Gas-Liq-Solids
Three-laws-Thermo

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Outline

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General Notice

- unit: Kelvin(K) & J$\cdot$K$^{-1}\cdot$mol^{-1}

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- formula transformation: molartity & density

Gas

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Why do we study kinetic molecular theory?

- Graham's law of effusion?

Understanding from A New Point of View

Here we will discuss the **ideal gas equation** from a new point of view, *i.e.*, **kinetic molecular theory**(KMT).

Understanding from A New Point of View

First we should get aware of the **prerequisite** of KMT.

[1] Sun, Ting, *CHEM2100J-FA21-Ch5-6*, pp. 35.

Understanding from A New Point of View

First we should get aware of the **prerequisite** of KMT. Recall what has been taught in lectures.

1. A gas is in continuous random motion
2. Gas molecules are infinitesimally small
3. They move in straight lines until collision
4. Gas molecules do not influence one another except during collisions
5. The collisions are elastic

Prerequisites of KMT shown in slides[1]

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- Gas molecules do not influence one another except during collisions.
- The collisions are elastic.

Understanding from A New Point of View

Example

For a model satisfying KMT, suppose there exists N gas molecules in a cubic box with length L. Each molecule has the mass of m, and the speed of u.

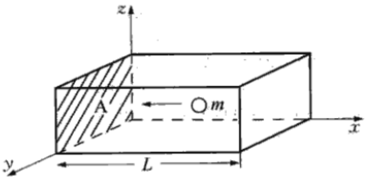


Figure 1.7 An elastic collision of molecule with a well.

Understanding from A New Point of View

(1) Calculate the average kinetic energy of each molecule $\bar{E}_k$.
(2) If the relationship between average molecule and the temperature is

$$\bar{E}_k = \frac{3}{2}kT$$

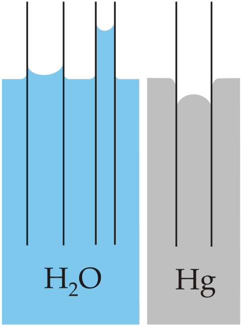
where k denotes the Boltzmann constant and satisfies $k = \frac{R}{N_A}$, what familar formula will derived?

Liquid

- viscosity

Liquid

- viscosity
- surface tension



Solid

- crystalline & amorphous

Solid

- crystalline & amorphous
- Molecular Solids & Network Solids & Metallic Solids

Closed-Packed Structures

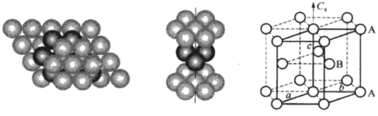


Figure 8. 17 Hexagonal closest packing (ABAB . . .).

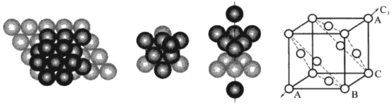


Figure 8. 20 Cubic closest packing (ABCABC···).

How to understand packed structures?

What is packed structures/closed-packed structures?
What does A, B, C mean?
How to calculate the occupied rate?

Intermolecular Forces

The key to understanding intermolecular forces is to understand the way to form chemical bonds.

Several ways to consider

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Several ways to consider

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- spacial geometries
- chemical elements

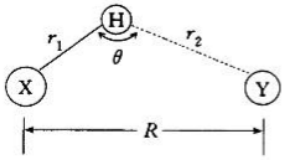
Intermolecular Forces

	Ion-Ion	Ion-Dipole	Dipole-Dipole
E_p dependence	$\frac{1}{r}$	$\frac{1}{r^2}$	$\frac{1}{r^3}$

	Dipole-Dipole (induced)	London	Hydrogen Bonding
E_p dependence	$\frac{1}{r^6}$	$\frac{1}{r^6}$	/

Remarks: In daily life, Total Price = Unit Price × Amount. So is chemistry.

Hydrogen Bonding



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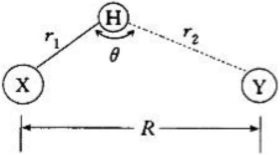

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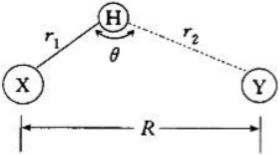

- Tend to be formed and can be formed easily.
- Both intermolecular or intramolecular.
- Depends on the geometry, the environment, and the nature of the specific donor and acceptor atoms, varying between a large range.

Hydrogen Bonding

Examples of hydrogen bond

- The density of water and ice.

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Examples of hydrogen bond

- The density of water and ice.
- The acidity of HF.
- Alcohol solution

Outline

Introduction

The key to understanding theomodynamics is to design thermodynamic cycle.

Key Concepts

- system & surrounding

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- work & heat & energy
  The First Law $\Delta U = q + w$

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- The Born-Haber Cycle

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- sign

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- free expansion

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- expansion at constant temperature

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- reversible expansion

Heat Capacity

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  - molar heat capacity: $C_m = \frac{C}{n}$

Enthalpy

- definition

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- origin

Enthalpy

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- constant pressure and constant volume

Enthalpy

- definition
- origin
- constant pressure and constant volume
- relationship between heat capacity

Expansion

Example

10 mol ideal gas expands at 300 K, with initial volume $V_1 = 25\ \mathrm{dm}^3$, final volume $V_2 = 100\ \mathrm{dm}^3$, experiencing the following four paths:

(1) free expansion;

(2) expands at final pressure when it is $100\ \mathrm{dm}^3$;

(3) first expands at the initial pressure until it is $50\ \mathrm{dm}^3$, then expands at the final pressure until final state;

(4) reversible expansion.

Hess's Law

Example

Given the thermochemical equations

$$X_2 + 3\,Y_2 \longrightarrow 2\,XY_3 \qquad \Delta H_1 = -340 \text{ kJ}$$

$$X_2 + 2\,Z_2 \longrightarrow 2\,XZ_2 \qquad \Delta H_2 = -120 \text{ kJ}$$

$$2\,Y_2 + Z_2 \longrightarrow 2\,Y_2Z \qquad \Delta H_3 = -220 \text{ kJ}$$

Calculate the change in enthalpy for the reaction.

$$4\,XY_3 + 7\,Z_2 \longrightarrow 6\,Y_2Z + 4\,XZ_2$$

The Born-Haber Cycle

Example

At $p^{\ominus}$ and 298.15 K, mix 1 mol CH_4 and 4 mol O_2 and fire them to make them explode under constant pressure. Suppose this reaction happens in an instaneous moment. Calculate the higher temperature this system may achieve.

Data:

$\Delta_{\mathrm{f}} H_{\mathrm{m}}^{\ominus}\left(\mathrm{CO_2},\ \mathrm{g}\right) = -393.51\ \mathrm{kJ \cdot mol^{-1}}$

$\Delta_{\mathrm{f}} H_{\mathrm{m}}^{\ominus}\left(\mathrm{H_2O}, \mathrm{g}\right) = -241.82\ \mathrm{kJ \cdot mol^{-1}}$

$\Delta_{\mathrm{r}} H_{\mathrm{m}}^{\ominus}\left(\mathrm{CH_4},\ \mathrm{g}\right) = -74.81\ \mathrm{kJ \cdot mol^{-1}}$

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- Process: constant pressure, constant volume, adiatic
- Example: vaporation, fusion, freezing, condensation, sublimation, deposition, expansion
- Know the concepts and design your cylce smartly.