Physical Chemistry (A)

S/N: 10421100-10421110
Classification: Specialized basic course
Applicable to: Chemical Engineering and Technics
Materials Science and Engineering
Pharmaceutical Engineering
Total Hours: 102 Credit Points: 6
Requirements on foundation courses: Advanced Mathematics
General Physics
Inorganic and Analytical Chemistry
Organic Chemistry
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A. Characteristics and Status

Physical chemistry is engaged in the research of basic principles of chemical changes, phase changes and physical changes concerned, mainly including the rules of equilibrium and change speed. As a specialized basic course for chemical engineering and technics, materials science and engineering, pharmaceutical engineering majors, etc, physical chemistry is not only an important part for cultivating integral knowledge structure and capability structure of engineering and technical talents of the said majors, but also a foundation for the subsequent specialized courses.

B. Teaching Targets

1. After studying this course, students shall master basic theoretical knowledge well, understand important concepts and basic principles, and master basic computational technique of physical chemistry.
2. After studying this course, students shall master theoretical research approaches of physical chemistry, especially the thermodynamics approaches, and understand methods of statistical thermodynamics basically.
3. After studying this course, students shall receive the training of general scientific approaches further and improve the ability of analyzing and resolving problems of physical chemistry. Training of scientific approaches shall be carried out through the course of teaching; therefore, particularly through learning of thermodynamics and dynamics, students will master general methods of inducing and deducing from experimental results, be familiar with methods of concluding theories from hypothesis and master general scientific approaches of resolving practical problems through theories and according to real conditions.

C. Teaching Contents, Basic Requirements and Time Allocation

Introduction

To find out research contents of physical chemistry, understand research approaches and the development trend and characteristics of modern physical chemistry, and master the learning approaches for the course of physical chemistry.

Major Contents:

0.1 Research contents of physical chemistry

0.2 Research approaches of physical chemistry

0.3 Establishment and development of physical chemistry

0.4 Development trend and characteristics of modern physical chemistry

0.5 Learning approaches for the course of physical chemistry

Key Points:

1. Intentions and contents of physical chemistry
2. Research approaches of physical chemistry
3. Learning approaches for the course of physical chemistry

Nodus:

1. Research approaches of physical chemistry
2. Learning approaches for the course of physical chemistry

Chapter 1 PVT property of gas

To master the perfect gas equation and mode, Dalton law and Amagat law, comprehend the liquefaction and critical properties of real gas, master perfect gas mode and its theoretical explanation, comprehend the principle of corresponding state diagram of compressibility factor and related calculations.

Major Contents:

1.1 Perfect gas equation and mode

1.2 Dalton law and Amagat law

1.3 PVT property of real gas

1.4 Van der Waals equation

1.5 Liquefaction and critical properties of real gas

1.6 Principle of corresponding state and diagram of compressibility factor

Key Points:

1. Perfect gas equation and mode
2. Dalton law and Amagat law
3. Liquefaction and critical properties of real gas
4. Principle of corresponding state and diagram of compressibility factor

Nodus:

1. Perfect gas mode and its theoretical explanations
2. Liquefaction and critical properties of real gas
3. Principle of corresponding state diagram of compressibility factor and related calculations

Chapter 2 The First Law of Thermodynamics and its applications

To comprehend the basic conceptions of thermodynamics below: equilibrium state, state function, reversible process, etc., comprehend the description and mathematical representation of the first law of thermodynamics, master the definitions of thermodynamic energy enthalpy standard enthalpy of foundation and their applications, to master the calculation principles and methods of heat work and variation of functions in all states when P V T changes, phase changes or during the chemical change process. When applying the general relation of thermodynamics in specific system, learn to use the state equations (mainly refers to perfect gas equation) and thermodynamic data (heat capacity heat of phase change saturated vapor pressure, etc .).

Major Contents:

2.1 Thermodynamic conspectus

2.2 The first law of thermodynamics

2.3 Quasistatic process and reversible process

2.4 Enthalpy

2.5 Heat capacity

2.6 Application of the first law of thermodynamics for perfect gas

2.7 Real gas

2.8 Thermochemistry

2.9 Hess's law

2.10 Kirchhoff's law

2.11 Adiabatic reaction

Key Points:

1. Basic conceptions of thermodynamics below: equilibrium state, state function, reversible process

2. Description and mathematical representation of the first law of thermodynamics

3. Definitions of thermodynamic energy enthalpy standard enthalpy of foundation and their applications.

4. Master the calculation methods of heat work and variation of thermodynamic energy and enthalpy when P V T changes, phase changes or during the chemical change process.

Nodus:

1. Definitions of thermodynamic energy enthalpy standard enthalpy of foundation and their applications.

2. Calculation methods of heat work and variation of thermodynamic energy and enthalpy when P V T changes, phase changes or during the chemical change process.

Chapter 3 The Second Law of Thermodynamics

Comprehend the descriptions and mathematical representations of the second and the third law of thermodynamics. Master the definitions of entropy, Gibbs function, Helmholz function, standard entropy and standard Gibbs function of formation and their applications. Master the calculation principles and methods of variation of entropy, Gibbs function, Helmholz function when P V T changes, phase changes or during the chemical change process. Comprehend the fundamental equation of thermodynamics and the derivation of Maxwell relation master the applicability of thermodynamic formula and general criterion of the principle of entropy increase and equilibrium.

Mayor Contents:

3.1 Common features of spontaneous variation

3.2 The second law of thermodynamics

3.3 Carnot cycle and Carnot theorem

3.4 Conception of entropy

3.5 Clausius inequality and principle of entropy increase

3.6 Calculation of entropy change

3.7 Essence of the second law of thermodynamics and statistic significance of entropy

3.8 Helmholz free energy and Gibbs free energy

3.9 Variation direction and equilibrium condition

3.10 Calculating demonstration of ΔG

3.11 Relation of thermodynamic functions

3.12 Clapeyron equation

3.13 The third law of thermodynamics and conventional entropy

Key Points:

1. Description and mathematical representation of the second law of thermodynamics
2. Definitions of entropy, Gibbs function, Helmholz function, standard entropy and standard Gibbs function of formation and their applications.
3. Calculation principles and methods of variation of entropy, Gibbs function, Helmholz function when P V T changes, phase changes or during the chemical change process.
4. Master the applicability of thermodynamic formula and general criterion of the principle of entropy increase and equilibrium.
5. Clapeyron equation and Clapeyron-Clausius equation and related calculations

Nodus:

1. Definitions of entropy, Gibbs function, Helmholz function, standard entropy and standard Gibbs function of formation and their applications.
2. Calculation principles and methods of functions in all states when P V T changes, phase changes or during the chemical change process.
3. General criterion of the principle of entropy increase and equilibrium.
4. Clapeyron equation and Clapeyron-Clausius equation

Chapter 4 Thermodynamics for multi-component system

Comprehend the conceptions of partial molar quantity and chemical potential, comprehend Raoult's law and Henry's law and related calculations. Comprehend the expressions of componental chemical potential in ideal system (ideal solution and ideal dilute solution). Master the colligative property of dilute solution, comprehend the conceptions of activity and activity coefficient and simple calculations of activity (fugacity).

Mayor Contents:

4.1 Introduction

4.2 Expression of solution composition

4.3 Partial molar quantity and chemical potential

4.4 Two empirical laws of dilute solution

4.5 Chemical potential of components in gas mixture

4.6 Chemical potential of components in dilute solution

4.7 Colligative coefficient of dilute solution

Key Points:

1. Conceptions of partial molar quantity and chemical potential
2. Raoult's law and Henry's law and related calculations
3. Expressions of componental chemical potential in ideal system (ideal solution and ideal dilute solution)
4. Colligative coefficient of dilute solution

Nodus:

1. Conceptions of partial molar quantity and chemical potential
2. Raoult's law and Henry's law
3. Conceptions of activity and activity coefficient and simple calculations of activity (fugacity)
4. Expressions of chemical potential of components

Chapter 5 Chemical equilibrium

Master the definition of standard constant. Comprehend the derivations of isothermal and isobaric equations in chemical reaction and their applications. Learn to calculate equilibrium constant and equilibrium composition by thermodynamic data. Learn to identify the possible reaction direction in certain conditions. Learn to analyze the effects of temperature, pressure, composition, etc. on equilibrium.

Mayor Contents:

5.1 Chemical equilibrium condition and compatible potential

5.2 Equilibrium constant and isothermal function of chemical reaction

5.3 Relation of equilibrium constant and chemical equation

5.4 Heterogeneous chemical equilibrium

5.5 Determination of equilibrium constant and calculation of equilibrium rate of conversion

5.6 Standard Gibbs free energy of formation

5.7 Calculation of equilibrium constant by partition function

5.8 Effects of temperature, pressure and inert gas on chemical equilibrium

5.9 Synchronous equilibrium

Key Points:

1. Definition of standard constant

2. Equilibrium constant and isothermal function of chemical reaction
3. Calculate equilibrium constant and equilibrium composition by thermodynamic data
4. Identify the possible reaction direction in certain conditions
5. Effects of temperature, pressure, composition, etc. on equilibrium
Nodus:
1. Calculate equilibrium constant and equilibrium composition by thermodynamic data
2. Synchronous equilibrium and related calculations

Chapter 6 Phase equilibrium

Comprehend the significance of phase rule and its applications and derivation. Master the features and applications of typical phase diagram of single-component and binary systems. Perform analysis and calculation by lever rule and comprehend the plotting method of phase diagram by experimental data.

Mayor Contents:
6.1 Introduction
6.2 Phase rule
6.3 Phase diagram of single component system
6.4 Phase diagram of binary system and its applications
Key Points:
1. Comprehend the significance of phase rule and its applications
2. Features and applications of typical phase diagram of single-component and binary systems
3. Analytical and calculation methods by lever rule
4. Plotting methods of phase diagram by experimental data
Nodus:
1. Significance of phase rule and its applications
2. Features and applications of typical phase diagram of binary systems
3. Analytical and calculation methods by lever rule

Chapter 7 Electrochemistry

Comprehend the physical quantities which represent the electric conductive characters of electrolytical solution (electrolytic conductivity, molar conductivity, ionic mobility, transport number), comprehend the definitions of ionic mean activity and mean activity coefficient. Comprehend the definition of ionic strength. Comprehend the conception of ionic atmosphere and Debye-Hukel limit formula. Comprehend the conception of reversible cell, master Nernst equation and the calculations and applications of cell electromotive force. Comprehend the conceptions of polarization and overpotential.

Mayor Contents:
7.1 Basic conception of electrochemistry and Faraday’s law
7.2 Ionic electromigration and transport number

7.3 Electric conductance
7.4 Theoretical introduction of strong electrolytical solution
7.5 Reversible cell
7.6 Determination of electromotive force
7.7 Writing method of reversible cell and sign of electromotive force
7.8 Thermodynamics of reversible cell
7.9 The mechanism of electromotive force production
7.10 Electrode potential and cell electromotive force
7.11 Concentration cell and contact potential
7.12 Applications of electromotive force measurement
7.13 Electrolyzation and polarization

Key Points:

1. Physical quantities which represent the electric conductive characters of electrolytical solution
2. Conception of reversible cell
3. Nernst equation and related calculations
4. Calculations and applications of cell electromotive force

Nodus:

1. Definitions of ionic mean activity and mean activity coefficient
2. Polarization and conception of overpotential
3. Concentration cell and related calculations

Chapter 8 Basic statistic thermodynamics

Comprehend the basic hypothesis of statistic thermodynamics and the significance and applications of Boltzmann distribution. Master the significance of partition function and the relations of partition function and thermodynamic function

Mayor Contents:

8.1 Introduction
8.2 Boltzmann statistic
8.3 Partition function
8.4 Calculations of partition functions
8.5 Contributions of partition functions to thermodynamic function
8.6 Calculations of monatomic perfect gas thermodynamic functions

Key Points:

1. Basic hypothesis of statistic thermodynamics
2. Significance and applications of Boltzmann distribution
3. Significance of partition function
4. Relations of partition function and thermodynamic function

Nodus:

1. Significance and applications of Boltzmann distribution
2. Calculations of partition function
3. Relations of partition function and thermodynamic function and related calculations

Chapter 9 Interfacial phenomenon

Comprehend the conceptions of surface tension and surface Gibbs function and the relations of contact angle wetting and spreading. Comprehend the effects of flexural liquid lever on thermodynamic properties and Laplace formula and the applications of Kelvin formula. Comprehend the relations of metastable state and new phase production. Comprehend the adsorption of solution interface and the effects of surfactant. Comprehend the significance and applications of Gibbs adsorption formula. Comprehend the significance and differences of physisorption and chemisorption. Comprehend Langmuir monolayer adsorption theory and adsorption isothermal formula.

Main contents:

9.1 Surface Gibbs free energy and surface tension

9.2 Additional pressure and vapor pressure of flexural liquid lever

9.3 Properties of liquid interface

9.4 Liquid-solid interfacial phenomenon

9.5 Adsorption of solid surface

9.6 Surfactant and its effects

Key Points:

1. Conceptions of surface tension and surface Gibbs function and the relations of contact angle wetting and spreading
2. Effects of flexural liquid lever on thermodynamic properties and Laplace formula and the applications of Kelvin formula
3. Adsorption of solution interface
4. Langmuir monolayer adsorption theory and isothermal formula

Nodus:

1. Effects of flexural liquid lever on thermodynamic properties and Laplace formula and the applications of Kelvin formula
2. Relations of metastable state and new phase production
3. Langmuir monolayer adsorption theory and isothermal formula and multilayer adsorption theory

Chapter 10 Basic chemical kinetics

Comprehend the conceptions of chemical reaction rate, reaction rate constant and reaction order. Master the methods to establish rate equations by experiments and the rate equations of first order and second order reactions and their applications. Comprehend the characters of typical complex reactions. Comprehend the kinetic methods dealing with opposing reaction, parallel reaction and consecutive reaction. Comprehend the conceptions of elementary reaction and molecularity of reaction. Comprehend the conceptions of steady state approximation, equilibrium approximation and control process and the kinetic features of chain reaction.

Mayor Contents:

10.1 Assignment and purpose of chemical kinetics

10.2 Expression of chemical reaction rate

10.3 Rate equation of chemical reaction

10.4 Reactions with simple orders
10.5 Some typical complex reactions
10.6 Effects of temperature on reaction rate
10.7 Effects of activation energy on reaction rate
10.8 Chain reaction
10.9 General methods to draft reaction mechanism
Key Points:
1. Conceptions of chemical reaction rate, reaction rate constant and reaction order
2. Rate equations of first order and second order reactions and their applications
3. Characters of typical complex reactions., comprehend the kinetic methods dealing with opposing reaction, parallel reaction and consecutive reaction.
4. Significance of Arrhenius equation and its applications
Nodus:
1. Methods to establish rate equations by experiments
2. Conceptions of steady state approximation, equilibrium approximation and control process and their applications
3. Features of complex reactions and related calculations

Chapter 11 Dynamics of special reaction

Comprehend the necessary process of multi phase reaction. Comprehend catalysis and the definitions of activation energy and pre-exponential factor. Comprehend the basic theory of elementary reaction rate. Comprehend the basic formulas of effective collision theory and transition state theory and related conceptions.
Mayor Contents:
11.1 Collision theory
11.2 Transition state theory
11.3 Unimolecular reaction theory
11.4 Photochemistry reaction
11.5 Catalytic reaction kinetics
Key Points:
1. Basic theory of elementary reaction rate
2. Basic formulas of effective collision theory and transition state theory and related conceptions.
3. Necessary process of multi phase reaction
4. Catalytic reaction kinetics
Nodus:
1. Basic theory of elementary reaction rate
2. Basic formulas of effective collision theory and transition state theory and related conceptions.

Chapter 12 Collochemistry

Comprehend the classification of disperse system and the definition of colloid.

Comprehend the reasons for colloid stabilization and destruction. Comprehend the classification and stabilization of emulsion.

Mayor Contents:

12.1 Preparation of colloid system
12.2 Optical properties of colloid system
12.3 Dynamic properties of colloid system
12.4 Electrical properties of colloidal sol system
12.5 Stabilization and coagulation of colloidal sol
12.6 Suspension and emulsion:

Key Points:

1. Classification of disperse system and definition of colloid
2. Optical and dynamic properties of colloid system
3. Classification and stabilization of emulsion

Nodus:

1. Optical and dynamic properties of colloid system
2. Electrical properties of colloidal sol system

The distribution of experimental hours: total 102. The distribution is listed as below:

SN	Teaching contents	Hours
1	Gas	4
2	The first law of thermodynamics	12
3	The second law of thermodynamics	12
4	Thermodynamics of multi-component system	8
5	Chemical equilibrium	8
6	Phase equilibrium	8
7	Electrochemistry	12
8	Statistic thermodynamics	8
9	Interfacial phenomenon	8
10	Chemical kinetics	12
11	Dynamics of special reaction	4
12	Collochemistry	6

D. Arrangement and Examination Methods for Teaching Segment

a. Classroom Lecturing

(1). Lecturing: Systematical lecturing shall be carried out for the part of basic theory of this course.

Great attentions shall be paid to the systematicness of contents and strictness of logic. Teachers shall impart correct concepts, give prominence to key points, write clearly, distinguish arrangement and consecution, inherit the past and usher in the future, and introduce the cases of scientific researches and engineering in practical use.

(2). The aim of exercise class is to improve students' understanding toward basic concepts and enhance practical ability of basic theory. Therefore, the selection of exercises shall be refined and have a strong aim. Great attentions shall be paid to lead and enlighten students' thinking and put forward discussions to cultivate students' ability of analyzing and resolving problems.

(3). Tutorship: We recommend that you arrange for time of answering problems, mainly through internet and after class.

(4). Teaching methods: Specific teaching form shall be determined by teachers, in conformity with teaching contents, teaching objects, teaching conditions and corresponding teaching experiences. In principle, we recommend that you adopt the form of combination between CAI courseware and blackboard class and use the teaching methods of problem teaching and project teaching reasonably.

Teachers shall impart knowledge and educate students, carry out strict requirements on students in all sectors, and train students' learning targets and style of study with combination of learning the course.

b. Exercise Requirements and Quantities

One of key factors for students to learn the course of physical chemistry well is to fulfill exercise independently in time. Teachers shall supervise and urge students to pay great attention to exercises and require students to review and understand lecturing contents well in advance before exercises, so that targets of lecturing will be consolidated.

(1). Requirements on students: To hand on exercise in time. Suitable ways of criticism shall be implemented on those who hand on exercises later, do not hand on exercise or plagiarize.

(2). Requirements on teachers:

Teachers shall comment on and correct every exercise and record the results as one of bases for scoring regular grades in the end of the term.

(3). Exercise quantities:

The exercise quantities shall be suitable; that is, 3 to 5 subjects will be allocated for every two class hours.

c. Examination Methods

(1). This course is a examination course, so closed-book exam shall be carried out in final examination.

(2). Questions shall be formulated unifiedly according to test question database in final examination.

(3). Grade in final examination shall account for a main factor of 80% of overall grade; while test grade in normal times (including exercise and learning status) shall account for 20%.

E. Recommended Teaching Materials and Bibliographies

1. Recommended teaching materials: *Physical Chemistry*, the fourth edition, edited by Tianjin University
2. Bibliographies: *Physical Chemistry*, edited by Fu Xiancai of Nanjing University
   Simple Physical Chemistry, edited by Yin Yongjia
   500 Cases for Physical Chemistry, edited by Li Guozhen