

FIRST SEMESTER 2022-2023 Course Handout (Part - II)

Date: 29/08/2022

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**Co-Instructor : **Dr. Balaji Gopalan**

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:

Lectu re 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 (6 th) 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 (6 th) 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	T1 : 16.1 – 16.7

		solids and electrolyte solutions	
Self Stud y	Rates of chemical reactions and analysis of kinetic data of simple reactions	Definition of rate, derivation of concentration time relationship for simple reactions, Determination of rate law, Half-life of reactions	T1 : 17.1 – 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
27-34	Statistical Thermodynamics	Partition function, thermodynamic information from canonical partition function, molecular partition function, equilibrium constants	T1 : 22.2 – 22.4, 22.6 – 22.8
35-37	Theories of reaction rates	Theoretical description of reaction rates: CT and TST	T1 : 23.1-23.2, 23.4-23.6
38-39	Reactions in solution	Extending the gas phase theories to the solution phase	T1 : 23.8 (b)
40-42	Molecular reaction Dynamics	Reaction trajectory	T1 : 23.3

5. Evaluation Scheme:

Component	Duratio	Weightage	Date Time	Nature of
Component	n	%	Dute Time	Component
Mid semester	1.5 hrs	35%	03/11 11.00 - 12.30PM	Closed Book
Test Class Tests &	TBA	20%	Evenly spaced throughout	Open Book
assignments			the	<u>.</u>

			Semester	
Comprehensiv	3 hrs	45%		Closed Book
e			24/12 AN	
Examination				

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.

- 6. **Chamber Consultation Hours**: To be announced later by the IC.
- 7. **Notices**: Notices, if any, concerning the course will be displayed on the **Chemistry Department Notice Board and course page on CMS**.
- 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.

^{*} There will be a total of 6 surprise tests, and the best 4 will be taken for evaluation.

Lectures 27-34: Find the origin of macroscopic thermodynamic observables in terms of statistical thermodynamics- partition functions.

Lectures 35-42: Consolidate and apply the concepts of rate theories to condensed phase reactions.

Instructor-in-charge CHEM F312