**BIRLA INSTITUTE OF TECHNOLOGY & SCIENCE, PILANI**
**HYDERABAD CAMPUS**
FIRST SEMESTER 2021-2022
**Course Handout (Part - II)**

**Date: 20/08/2021**

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",** 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 |
| 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 | **T1**: 17.1 – 17.4 |
| 14-16 | Elementary reactions, Complex | Elementary reactions, consecutive reactions, steady-state approximation, | **T1**: 17.5 – 17.6, 17.9 |

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|---|---|---|---|
| | reactions | rate determining 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, 17.10 |
| 18 – 20 | Rate laws and reaction mechanisms | Unimolecular reactions, bimolecular reactions, Lindemann-Hinshelwood mechanism | **T1**: 17.11 – 17.12 |
| 21 | Chain reactions | Polymerization kinetics, chain polymerization reactions | **T1**: 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 | **T1**: 17.14 – 17.15 |
| 24-25 | Homogeneous catalysis | Details of enzyme catalysis, Michaelis-Menton equation | **T1**: 17.16 – 17.17 |
| 26-28 | Adsorption of gases on solids | Extent of adsorption, Physisorption and chemisorptions, Adsorption isotherms | **T1:** 13.5 **16.18 (6th)** |
| 29-31 | Heterogeneous catalysis | Extent of adsorption, rates of surface processes | **T1**: 17.18 |
| 32-37 | Statistical Thermodynamics | Partition function, thermodynamic information from canonical partition function, molecular partition function, equilibrium cosntants | **T1**: 22.2 – 22.4, 22.6 – 22.8 |
| 38-39 | Theories of reaction rates | Theoretical description of reaction rates: CT and TST | **T1**: 23.1-23.2, 23.4-23.6 |
| 40 | Reactions in solution | Extending the gas phase theories to the solution phase | **T1**: 23.8 (b) |
| 41-42 | Molecular reaction Dynamics | Reaction trajectory | **T1**: 23.3 |

## 5. Evaluation Scheme:

| Component | Duration | Weightage % | Date Time | Nature of Component |
|---|---|---|---|---|
| Midsemester Test | 1.5 hrs | 35% | 19/10/2021 9.00 - 10.30AM | Open Book |
| Assignments* | TBA | 25% | Evenly spaced throughout the Semester (To be completed by November) | Open Book |
| Comprehensive Examination | 2 hrs | 40% | 14/12 FN | 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 (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 11-21:** 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 22-23:** 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 24-25; 29-31:** Model the kinetics of catalytic reactions, homogeneous, heterogeneous and enzyme catalysis.

**Lectures 26-28:** Understand the phenomenon of adsorption in general, generate adsorption isotherms and their experimental importance in characterization of interfaces.

**Lectures 32-37:** Find the origin of macroscopic thermodynamic observables in terms of statistical thermodynamics- partition functions.

**Lectures 38-42:** Consolidate and apply the concepts of rate theories to condensed phase reactions.

**Instructor-in-charge**
CHEM F312