Birla Institute of Technology & Science, Pilani
Hyderabad Campus

SECOND SEMESTER 2024-2025

Course Handout (Part - II)

Date: 06-01-2025

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 F111**
Course Title : **General Chemistry**
Instructor-in-charge : **Prof. Subit K Saha**
Instructors : **Profs. Subit K Saha, Nilanjan Dey, Amit Nag, Abhishek Saha, Arijit Mukherjee, Balaji Gopalan, Pralok Kumar Samanta, Sourav Bag, Suryoday Prodhan**

1. Scope and Objective of the Course: This course highlights the comprehensive study of the electronic structure of atoms, molecules, and chemical reactions via the introduction of quantum chemistry, molecular spectroscopy, thermodynamics, chemical equilibrium, and chemical kinetics as a part of general physical chemistry. It also provides a comprehensive survey of the concepts involved in the study of conformations, stereochemistry, reaction mechanisms, electrocyclic reactions, and coordination chemistry as a part of organic and inorganic chemistry.

2. Text Books:
T1: P.W. Atkins & Julio de Paula, '**The Elements of Physical Chemistry',** Fifth/International edition (Oxford University Press, 2017).
T2: T. W. Graham Solomons and Craig B. Fryhle, '**Organic Chemistry'**, 10th Edition, John Wiley & Sons, Inc. New York, 2011.
T3: J. D. Lee, '**Concise Inorganic Chemistry'**, 5th Edition, Blackwell Science, Oxford, 1999.

3. Reference Books:
R1: L. G. Wade, Jr. and M. S. Singh, **'Organic Chemistry'**, 6th Edition, Pearson Education Inc., 2006.
R2: D. W. Ball, **'Physical Chemistry',** First Edition, India Edition (Thomson, 2007).
Additional materials include lecture slides and tutorial class notes.

4. Course Plan (SS stands for 'self study'):
Note: The sections of the Chapters in the **T1** are given below based on **the 5th Edition (and international edition in bracket) of P.W. Atkins & Julio de Paula.**

Lec. No.	Learning Objectives	Topics to be Covered	Learning Outcomes of the Lectures	Chapter in the Text Book

1-3	Quantum Theory	Origin of quantum mechanics; Black body radiation, Wavefunction, Uncertainty principle, Schrodinger equation - Simple Applications	Discuss historical developments and the role of quantum theory. Understand the importance of quantization through simple model systems.	**T1** 12.1-12.7, 12.9 **(7A, 7B, 7C, 7E)**
4-10	Atomic Structure and Spectra	Hydrogenic Atoms: Energy levels and Wavefunctions, Orbitals, spectral transitions, many-electron atoms: orbital approximation, Pauli principle, Aufbau principle, term symbols, (simple systems only), selection rule	Identify the atomic orbital picture of H-atom from quantum mechanics; spin orbit coupling and atomic term symbols. Identify spin as another coordinate.	**T1** 13.1-13.11, 13.17-13.19. **(8A, 8B, 8D)** 13.15-13.16 **(8C)**
11-13	Chemical Bonding: Valence Bond and Molecular Orbital Theories	VB Theory: electron pair bond, hybridization, resonance, MO theory: LCAO, bonding and antibonding orbitals, homonuclear and heteronuclear diatomic molecules. ***Lewis theory and VSEPR model (self-study)***	Demonstrate successful description of chemical bond; examine the application of molecular orbital theory to diatomic molecules.	**T1** 14.1-14.14 **(9A, 9B, 9C)**
14	Thermodynamics: the First Law, Internal Energy and Enthalpy	Thermodynamic systems, state functions, thermal equilibrium and temperature, work, internal energy and heat transfer, heat capacity.	Comprehend the concept of energy transormations and the role of temperature and pressure on thermodynamic functions.	**T1** 2.1-2.9 **(2A, 2B, 2C, 2D)**
15-16	Thermodynamics: the Second Law, Entropy, Gibbs Energy	Natural and reversible processes, entropy and second Law, Calculation of entropy changes, absolute entropies, Gibbs energy.	Understand the direction of spontaneous changes. Evaluate the entropy changes with various physical processes. Molecular disorder/statistical entropy, Third law and residual entropy. Spontaneity of a process in a closed system - concept of Gibbs free energy.	**T1** 4.1-4.13 **(3A, 3B, 3C, 3D)**
17	Spontaneity and Equilibrium	Applications of entropy and Gibbs free energy in chemical reactions	The variation of Gibbs free energy with pressure and temperature. Predict the spontaneity of a reaction, Role of temperature on the spontaneity of physical & chemical changes. Relate and apply concept of chemical equilibrium and response of chemical equilibria to temperature and pressure.	**T1** 5.1 – 5.3, 7.1-7.4 **(4A, 5A)** 7.5-7.6, 7.8 **(5B, 5C) (SS)**

18 (partial portion is S.S.)	Chemical Kinetics: Experimental Methods, Reaction Rates, Temperature Dependence	*Rate laws, order, rate constants, Arrhenius equation; rate-determining step, reaction mechanisms*; steady-state approximation. **(except the steady-state approximation, remaining portions are self-study).**	Effect of temperature on the rates of reaction. Understanding reaction mechanisms involving elementary reactions. Formulation of rate laws with steady state approximation..	**T1** 10.1-10.9, **T1** 11.4-11.7 **(6A, 6B, 6C, 6D-1, 6F)**
19-21	Vibrational and Electronic Spectroscopy	General features, vibrational energy levels and spectra; electronic spectra: Franck-Condon principle, types of transitions	Relating the interaction of IR, UV-Vis radiations and molecules, vibrational frequency and transitions. Detailed understanding of vibrational and electronic spectra of small molecules, Electronic transition probabilities and Franck-Condon principle.	**T1** 12.9, 19.6 – 19.8; 19.11; 20.1 – 20.4 **(7E, 13A, 13C.1-13C.3, 13C.5, 13D)** **T3:** 2.15 – 2.16
22-25	Nuclear Magnetic Resonance Spectroscopy	Principles, chemical shift, fine structure, applications (identification of organic compounds).	Understand the basic principles and techniques of nuclear magnetic resonance spectroscopy and identification of organic molecules.	**T1** 21.1 – 21.4 **(14A, 14B.1-14B.2)** **T2:** 9.1-9.8
26-27	Conformations	Rotation around sigma bonds, conformational analysis of butane, cyclohexane, and substituted cyclohexanes.	Classify structural and constitutional isomers. Understand conformations and explain torsional energy, torsional strain, and angle strain. Judge the stabilities of various conformations and identify cis and trans relationships for the substituents on cyclohexanes. Draw chair forms of cyclohexane with unambiguous representations of axial and equatorial substituents and the reason for the stability between the two isomers.	**T2:** 4.8-4.9, 4.10 **(SS)**, 4.11-4.14
28-29	Stereochemistry	Isomerism, chirality, origin of optical activity, stereochemistry of cyclic compounds, resolution.	Define stereochemistry, outline different types of isomerism, differentiate between configurational and conformational isomers, enantiomers, chirality, specific rotation, optical activity, diastereomers, meso compounds, and racemic mixtures, designate the R and S configurations, explain geometrical isomerism, optical resolution.	**T2:** 5.1-5.13, 5.15-5.18, 7.2
30-31	Substitution reactions	Nucleophilic substitution reactions (both S_N1 and S_N2) of alkyl halides.	List the types of substitution reactions (mechanism). Analyze the role of substrate, solvent, and nucleophile.	**T2:** 6.2-6.13

32-33	Elimination reactions	Elimination reactions of alkyl halides; Hoffmann and Cope elimination.	Outline the types of elimination reactions and their differences. Explain the difference between Hoffman and Zeitsev products. Identify the importance of substrate, solvent, and base. Examine the difference between nucleophile and base; Hoffman and Cope elimination mechanism. Compare substitution and elimination reactions.	**T2:** 6.15-6.19, 7.5-7.8, 20.12
34-36	Electrocyclic reactions	Introduction to pericyclic reactions with emphasis on electrocyclic reactions	Identifying pericyclic reactions and various types of pericyclic reactions. Electrocyclic reaction types and conditions. Understanding the outcome of electrocyclic reactions by FMO approach.	Lecture notes
S.S.	Introduction to coordination compounds	*Double salts and coordination compounds. Werner's work; identification of structure by isomer counting. Effective atomic no. concept.* (**Self-study**)	Demonstrate comprehensive and well-founded knowledge of structure and bonding theories relevant to inorganic molecular compounds. Interpret Werner's theory, coordination compound, ligand, and valency, describe coordination compounds, and deduct the effective atomic number.	**T3:** p194-201 (**S.S.**)
37-38	VB theory and Crystal field theory for octahedral complexes	Explanation for the stability of complexes according to crystal field theory.	To understand the basic model behind the crystal field theory. Using the crystal field theory to explain and measure the stabilities of coordination complexes.	**T3:** p203-213
39-41	Jahn-Teller distortions; square planar and tetrahedral complexes	How do geometrical distortions stabilize the system? Stability in other geometries.	Understand the reason behind the Jahn-Teller distortion and its structural consequences. Formulate the crystal field theory to understand square planar and tetrahedral complexes.	**T3:** p214-222
42	Chelates & Isomerism	Different types of ligands and stabilization due to entropy factors and electron delocalization in the rings.	Distinguish various types of ligands and isomerism in coordination compounds.	**T3**: p222-224, 307, 351-352, 389, 793, 807; p232-236

5. Evaluation Scheme:

Component	Duration	Weightage (%)	Date and Time	Nature of component
Midsemester Test	90 min	30	07/03 2.00 - 03.30PM	Closed Book
Class Tests[#]	-	20	To be announced	Open Book
Class Interaction**	-	10	Continuous	Open Book
Comprehensive Examination	180 min	40	13/05FN	Closed Book

Minimum pass-mark criteria for getting a valid grade: 15% of the total marks.

Tutorials: The tutorial hour will be used for a quick review of the material covered in the lectures, clarification of doubts, and problem-solving.

[#] **Two announced class tests** will be held during regular tutorial hours. Specific dates and times will be announced separately. Make-up tests are not permissible for this evaluation component.

****This evaluation is based on the classroom interaction of the students with the instructor in the respective tutorial section only. For the evaluation under this component, it is solely the student's responsibility to attend his/her registered tutorial section only. Biometric attendance in tandem with the physical attendance, collected by the instructor shall be taken into account for marks and grading. Therefore, it is the individual student's responsibility to ensure providing the attendance via both methods.**

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

7. **Notices**: Notices concerning the course will be displayed on the **LMS** and or appropriate online platforms.

8. 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.

9. Make-up-policy: Make-up would be considered by the Instructor in charge & the team only for **very genuine reasons, with valid documents**.

Instructor-In charge

Subit K Saha