

BIRLA INSTITUTE OF TECHNOLOGY & SCIENCE, PILANI
HYDERABAD CAMPUS
Second Semester 2019-2020
Course Handout (Part - II)

Date: 06/01/2020

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 G553**
Course Title : **Advanced Physical Chemistry**
Instructor-in-charge : **K. Sumithra**
Instructors : **K. Sumithra, Subit Kumar Saha**

Course Description: Equilibrium: The laws of Thermodynamics, applications to phase equilibrium, reaction equilibrium, and electrochemistry; Structure: Principles and techniques of quantum mechanics, applications to atomic and molecular structure and spectroscopy, statistical thermodynamics, molecular interactions, macromolecules, solid state; Dynamics: Molecular motion in gases and liquids, reaction rate laws, mechanisms and rate theories of complex reactions, molecular reaction dynamics, surface processes, electron transfer dynamics.

1. Scope and Objective of the Course: The course is concerned with the advanced/next level understanding of physical chemistry for the students of post post-graduate level, currently pursuing PhD. It includes chemical thermodynamics and its applications to solutions, phase and chemical equilibria and electrochemical systems. Emphasis is given on the structure elucidation of materials in atomic and molecular level using concepts of quantum mechanics and spectroscopy. 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. (i) Text Book 1 (TB1): ‘Atkins Physical Chemistry’, P. W. Atkins & Julio de Paula, 8th and 9th editions (Oxford University Press 2009 & 2010, respectively).

(ii) Text Book 2 (TB2): ‘Physical Chemistry’, Ira N. Levine, Fifth Edition, Special Indian Edition (Tata McGraw-Hill, 2002).

3. Reference Book:

‘Physical Chemistry’, David W. Ball, First Edition, India Edition (Thomson, 2007).

4. Course Plan:

L N	Topic	Text
1- 4	Quantum theory and atomic structure	TB1 Ch 8 & 9
5-8	Chemical Bonding: Valence Bond and Molecular Orbital Theories	TB1 Ch 11
9-11	Vibrational and electronic transitions	TB1 Ch 13
12-14	Magnetic Resonance-NMR	TB1 Ch 15

15-17	Statistical Thermodynamics: Basics of Partition functions, Maxwell Boltzmann distribution and Molecular partition function for an ideal gas, translational, rotational, vibrational	TB1 Ch 16 & 17
18-21	Chemical Kinetics: Experimental Methods,-Stopped flow methods, Reaction rates, Arrhenius equation, steady state approximations	TB1 Ch 22
22 – 23	Thermodynamic systems, states, properties, equations of state, First Law of Thermodynamics	TB2 Ch 1&2; TB1 Ch 2
24-25	Thermochemistry, Hess law, Kirchhoff law, Change of enthalpy, Change of internal energy	TB2 Ch 5; TB1 Ch2
26-29	Second Law of Thermodynamics, Entropy, Gibbs Energy	TB2 Ch 3&4; TB1 Ch3
30 –32	Phase Equilibria of Pure Substances: Gibbs phase Rule, Phase Diagrams, Clausius-Clapeyron Equation	TB2 Ch 7, TB1 Ch 4
33-36	Mixtures: Thermodynamic description, Phase equilibrium, Reaction equilibria, Partial molar properties, Ideal, Ideally dilute and Non-ideal solutions, Activity coefficients	TB2 Ch4, Ch6, Ch9 &10
37-38	Colligative properties, Two-component phase equilibria, Lever rule	TB2 Ch12
39-40	Electrochemistry: Processes at electrodes	TB2 Ch 14
41-42	Adsorption phenomena, Langmuir and BET Isotherms, Rates of surface processes, Catalysis	TB1 Ch23

5. Evaluation Scheme:

Component	Duration	Weightage (%)	Date and Time	Nature of component
Mid-Sem Test	1.5 hrs	20	4/3 9 to 10:30 AM	Closed Book
Assignments (open book)	-	40	Continuous	Open Book [#]
Comprehensive Examination	3 hrs	40	06/05 AN	Closed Book and 50% Open Book

[#]Assignments can be problem solving/presentation/tests.

6. **Chamber Consultation Hours:** To be announced through a notice.

7. **Notices:** Notices, if any, concerning the course will be displayed on the **Chemistry Group Notice Board Only**.

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.

K. Sumithra
Instructor-in-charge
CHEM G553