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THERMOCHEMISTRY

Syllabus Learning Outcomes : 1, 7

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Heat, Energy & Chemistry

- Burning peanuts supply sufficient energy to boil a cup of water.
- Burning sugar (sugar reacts with $KClO_3$, a strong oxidizing agent)

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Heat, Energy & Chemistry

- Product favored reactions: make more products (perhaps with outside assistance) and usually give off energy as heat.

Driving forces from Chem I

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Energy: is ability to do work or transfer heat.

HEAT: energy that flows between 2 objects because of a temperature difference.

Other forms of energy —

- light
- electrical
- kinetic and potential

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Potential energy (PE) comes from position

Energy a motionless body has from its position.

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Atoms have potential energy

- Positive and negative ions attract.
- Ions can bond
- Bonding lowers potential energy

Kinetic energy (KE) comes from motion

Atoms also have kinetic energy because they vibrate, rotate, and move

Internal Energy (E or U)= KE+PE

E for a chemical system depends on:

- number of particles (n or m)
- temperature (T)
- type of particles

Thermodynamics

uses temperature changes (ΔT) and mass (m) to calculate changes in E (ΔE).

Thermodynamics

is the science of heat transfer (energy) transfer.

Heat comes from molecular motion.
transfers to achieve thermal equilibrium.

Heat transfer can be measured by ΔT.

System is the object under study

- Surroundings
  - Everything outside the system

Heat transfers from a hotter object to a cooler one

Exothermic: heat transfers from system to surroundings.

Exothermic systems feel warm or hot to the touch

T_{system} goes down and $T_{surroundings}$ goes up

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Endothermic: heat transfers from surroundings to system.

Endothermic systems feel cool or cold to the touch

T_{system} goes up and $T_{surroundings}$ goes down

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Thermodynamics depends on conservation of energy

- E is unchanged by chemistry.
- If PE of products is less than reactants, the difference must be released as KE (an increase in T).

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Energy has Units

1 calorie = heat required to raise temp. of 1.00 g of H_2O by 1.0 ^oC.

1000 cal = 1 kilocalorie = 1 kcal

1 kcal = 1 Calorie (a food "calorie")

But we use the unit called the JOULE

1 cal = 4.184 joules

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Predict Chemical Reactivity

What drives chemical reactions? How do they occur (and how fast)?

First question is answered by Thermodynamics and the second by Kinetics.

"Driving forces" for Product-Favored reactions.

- precipitation
- gas formation
- H_2O formation (acid-base reaction)
- redox, electron transfer in a battery
- Heat

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Predict Chemical Reactivity

Reactions that transfer energy to their surroundings are usually product favored.

Exothermic reactions are usually product favored.

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HEAT CAPACITY is

heat to raise T of a substance by 1 °C.

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Specific Heat Capacity (Cp) is heat to raise 1g by 1°C

Heat (*q*) is related to

a) sample mass (m)
b) change in T and
c) specific heat capacity, Cp

$$q\ (J) = m\ (g) * Cp\ (J/g°C) * \Delta T\ (°C)$$

$$\Delta T = T_{final} - T_{initial}$$

Note: for temperature changes, 1K = 1°C

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Find specific heat capacities in tables

Substance	Spec. Heat (J/g•K)
H_2O	4.184
Ethylene glycol	2.39
Al	0.897
glass	0.84

Look in your book or on the exam for the Cp value for the substance

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Example: Calculate "q"

Calculate the joules of heat lost (or transferred) when 25.0 g of Al cool from 310 °C to 37 °C.

$$q = m\ C_p\ \Delta T$$

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Example: Calculate "q"

Calculate the joules of heat lost when 25.0 g of Al cool from 310 °C to 37 °C.

$q = (25.0\ g)\ (0.897\ J/g•K)\ (37 - 310)K$

$q = - 6120\ J$

Negative sign means heat is lost by Al.

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Equation applies for heat/ energy transfer with no change in state (s,l,g)

$$q = m\ Cp\ \Delta T$$

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Example: Calculate Cp

- Take 55.0 g Fe at 99.8 °C
- Drop into 225 g water at 21.0 °C
- Water and metal come to 23.1 °C
- Calculate the experimental specific heat capacity of Fe

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Example: Calculate C_p

Because of conservation of energy,

$q(Fe) = -q(H_2O)$ (heat out of Fe = heat into H_2O)

or $q(Fe) + q(H_2O) = 0$

$q(Fe) = (55.0\ g)(C_p)(23.1\ ^{\circ}C - 99.8\ ^{\circ}C) = -4219 \cdot C_p$

$q(H_2O) = (225\ g)(4.184\ J/K \cdot g)(23.1\ ^{\circ}C - 21.0\ ^{\circ}C) = 1977\ J$

$q(Fe) + q(H_2O) = -4219\ C_p + 1977 = 0$

$C_p = 0.469\ J/g \cdot K$

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Heat transfer with change of state

Changes of state involve energy (at constant T)

Ice + 333 J/g (heat of fusion) → Liquid water

$q = \Delta H_{fusion} \cdot m$

ΔH_{fusion} values may be given in J/mol, in which case multiply the heat by mol (n) instead of mass

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Heat transfer with change of state

Changing a liquid to a gas (vapor) requires energy, $\Delta H_{vaporization}$.

To boil water on a stove __________ energy.

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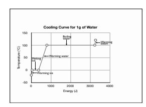
Heating/Cooling Curve for Water



T is constant as ice melts or as water boils

T changes when warming solids, liquids or gases

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Example: Heat with state change

Calculate the heat to melt 500.g of ice to steam at 100 ^{o}C

Heat of fusion of ice, ΔH_{fus} = 333 J/g
Specific heat capacity of water, Cp = 4.184 J/g•K
Heat of vaporization, ΔH_{vap} = 2260 J/g

$$\text{Ice} \xrightarrow[+333\ J/g]{} \text{Water} \xrightarrow[+2260\ J/g]{} \text{Steam}$$

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Example: Heat with state change

Calculate the heat to melt 500.g of ice to steam at 100 ^{o}C

1. Melting ice at 0°C
   $q = (500.\ g)(333\ J/g) = 1.67 \times 10^5\ J$
2. Warming water from 0 ^{o}C to 100 ^{o}C
   $q = (500.\ g)(4.2\ J/g \cdot K)(100 - 0)K = 2.1 \times 10^5\ J$
3. Evaporating water at 100 ^{o}C
   $q = (500.\ g)(2260\ J/g) = 1.13 \times 10^6\ J$
4. Total heat energy = 1.51×10^6 J = 1510 kJ

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Transfer heat (and work) in a physical process

CO_2 (s, -78 °C) → CO_2 (g, -78 °C)

Subliming CO2 requires energy, so it is an endothermic process.
Endothermic process: heat transfers from surroundings to system

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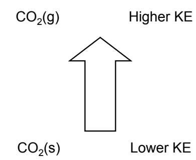
Energy diagram for heat transfer



Heat energy to sublime CO_2 comes from the surroundings.
CO_2 molecules gain kinetic energy and move faster.

It is possible to do work with the energy

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First Law of Thermodynamics: Energy is conserved

$$\Delta E = q + w$$

Energy change — ΔE

Work done on or by system — w

Heat energy transferred — q

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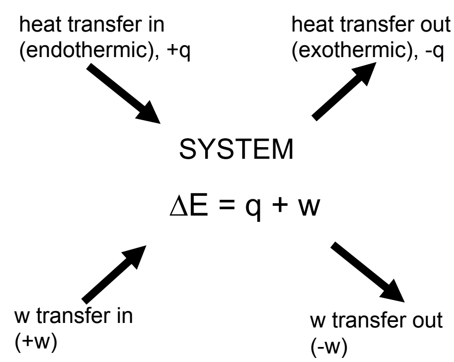

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Enthalpy(ΔH) is the change in heat content of system

Most chemical reactions occur at constant P, so

Heat transferred at constant P = q_p, and

$$\Delta H = q_p$$

giving $\Delta E = \Delta H + w$ (w is usually small), so

$$\Delta H = q_p \approx \Delta E$$

ΔH = change in heat content of the system

$$\Delta H = \Delta H_{final} - \Delta H_{initial}$$

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Calculating Enthalpy

$\Delta H = \Delta H_{final} - \Delta H_{initial}$

If $\Delta H_{final} > \Delta H_{initial}$ then ΔH is positive
Process is Endothermic

If $\Delta H_{final} < \Delta H_{initial}$ then ΔH is negative
Process is Exothermic