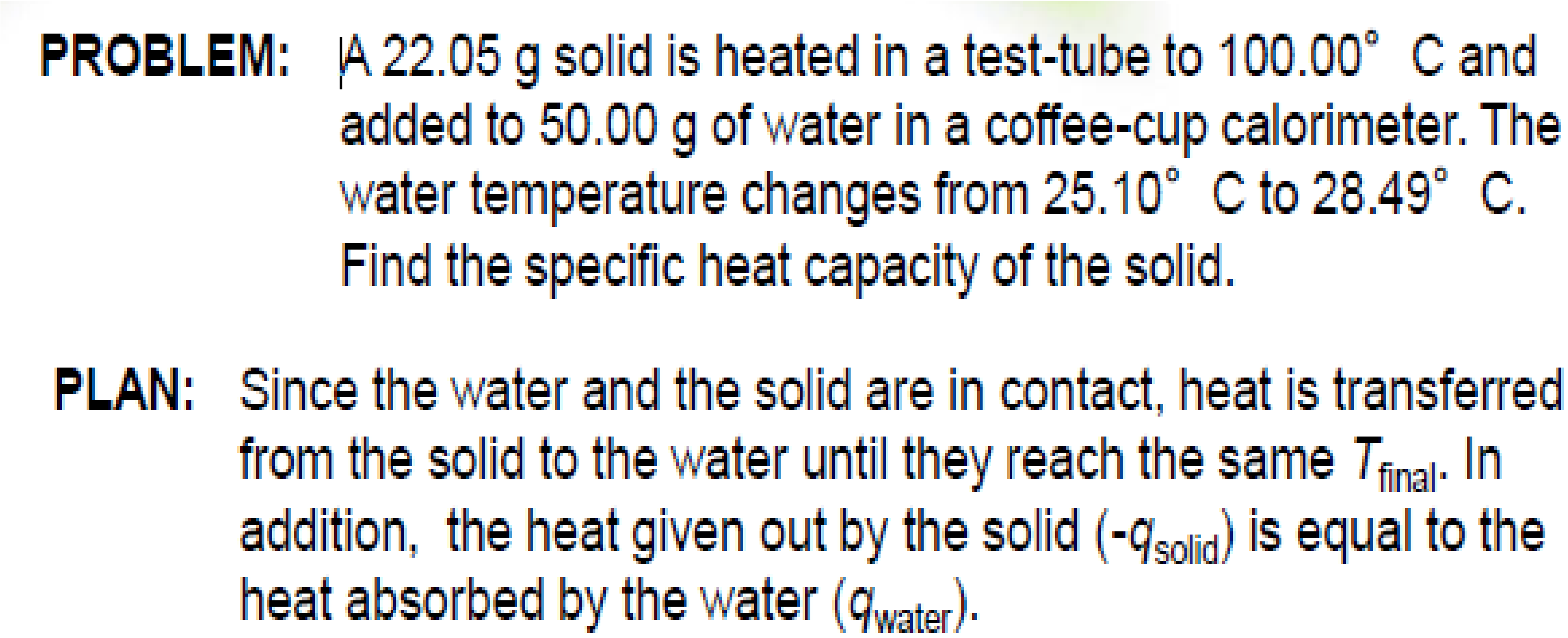
PROBLEM: A layer of copper welded to the bottom of a skillet weighs 125 g. How much heat is needed to raise the temperature of the copper layer from 25° C to 300° C? The specific heat capacity (*c*) of Cu is 0.387 J/g·K.

PLAN: We know the mass (125 g) and *c* (0.387 J/g·K) of Cu and can find ΔT in ° C, which equals ΔT in K. We can use the equation $q = cm\Delta T$ to calculate the heat.

SOLUTION: $\Delta T = T_{\text{final}} - T_{\text{initial}} = 300 - 25 = 275°\ \text{C} = 275\ \text{K}$

$$q = cm\Delta T = \frac{0.387\ \text{J}}{\cancel{\text{g}}\cdot\cancel{\text{K}}} \times 125\ \cancel{\text{g}} \times 275\ \cancel{\text{K}} \quad \boxed{= 1.33\text{x}10^4\ \text{J}}$$

Example



PROBLEM: A 22.05 g solid is heated in a test-tube to 100.00° C and added to 50.00 g of water in a coffee-cup calorimeter. The water temperature changes from 25.10° C to 28.49° C. Find the specific heat capacity of the solid.

PLAN: Since the water and the solid are in contact, heat is transferred from the solid to the water until they reach the same T_{final}. In addition, the heat given out by the solid ($-q_{solid}$) is equal to the heat absorbed by the water (q_{water}).

Solution

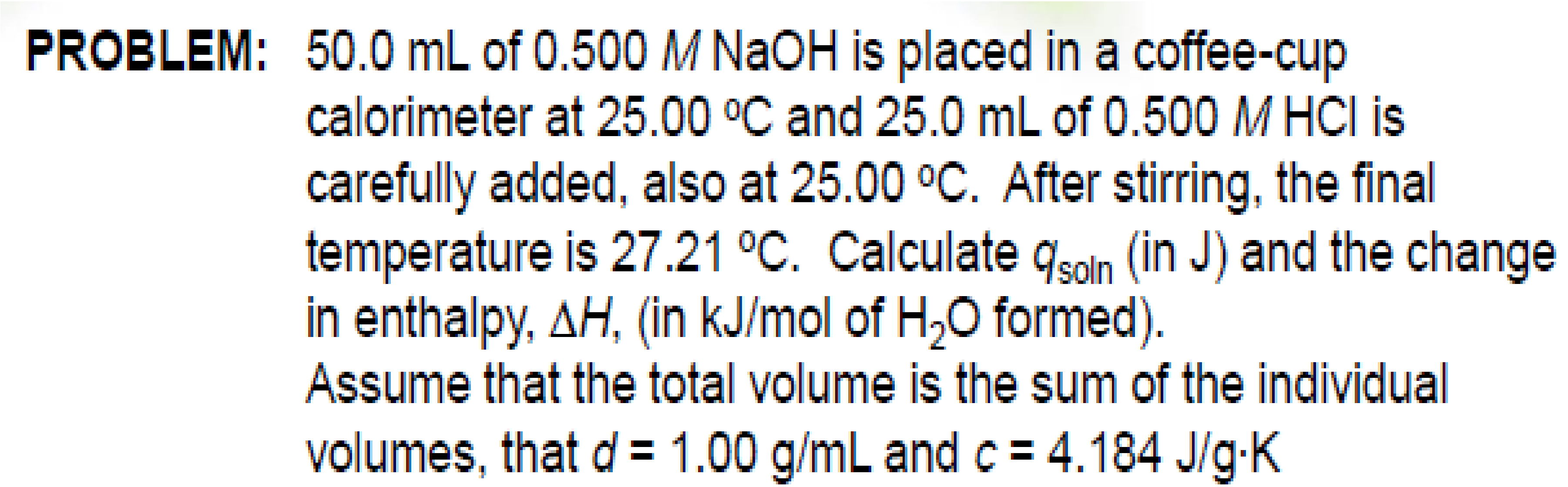
$$\Delta T_{water} = T_{final} - T_{initial} = (28.49^\circ\ \mathrm{C} - 25.10^\circ\ \mathrm{C}) = 3.39^\circ\ \mathrm{C} = 3.39\ \mathrm{K}$$

$$\Delta T_{solid} = T_{final} - T_{initial} = (28.49^\circ\ \mathrm{C} - 100.00^\circ\ \mathrm{C}) = -71.51^\circ\ \mathrm{C} = -71.51\ \mathrm{K}$$

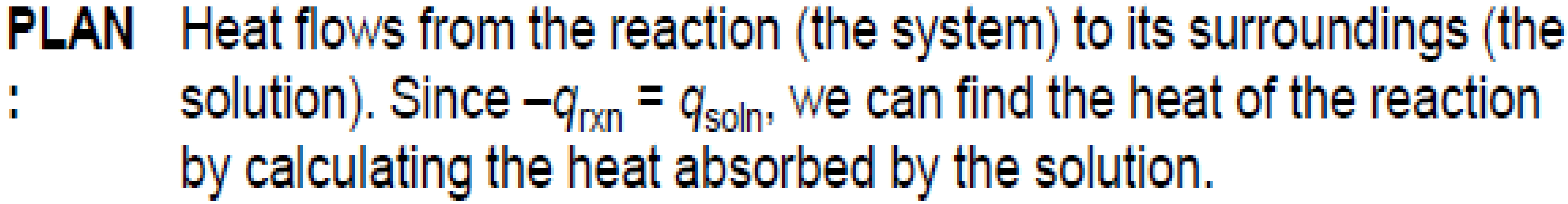
$$c_{solid} = \frac{c_{H_2O} \times \text{mass}_{H_2O} \times \Delta T_{H_2O}}{\text{mass}_{solid} \times \Delta T_{solid}}$$

$$= \frac{4.184\ \mathrm{J/g{\cdot}K} \times 50.00\ \mathrm{g} \times 3.39\ \mathrm{K}}{22.05\ \mathrm{g} \times (-71.51\ \mathrm{K})} \quad \boxed{= 0.450\ \mathrm{J/g{\cdot}K}}$$

EXAMPLE 3



PROBLEM: 50.0 mL of 0.500 *M* NaOH is placed in a coffee-cup calorimeter at 25.00 °C and 25.0 mL of 0.500 *M* HCl is carefully added, also at 25.00 °C. After stirring, the final temperature is 27.21 °C. Calculate q_{soln} (in J) and the change in enthalpy, ΔH, (in kJ/mol of H_2O formed).
Assume that the total volume is the sum of the individual volumes, that d = 1.00 g/mL and c = 4.184 J/g·K



PLAN: Heat flows from the reaction (the system) to its surroundings (the solution). Since $-q_{rxn} = q_{soln}$, we can find the heat of the reaction by calculating the heat absorbed by the solution.

Solution

(a) To find q_{soln}:

Total mass (g) of the solution = (25.0 mL + 50.0 mL) x 1.00 g/mL = 75.0 g

$$\Delta T_{\mathrm{soln}} = 27.21^\circ\ \mathrm{C} - 25.00^\circ\ \mathrm{C} = 2.21^\circ\ \mathrm{C} = 2.21\ \mathrm{K}$$

$$q_{\mathrm{soln}} = c_{\mathrm{soln}} \times \mathrm{mass}_{\mathrm{soln}} \times \Delta T_{\mathrm{soln}} = (4.184\ \mathrm{J/g{\cdot}K})(75.0\ \mathrm{g})(2.21\ \mathrm{K})\ \boxed{= 693\ \mathrm{J}}$$

(b) To find ΔH_{rxn} we first need a balanced equation:

$$\mathrm{HCl}(aq) + \mathrm{NaOH}(aq) \longrightarrow \mathrm{NaCl}(aq) + \mathrm{H_2O}(l)$$

For HCl:

$$25.0\text{ mL HCl} \times \frac{1\text{ L}}{10^3\text{ mL}} \times \frac{0.500\text{ mol}}{1\text{ L}} \times \frac{1\text{ mol H}_2\text{O}}{1\text{ mol HCl}} = 0.0125\text{ mol H}_2\text{O}$$

For NaOH:

$$50.0\text{ mL NaOH} \times \frac{1\text{ L}}{10^3\text{ mL}} \times \frac{0.500\text{ mol}}{1\text{ L}} \times \frac{1\text{ mol H}_2\text{O}}{1\text{ mol NaOH}} = 0.0250\text{ mol H}_2\text{O}$$

HCl is limiting, and the amount of H_2O formed is 0.0125 mol.

$$\Delta H_{rxn} = \frac{q_{rxn}}{\text{mol H}_2\text{O}} = \frac{-693\text{ J}}{0.0125\text{ mol}} \times \frac{1\text{ kJ}}{10^3\text{J}} \boxed{= -55.4\text{ kJ/mol H}_2\text{O}}$$

CONCEPT CHECK!

A 100.0 g sample of water at 90° C is added to a 100.0 g sample of water at 10° C.

The final temperature of the water is:

a) Between 50° C and 90° C

[✓ b) 50° C]

c) Between 10° C and 50° C

CONCEPT CHECK!

A 100.0 g sample of water at 90.° C is added to a 500.0 g sample of water at 10.° C.

The final temperature of the water is:

a) Between 50° C and 90° C

b) 50° C

[✓ c) Between 10° C and 50° C]

Calculate the final temperature of the water.

23° C

CONCEPT CHECK!

You have a Styrofoam cup with 50.0 g of water at 10.° C. You add a 50.0 g iron ball at 90. ° C to the water. (s_{H2O} = 4.18 J/° C·g and s_{Fe} = 0.45 J/° C·g)

The final temperature of the water is:

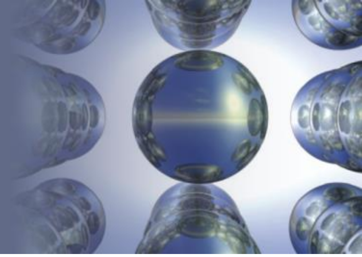
a) Between 50° C and 90° C

b) 50° C

c) Between 10° C and 50° C

Calculate the final temperature of the water.

18° C



EXERCISE!

- A metal pellet with mass 100.0 g, originally at 88.4 °C, is dropped into 125 g of water originally at 25.1 °C. The final temperature of both the pellet and the water is 31.3 °C. Calculate the heat capacity C (in J/°C) and specific heat capacity Cs (in J/g•°C) of the pellet. The specific heat of water is 4.184 J/g•°C.

- When 200.0 g of a $AgNO_3$ solution mixes with 150.0 g of NaI solution, 2.93 g of AgI precipitates, and the temperature of the solution rises by 1.34°C. Assume 350. g of solution and a specific heat capacity of 4.184 J/g•°C. Calculate ΔH for the following:

$$Ag^+(aq) + I^-(aq) \rightarrow AgI(s)$$

Standard Enthalpy of Formation (ΔH_f°)

- Change in enthalpy that accompanies the formation of one mole of a compound from its elements with all substances in their standard states.
- Enthalpy change when 1 mole of a compound is formed at 1 atm and 25° C from the elements in their stable states

Conventional Definitions of Standard States

- For a Compound
  - For a gas, pressure is exactly 1 atm.
  - For a solution, concentration is exactly 1 *M*.
  - Pure substance (liquid or solid)
- For an Element
  - The form [$N_2(g)$, $K(s)$] in which it exists at 1 atm and 25° C.

$Ag_{(s,\ 25°C)} + ½\ Cl_{2\ (g,\ 25°C,\ 1\ atm)} \rightarrow AgCl_{(s)}$ $\Delta H_f° = -127.1$ kJ

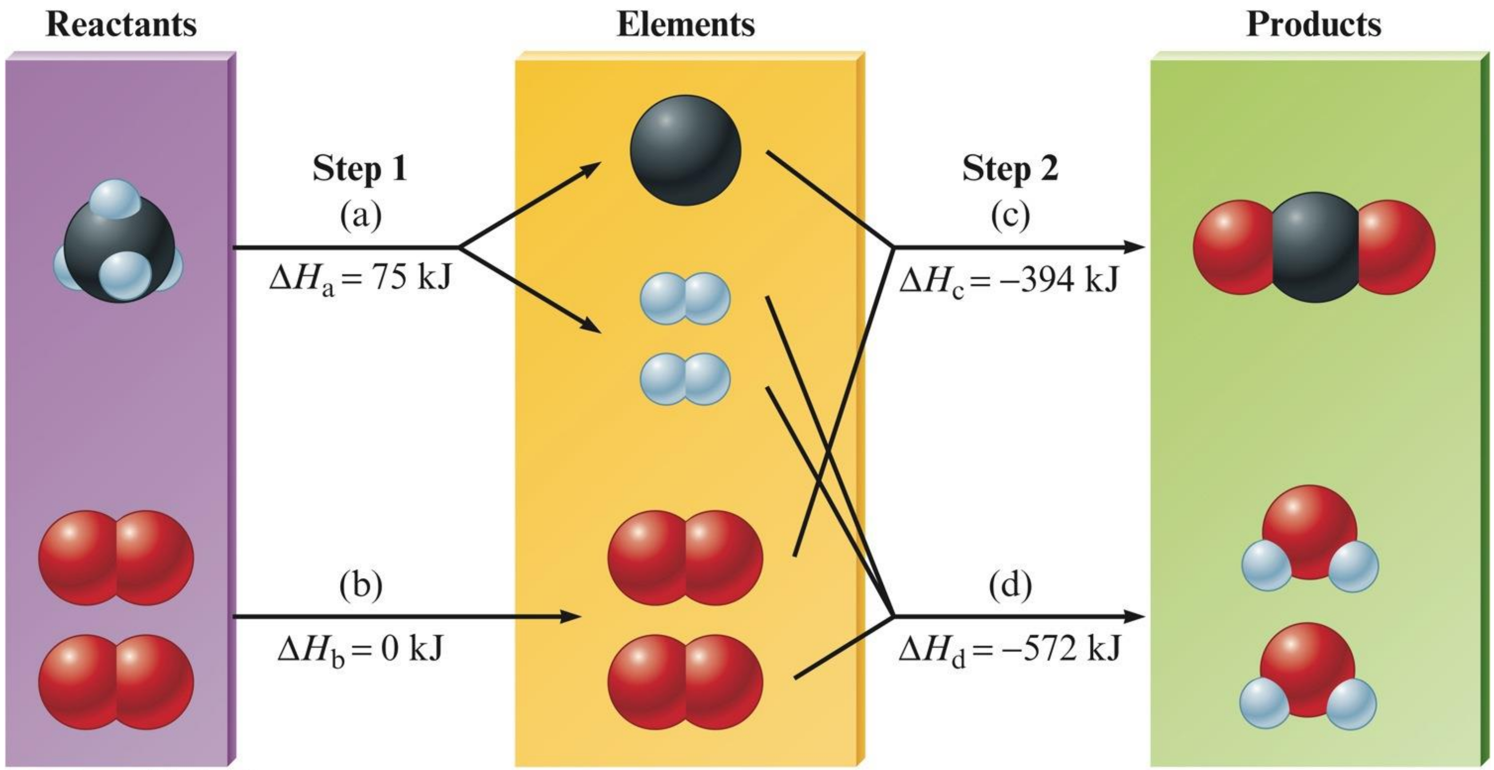
- Most $\Delta H_f°$ are negative values, meaning that the formation of most compounds is exothermic.
- The $\Delta H_f°$ of an element in its stable state at 25°C and 1 atm is zero.
  - $\Delta H_f°$ for $Br_{2\ (l)} = 0$

    $O_{2\ (g)} = 0$

A Schematic Diagram of the Energy Changes for the Reaction

$$CH_4(g) + 2O_2(g) \longrightarrow CO_2(g) + 2H_2O(l)$$

$$\Delta H^\circ_{\text{reaction}} = -(-75\text{ kJ}) + 0 + (-394\text{ kJ}) + (-572\text{ kJ}) = -891\text{ kJ}$$



Problem-Solving Strategy: Enthalpy Calculations

Keep in Mind the Following Key Concepts When Doing Enthalpy Calculations:

- When a reaction is reversed, the magnitude of ΔH remains the same, but its sign changes.
- When the balanced equation for a reaction is multiplied by an integer, the value of ΔH for that reaction must be multiplied by the same integer.
- The change in enthalpy for a given reaction can be calculated from the enthalpies of formation of the reactants and products:

$$\Delta H^\circ_{\text{reaction}} = \Sigma n_{\text{p}} \Delta H^\circ_{\text{f}}(\text{products}) - \Sigma n_{\text{r}} \Delta H^\circ_{\text{f}}(\text{reactants})$$

- Elements in their standard states are not included in the $\Delta H_{\text{reaction}}$ calculations. That is, $\Delta H^\circ_{\text{f}}$ for an element in its standard state is zero.

Calculation of ΔH°

The standard enthalpy change for a given equation is equal to the sum of ΔH_f° for the products minus ΔH_f° for the reactants.

- $\Delta H_f^\circ{}_{\text{rxn}} = \sum \Delta H_f^\circ{}_{\text{products}} - \sum \Delta H_f^\circ{}_{\text{reactants}}$
- *Elements in their standard form can be omitted. ($Fe_{(s)}$, $O_{2\,(g)}$, ...)*
- The coefficients from the balanced equation must be taken into account.

Example

Using enthalpies of formation, calculate the standard change in enthalpy for the thermite reaction:

$$2\text{Al}(s) + \text{Fe}_2\text{O}_3(s) \longrightarrow \text{Al}_2\text{O}_3(s) + 2\text{Fe}(s)$$

This reaction occurs when a mixture of powdered aluminum and iron(III) oxide is ignited with a magnesium fuse.

Solution

$$\Delta H^\circ = \Sigma n_p \Delta H_f^\circ(\text{products}) - \Sigma n_r \Delta H_f^\circ(\text{reactants})$$

where

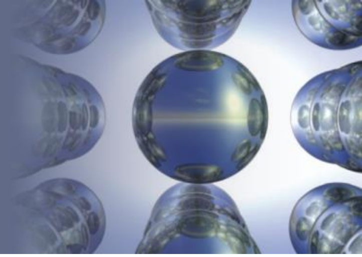
$$\Delta H_f^\circ \text{ for } Fe_2O_3(s) = -826 \text{ kJ/mol}$$

$$\Delta H_f^\circ \text{ for } Al_2O_3(s) = -1676 \text{ kJ/mol}$$

$$\Delta H_f^\circ \text{ for } Al(s) = \Delta H_f^\circ \text{ for } Fe(s) = 0$$

Thus

$$\begin{aligned}\Delta H^\circ{}_{\text{reaction}} &= \Delta H_f^\circ \text{ for } Al_2O_3(s) - \Delta H_f^\circ \text{ for } Fe_2O_3(s)\\ &= -1676 \text{ kJ} - (-826 \text{ kJ}) = -850. \text{ kJ}\end{aligned}$$



EXERCISE!

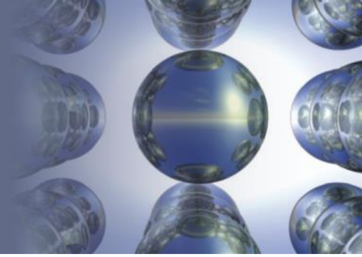
Calculate $\otimes H^\circ$ for the following reaction:

$2Na(s) + 2H_2O(l) \rightarrow 2NaOH(aq) + H_2(g)$

Given the following information:

	$\otimes H_f^\circ$ (kJ/mol)
$Na(s)$	0
$H_2O(l)$	–286
$NaOH(aq)$	–470
$H_2(g)$	0

$\otimes H^\circ = –368\text{ kJ}$



Phase changes

- Although phase changes are not chemical reactions, a quantity of heat is still required, for example, to transform ice at 0^{o}C to water at 0^{o}C. This quantity of heat is called the enthalpy of fusion:

$$H_2O(s) \longrightarrow H_2O(l) \qquad \Delta H_{\text{fus}} = +6.007\ \text{kJ}$$

- Similarly, a quantity of heat is needed to transform water at 100^{o}C to steam at 100^{o}C. This quantity of heat is known as the enthalpy of vaporization:

$$H_2O(l) \longrightarrow H_2O(g) \qquad \Delta H_{\text{vap}} = +40.7\ \text{kJ}$$

Bond Enthalpy – “Bond energy”

- ΔH when 1 mol of bonds is broken in the gaseous state

$H_{2\,(g)} \rightarrow 2\ H_{(g)}$ $\Delta H = 436\ kJ$

$Cl_{2\,(g)} \rightarrow 2\ Cl_{(g)}$ $\Delta H = 243\ kJ$

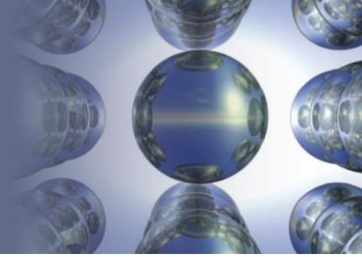
- Allows us to predict the likely energy change in a chemical reaction
- Reactions will be endothermic when:

Bonds of reactants are stronger than those of products.

$2HF_{(g)} \rightarrow H_{2\,(g)} + F_{2\,(g)}$ $\Delta H_f^\circ = +542.2\ kJ$

There are more bonds in the reactants than in the products.

$2\ H_2O_{(g)} \rightarrow 2\ H_{2\,(g)} + O_{2\,(g)}$ $\Delta H_f^\circ = +483.6\ kJ$



Bond Enthalpy – “Bond energy”

- Energy will be absorbed to break bonds.
- Energy will be released when bonds form.
- Bond energies between 2 different atoms are approximations.
- They are averages taken from multiple species.
- Bond energies are stronger for multiple bonds (double and triple bonds)
  - $C - C = 347$ kJ
  - $C = C = 612$ kJ
  - $C \equiv C = 820$ kJ

Bond Enthalpies and Enthalpy of Reaction

- Enthalpy change for a chemical reaction is the difference between energy required to break bonds and that released in the formation of new ones
- To obtain an estimate of ΔH_{rxn}

I. Add bond energy for all bonds made (+)

II. Subtract from bond energy for all bonds broken (–)

$$\Delta H_{rxn} = \Sigma\,(\text{bond enthalpies of bonds broken}) - \Sigma\,(\text{bond enthalpies of bonds formed})$$

OR

$$\Delta H_{rxn} = \sum \mathrm{BE}(\text{reactants}) - \sum \mathrm{BE}(\text{products})$$

Note: BE = Bond energy

Note

- Bond dissociation energy is defined as the amount of energy required to break one mole of covalent bonds in gaseous species e.g.

$$CO_2(g) \rightarrow C(g) + 2O(g) \qquad \Delta H_d^\circ = 1609\ \text{kJ mol}^{-1}$$

- If there are four C-H bonds in the molecule,
- Successive breaking of the bonds gives different enthalpy change.

$$CH_4(g) \rightarrow CH_3(g) + H(g) \qquad \Delta H_d^\circ = +427\ \text{kJ mol}^{-1}$$

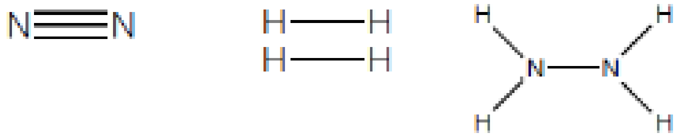
$$CH_3(g) \rightarrow CH_2(g) + H(g) \qquad \Delta H_d^\circ = +371\ \text{kJ mol}^{-1}$$

Example 1

Calculate the heat of formation ΔH_f of hydrazine N_2H_4 Using the bond energies given.

	KJ
N—N	159
N≡N	946
N—H	389
H—H	436

$$N_2 \quad + \quad 2H_2 \rightarrow \quad N_2H_4$$



Need to be broken bonds made

946+ 2(436) -(159 + 4(389))

$$= \sum BE(\text{reactants}) - \sum BE(\text{products})$$

$$= 1818 - 1715$$

$$= 103 \text{ KJ}$$

Example 2

Calculate the enthalpy of combustion of ethene gas at 298.15 K.
Bond energies are given.

Solution

$$C_2H_4(g) + 3O_2(g) \rightarrow 2CO_2(g) + 2H_2O(l)$$

$$H_2C{=}CH_2 + 3(O{=}O) \rightarrow 2(O{=}C{=}O) + 2(H-O-H)$$

$$\Delta H = \sum BE(\text{reactants}) - \sum BE(\text{products})$$

$$= (4C-H + C=C) + (3O=O) - 4C=O + 4O-H$$

$$= (4x413 + 1x614 + 3x495) - (4x745 + 4x467)$$

$$= (3751 - 4848)$$

$$= -1097\,\mathrm{k\,mol^{-1}}$$

Example 3

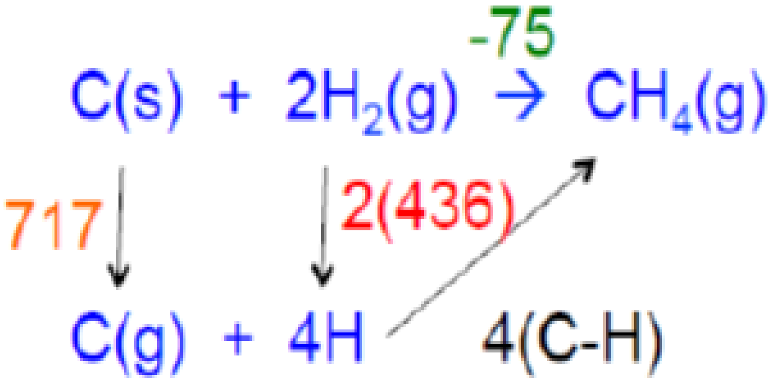
Given: $H + H \rightarrow H_2(g)$ $\Delta H = -436$ kJ

$C(s) \rightarrow C(g)$ $\Delta H = 717$ kJ (sublimation)

Heat of formation of methane is: $\Delta H_f = -75\ kJmol^{-1}$

What is the bond energy of a CH bond?

Sketch an energy cycle:



-75

$C(s) + 2H_2(g) \rightarrow CH_4(g)$

717 2(436)

$C(g) + 4H$ 4(C-H)

$-75\ kJ = 717kJ + 2(436kJ) - 4(C\text{-}H)$

$4(C\text{-}H) = 1664\ kJ$

$(C\text{-}H) = 416\ kJ$

Exercise

- Use the bond enthalpies to calculate the enthalpy of reaction for the combustion of ethane.

$2C_2H_{6\,(g)} + 7O_{2\,(g)} \rightarrow 4\ CO_{2\,(g)} + 6\ H_2O_{(g)}$ $\Delta H =$ [redacted]

Bond	ΔH (kJ)	Bond	ΔH (kJ)
H-H	436	C=O	715
C-H	414	O-O	138
C-C	347	O=O	498
C-O	351	O-H	464