FIRST SEMESTER 2023-2024

Course Handout (Part - II)

Date: 11/08/2023

In addition to part-I (General Handout for all courses appended to the time table) this portion gives further specific details regarding the course.

Course No. : **CHEM F312**

Course Title : **Physical Chemistry IV**

Instructor-in-charge : **Dr. Amit Nag**

1. Scope and Objective of the Course: The course provides a comprehensive survey of the concepts involved in the study of forces responsible for interaction between molecules, and its effect on the transport properties of matter like diffusion, viscosity etc. The course will also cover physical properties of colloids and micelles. Surface phenomenon like adsorption and adsorption isotherms would be discussed. Rates of chemical reactions, theories of reaction rates and statistical thermodynamics would be covered.

2. Text Books :

T1. **I. N. Levine, "Physical Chemistry",** 5th Edition, Tata McGraw-Hill, 2011.

3. Reference Books :

R1. P.W. Atkins & Julio de Paula, **"Atkins' Physical Chemistry",** Ninth edition (Oxford University Press, Oxford 2010).

4. Course Plan :

Lecture No.	**Topics to be covered**	**Learning Objectives**	**Chapter in the Text Book**
1-3	Weak forces	Electric dipole moment, Polarization, Interaction between dipoles, Interaction between induced dipoles, Hydrogen bonding, Total attractive and repulsive interactions	**T1**: 14.15, 22.10 **13.14, 21.10 (6th)** **R1**:17.1 - 17.6
4-5	Surface Chemistry	Molecular interactions in gases, Liquid-vapour interface, surface films, Thermodynamics of surface layers	**T1**: 13.1-13.4 **7.6 - 7.8 (6th)** **R1**: 17.7 – 17.10
6-7	Colloids, micelles, and reverse micellar structures	Classification, Preparation, Structure & stability of colloids, Micelle formation, Reverse micellar structures, bilayers, Determination of size & shape	**T1**: 13.6 **7.9 (6th)** **R1**: 18.6 – 18.9 (b)
8-10	Transport processes	Kinetics, viscosity, diffusion, sedimentation, electrical conductivity of solids and electrolyte solutions	**T1**: 16.1 – 16.7
Self	Rates of chemical	Definition of rate, derivation of	**T1**: 17.1 –

Study	reactions and analysis of kinetic data of simple reactions	concentration time relationship for simple reactions, Determination of rate law, Half-life of reactions	17.4
11-13	Elementary reactions, Complex reactions	Reactions approaching equilibrium, Elementary reactions, consecutive reactions, steady-state approximation, rate determining step, rate constants and equilibrium constants	**T1**: 17.5 – 17.6, 17.9
14	Effect of temperatures on reaction rates, rate law in non-ideal systems	To get an insight about the activation energy	**T1**: 17.8, 17.10
15-17	Rate laws and reaction mechanisms	Unimolecular reactions, bimolecular reactions, Lindemann-Hinshelwood mechanism	**T1**: 17.11 – 17.12
18	Chain reactions	Polymerization kinetics, chain polymerization reactions	**T1**: 17.13
19-20	Fast reaction kinetics, reactions in solutions, diffusion-controlled reactions	Techniques to study the reaction at extreme rate, reaction rates in solution and diffusion controlled reactions	**T1**: 17.14 – 17.15
21-22	Homogeneous catalysis	Details of enzyme catalysis, Michaelis-Menton equation	**T1**: 17.16 – 17.17
23-24	Adsorption of gases on solids	Extent of adsorption, Physisorption and chemisorptions, Adsorption isotherms	**T1:** 13.5 **16.18 (6th)**
25-26	Heterogeneous catalysis	Extent of adsorption, rates of surface processes	**T1**: 17.18
27-33	Statistical Thermodynamics	Partition function, thermodynamic information from canonical partition function, molecular partition function, equilibrium constants	**T1**: 22.2 – 22.4, 22.6 – 22.8
34-36	Theories of reaction rates	Theoretical description of reaction rates: CT and TST	**T1**: 23.1-23.2, 23.4-23.6
37-38	Reactions in solution	Extending the gas phase theories to the solution phase	**T1**: 23.8 (b)
39-40	Molecular reaction Dynamics	Reaction trajectory	**T1**: 23.3

5. Evaluation Scheme:

Component	Duration	Weightage%	Date & Time	Nature of Component
Mid semester Test	1.5 hrs	35%	10/10 - 11.30 - 1.00PM	Closed Book
Class Tests*	Will be announced in the class	10%	Evenly spaced throughout the Semester	Open Book
Lab	Will be	10%	Will be announced in	Open Book

experiments #	announced in the class		the class	
Comprehensive Examination	3 hrs	45%	08/12 AN	Closed Book

Tutorials: The tutorial hour will be used for a quick review of the highlights of the material covered in the lectures, clarification of doubts, and problem solving.

* There will be a total of six surprise tests, and the best four will be taken for evaluation.

Two Lab experiments will be conducted/demonstrated on few selected phenomena, discussed in the lecture class. Attendance is mandatory. Evaluation pattern will be announced in the class. **No makeup is permitted.**

6. **Chamber Consultation Hour**: Monday, 4 pm - 5 pm.
7. **Notices**: Notices, if any, concerning the course will be uploaded on the **course page on CMS or sent via email to all the students registered in the course**.
8. **Make-up-policy**: Make up would be considered only for **genuine reasons**.

9. **Academic Honesty and Integrity Policy**: Academic honesty and integrity are to be maintained by all the students throughout the semester and no type of academic dishonesty is acceptable.

Learning Outcomes (Lecture wise):

By the end of the course, the students should be able to:

Lectures 1-3: Describe the types of intermolecular forces possible between atoms or molecules in condensed phases (dispersion forces, dipole-dipole attractions, and hydrogen bonding).

Lectures 4-7: Identify the types of intermolecular forces experienced by specific molecules based on their structures. Would be able to understand the origin of interfacial properties like surface tension, adsorption and their applications. Would be able to classify systems based on the relative sizes of solute and solvent: solutions and colloidal systems, their characterization and properties like light scattering, concept of critical micelle concentration etc.

Lectures 8-10: Explain the relation between the intermolecular forces present within a substance and the activation barrier associated with the transport phenomena like viscosity, diffusion, conductivity etc.

Lectures 11-18: Model the kinetics of basic chemical reactions. Model the effect of temperature on reaction rates and transition probability: the collision theory and transition state theory. Modeling of unimolecular reactions and polymerization reactions.

Lectures 19-20: Understand experimental strategies to study rates of ultrafast reactions happening in pico- and/or femtosecond time scale. Model rates of diffusion controlled reactions as happening in electrochemical cells, discussion of diffusion control in electron-transfer reactions, Marcus theory and the presence of inverted parabola.

Lectures 21-22; 25-26: Model the kinetics of catalytic reactions, homogeneous, heterogeneous and enzyme catalysis.

Lectures 23-24: Understand the phenomenon of adsorption in general, generate adsorption isotherms and their experimental importance in characterization of interfaces.

Lectures 27-33: Find the origin of macroscopic thermodynamic observables in terms of statistical thermodynamics- partition functions.

Lectures 34-40: Consolidate and apply the concepts of rate theories to condensed phase reactions.

Lab experiments: Employ the theoretical concept learnt in the lecture class to gain practical knowledge.

Instructor-in-charge
CHEM F312