

## FIRST SEMESTER 2020-2021 Course Handout Part II

Date: 17/08/2020

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. Durba Roy** 

**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",** 5<sup>th</sup> 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:

LN	Topic	Learning Objectives	Text	
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 <sup>th</sup> ) R1:17.1 - 17.6	
4-5	Surface Chemistry	Molecular interactions in gases, Liquid-vapour interface, surface films, Thermodynamics of surface layers		
6-7	Colloids, micelles, and reverse micellar structures	Classification, Preparation, Structure & stability of colloids, Micelle formation, Reverse micellar structures, bilayers, Determination of size & shape	<b>T1</b> : 13.6 <b>7.9 (6<sup>th</sup>)</b> <b>R1</b> : 18.6 – 18.9 (b)	
8-10	Transport processes	Kinetics, viscosity, diffusion, sedimentation, electrical conductivity of solids and electrolyte solutions	<b>T1</b> : 16.1 – 16.7	
11-13	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, reactions approaching equilibrium	<b>T1</b> : 17.1 – 17.4	
14-16	Elementary reactions, Complex reactions	Elementary reactions, consecutive reactions, steady-state approximation, rate determining	<b>T1</b> : 17.5 – 17.6, 17.9	

		step, rate constants and equilibrium constants		
17	Effect of temperatures on reaction rates, rate law in non-ideal systems	To get an insight about the activation energy  T1: 17.8, 17		
18 –20	Rate laws and reaction mechanisms	Unimolecular reactions, bimolecular reactions, Lindemann-Hinshelwood mechanism	<b>T1</b> : 17.11 – 17.12	
21	Chain reactions	Polymerization kinetics, chain polymerization reactions	<b>T1</b> : 17.13	
22-23	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	<b>T1</b> : 17.14 – 17.15	
24-25	Homogeneous catalysis	Details of enzyme catalysis, Michaelis-Menton equation	<b>T1</b> : 17.16 – 17.17	
26-28	Adsorption of gases on solids	Extent of adsorption, Physisorption and chemisorptions, Adsorption isotherms	T1: 13.5 16.18 (6 <sup>th</sup> )	
29-31	Heterogeneous catalysis	Extent of adsorption, rates of surface processes	<b>T1</b> : 17.18	
32-37	Statistical Thermodynamics	Partition function, thermodynamic information from canonical partition function, molecular partition function, equilibrium cosntants	<b>T1</b> : 22.2 – 22.4, 22.6 – 22.8	
38-39	Theories of reaction rates	Theoretical description of reaction rates: CT and TST	<b>T1</b> : 23.1-23.2, 23.4-23.6	
40	Reactions in solution	Extending the gas phase theories to the solution phase	<b>T1</b> : 23.8 (b)	
41-42	Molecular reaction Dynamics	Reaction trajectory	<b>T1</b> : 23.3	

# 5. Evaluation Scheme:

Component	Duration(min )	Weightage%	Date Time	Remarks
Test1	30	15%	September 10 –September 20 (During scheduled class hour)	Open Book
Test2	30	15%	October 09 –October 20 (During scheduled class hour)	Open Book
Test3	30	15%	November 10 – November 20 (During scheduled class hour)	Open Book
Assignments*	TBA	20%	Evenly spaced throughout the Semester (To be completed by November 20)	Open Book
Comprehensive Examination	120	35%	ТВА	Open 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.

- \* The nature and title of the assignments will be announced by I/C during the class.
- 6. **Chamber Consultation Hours**: Monday, 11 am to 11:50 am.
- 7. **Notices**: Notices, if any, concerning the course will be displayed on the **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:**

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

- 1. Describe the types of intermolecular forces possible between atoms or molecules in condensed phases (dispersion forces, dipole-dipole attractions, and hydrogen bonding).
- 2. Identify the types of intermolecular forces experienced by specific molecules based on their structures.
- 3. 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.
- 4. Model the kinetics of chemical reactions including ultrafast processes, catalytic reactions, heterogeneous and enzyme catalysis.
- 5. Model the effect of temperature on reaction rates: the collision theory and transition state theory.
- 6. Find the origin of macroscopic thermodynamic observables in terms of statistical thermodynamics- partition functions.
- 7. Consolidate and apply the concepts of rate theories to condensed phase reactions.

Instructor-in-charge CHEM F312

