



6A Thermochemistry

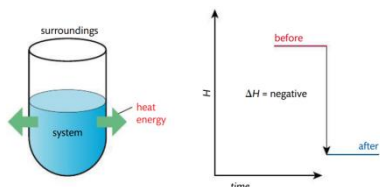
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考点一：Definition

- 6.1 write and balance **chemical equations** for combustion reactions of **alkanes**
 6.2 define **endothermic reaction, exothermic reaction, specific heat, enthalpy, bond energy, heat of reaction, and molar enthalpy**
 6.5 illustrate changes in energy of various chemical reactions, using **potential energy diagrams**

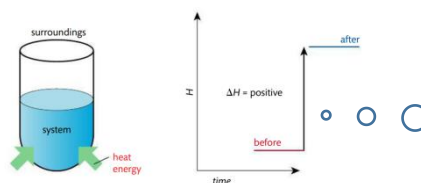
1. Endothermic reaction, exothermic reaction

Enthalpy (H) is a measure of the amount of heat energy contained in a substance. Changes in enthalpy are denoted by ΔH



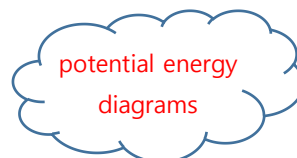
注：绝大多数的反应是放热的！包括 **combustion and all neutralization reactions**.

Exothermic reactions



注：只有极少数的反应是吸热的。

Endothermic reactions



Chemical potential energy is energy stored in a substance because of its composition

2. Specific heat

The **specific heat** of any substance is the amount of heat required to raise **one gram** of that substance **one degree** Celsius.

Table 21.1 Specific Heat Capacities		
Material	(J/g°C)	(cal/g°C)
Water	4.186	1.00
Aluminum	0.900	0.215
Clay	1.4	0.33
Copper	0.386	0.092
Lead	0.128	0.031
Olive Oil	1.97	0.471
Silver	0.23	0.056
Steel (iron)	0.448	0.107

3. Thermochemical equations



One mole of **methane** gas reacts with *two moles* of **oxygen** gas to give *one mole* of gaseous **carbon dioxide** and *two moles* of liquid **water** and *releases 890 kJ* of heat energy

1) **Standard enthalpy change of reaction, $\Delta_r H$** , is the enthalpy change when the reaction occurs in the **molar quantities** shown in the **chemical equation**, under standard conditions.

2) **Standard enthalpy change of formation, $\Delta_f H$** , is the enthalpy change when **1 mole** of a **compound** is formed from its **elements** in their standard states, under standard conditions, e.g. $2\text{C}(\text{s}) + 3\text{H}_2(\text{g}) + \frac{1}{2}\text{O}_2(\text{g}) \rightarrow \text{C}_2\text{H}_5\text{OH}(\text{l})$.

3) **Standard enthalpy change of combustion, $\Delta_c H$** , is the enthalpy change when **1 mole** of a substance is completely **burned in oxygen**, under standard conditions.

4) **Standard enthalpy change of neutralisation, $\Delta_{\text{neut}} H$** , is the enthalpy change when an acid and an alkali react together, under standard conditions, to form **1 mole of water**.



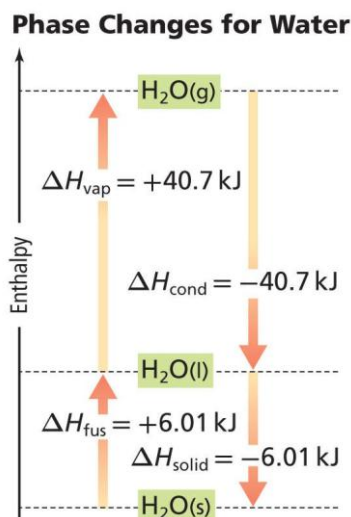
考点二：Calculation

- 6.3 calculate and compare the energy involved in **changes of state** that occur in chemical reactions
 6.4 calculate the changes in energy of various chemical reactions using **bond energy**, **heats of formation**, and **Hess's law**
 6.6 determine **experimentally** the **changes in energy** of various chemical reactions
 6.7 compare the **molar enthalpies** of several **combustion reactions** involving organic compounds

1. Changes of State

Molar enthalpy (heat) of vaporization refers to the heat required to **vaporize** one mole of a liquid substance.

Molar enthalpy (heat) of fusion is the amount of heat required to **melt** one mole of a solid substance.



SAMPLE PROBLEM 1

How much energy is needed to melt 25.0 g of ice?

$$\Delta H = n\Delta H_{\text{fus}}$$

In this formula, n is the number of moles of ice and ΔH_{fus} is the molar heat of fusion for water.

$$\Delta H = 25.0 \text{ g H}_2\text{O} \times \frac{1 \text{ mol}}{18.01 \text{ g}} \times 6.03 \text{ kJ/mol} = 8.38 \text{ kJ}$$

SAMPLE PROBLEM 2

If 15.0 kJ of energy is available to boil water, how many g of water can be boiled?

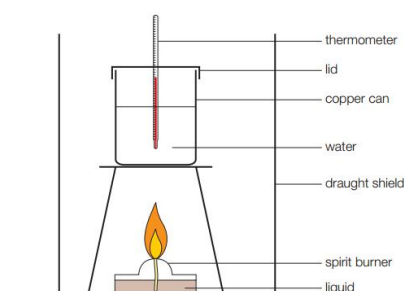
$$\Delta H = n\Delta H_{\text{vap}}$$

$$15.0 \text{ kJ} = n \times 40.8 \text{ kJ/mol}$$

$$n = 0.368 \text{ mol} \quad \text{since } n = \frac{\text{mass}}{\text{molar mass}}$$

$$\text{mass} = 0.368 \text{ mol H}_2\text{O} \times \frac{18.01 \text{ g H}_2\text{O}}{1.0 \text{ mol H}_2\text{O}} = 6.63 \text{ g H}_2\text{O}$$

1. Enthalpy change of combustion



CALCULATING ENTHALPY CHANGE OF COMBUSTION

Stage 1: $Q = mc\Delta T$

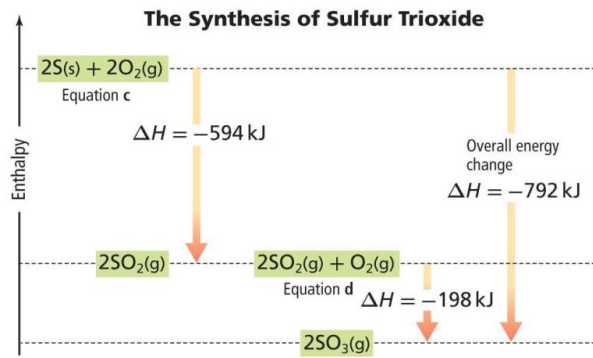
Stage 2: Calculate the **amount, n** , of ethanol burned

Stage 3: Calculate ΔH , using the equation $\Delta H = -\frac{Q}{n}$



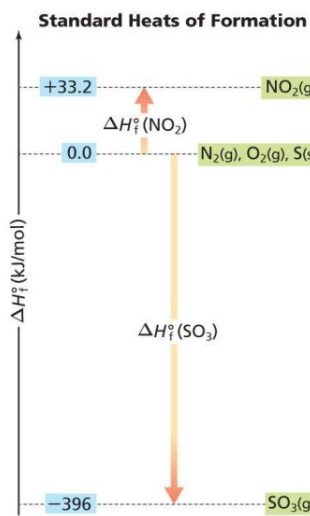
2. HESS'S LAW

Hess's law states that if you can add **two or more** thermochemical equations to produce a final equation for a reaction, then the **sum of the enthalpy changes** for the individual reactions is the **enthalpy change** for the **final reaction**.



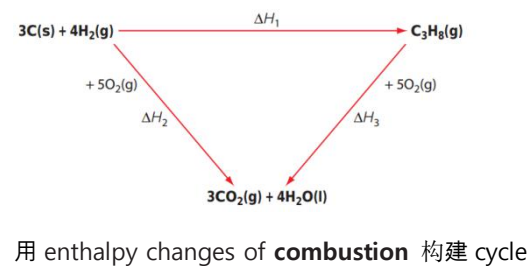
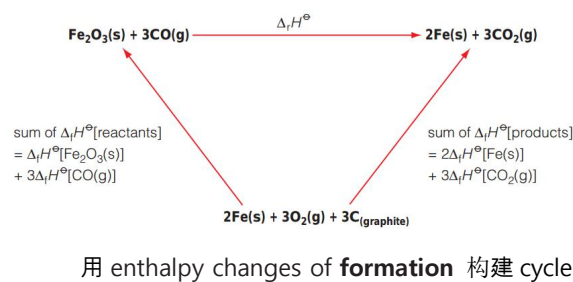
The standard enthalpy (heat) of formation

- **Elements** in their **standard states** have a ΔH_f° of 0.0 kJ
- The formation of compounds are placed above or below elements in their standard states.



$$\Delta H_{rxn}^\circ = \sum \Delta H_f^\circ(\text{products}) - \sum \Delta H_f^\circ(\text{reactants})$$

Standard enthalpies of formation can be used to calculate the **enthalpies** for many reactions under standard conditions by using **Hess's law**.



3. BOND ENTHALPY

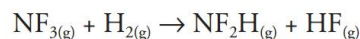
Bond enthalpy the enthalpy change when one mole of a bond in the gaseous state is broken;

mean bond enthalpy the enthalpy change when one mole of a bond, averaged out over many different molecules, is broken

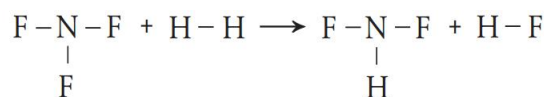
计算方法: 1, Calculate $\Sigma(\text{bonds broken})$ 断键吸热为**正**; 2, Calculate $\Sigma(\text{bonds made})$ 成键放热为**负**; 3, 相加。

SAMPLE PROBLEM

Calculate the ΔH for the following chemical reaction using the table of average bond energies



First, draw structural formulas for all the reactants and products.



First, draw structural formulas for all the reactants and products. For reactants there are:

3 mol of N-F bonds

1 mol of H-H bonds

For products there are:

2 mol of N-F bonds

1 mol of N-H bonds

1 mol of H-F bonds

$$\Delta H = (3 \times 272 \text{ kJ} + 1 \times 432 \text{ kJ}) - (2 \times 272 \text{ kJ} + 1 \times 391 \text{ kJ} + 1 \times 565 \text{ kJ}) = -252 \text{ kJ}$$

考点三：补充 Reaction Spontaneity

spontaneous process

entropy

second law of thermodynamics

free energy

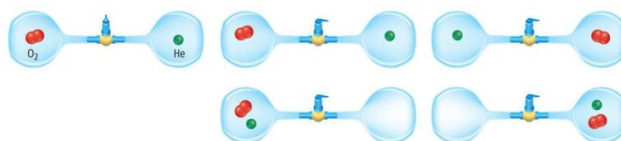
1. Spontaneous process

A **spontaneous process** is a physical or chemical change that once begun, occurs with **no outside intervention**.

- Many **spontaneous processes** require some energy from the surroundings to **start the process**.

2. Entropy

Entropy is a measure of the **possible ways** that the energy of a system can be distributed, and this is related to the **freedom of the system's particles** to move and the number of ways they can be arranged.



3. The second law of thermodynamics

- The **second law of thermodynamics** states that **spontaneous processes** always proceed in such a way that the **entropy** of the universe **increases**.
- Entropy is sometimes considered **a measure of disorder** or **randomness of the particles** in a system.
- The **more spread out** the particles are, the **more disorder**.

If a total entropy change increases ($\Delta S_{\text{total}} > 0$), the total reaction will be **spontaneous**.

$$\Delta S_{\text{total}} = \Delta S_{\text{system}} - \frac{\Delta H}{T}$$

4. Free energy

- **Free energy** is energy that is **available to do work**.
- Gibbs free energy equation

$$\Delta G_{\text{system}} = \Delta H_{\text{system}} - T\Delta S_{\text{system}}$$

- If the sign of the energy change, ΔG° , is **positive**, the reaction is **nonspontaneous**.
- If the sign of the energy change is **negative**, the reaction is **spontaneous**.

ΔH_{system}	ΔS_{system}	ΔG_{system}	Reaction Spontaneity
negative	positive	always negative	always spontaneous
negative	negative	negative or positive	spontaneous at lower temperatures
positive	positive	negative or positive	spontaneous at higher temperatures
positive	negative	always positive	never spontaneous