

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

Date: 01/8/2018

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 : **Durba Roy**

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 will touch upon concepts of 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. It further includes chemical thermodynamics and its applications to solutions, equilibrium 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. Text Book: ‘Atkins Physical Chemistry’, P. W. Atkins & Julio de Paula, 8th edition (Oxford University Press 2009).

3. Reference Books:

1. ‘Physical Chemistry’, David W. Ball, First Edition, India Edition (Thomson, 2007).
2. ‘Physical Chemistry’, Ira N. Levine, Fifth Edition, Special Indian Edition (Tata McGraw-Hill, 2002).

4. Course Plan:

L N	Topic	Text
1 – 3	First Law of Thermodynamics	TB Ch 2
4-6	Thermochemistry, Hess law, Kirchhoff law, Change of enthalpy, Change of internal energy	TB Ch 2

7-10	Thermodynamics: The Second Law, Entropy, Gibbs Energy	TB Ch 3
11 –14	Phase Equilibria: Pure Substances, Phase, components, Gibbs phase Rule and Phase Diagrams	TB Ch 6
15-17	Mixtures: Thermodynamic description, Phase equilibrium, chemical equilibria	TB Ch 7
18-20	Electrochemistry: Processes at electrodes	TB Ch 25
21-24	Quantum theory and atomic structure	TB Ch 8 & 9
25-28	Chemical Bonding: Valence Bond and Molecular Orbital Theories	TB Ch 11
29-31	Vibrational and electronic transitions	TB Ch 13
32-34	Magnetic Resonance-NMR	TB Ch 15
35-37	Statistical Thermodynamics: Basics of Partition functions, Maxwell Boltzmann distribution and Molecular partition function for an ideal gas, translational, rotational, vibrational	TB Ch 16 & 17
38-40	Chemical Kinetics: Experimental Methods,- Stopped flow methods, Reaction rates, Arrhenius equation, steady state approximations	TB Ch 22

5. Evaluation Scheme:

Component	Duration	Weightage (%)	Date and Time	Nature of component
Midsem	1.5 hrs	25	-	Closed Book
Class Tests(open book)	-	40	Continuous	Open Book [#]
Comprehensive Examination	3 hrs	35	-	Closed Book

[#]Assignments can be problem solving or presentation.

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**.

Durba Roy
Instructor-in-charge
CHEM G553