Birla Institute of Technology & Science, Pilani
Hyderabad Campus

FIRST SEMESTER 2022-2023

<u>Course Handout (Part - II)</u>

Date: 18-10-2022

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 : **Jayanty Subbalakshmi**
Instructors (Prof./Dr.) : **N. Rajesh, K. Sumithra, Anupam Bhattacharya, J. Subbalakshmi, Balaji Gopalan, Durba Roy, Arijit Mukharjee, Mudit Dixit, Satyanarayan Guin**

1. Scope and Objective of the Course: This course highlights the comprehensive study of the electronic structure of atoms, molecules, and chemical reactions via introducing quantum chemistry, spectroscopy (the study of the interaction between matter and electromagnetic radiation), 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, functional groups, reaction mechanisms, 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,'** 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, Wiley, 2008.

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).
The syllabus also includes lectures and tutorial class notes.

4. Course Plan (SS stands for 'self-study'):

Lect. No.	Learning Objectives	Topics to be Covered	Learning Outcomes of the Lectures	Chapter in the Text Book
1-4	Quantum Theory	Origin of quantum mechanics; Black body radiation, Wavefunction, Schrodinger equation, Uncertainty principle - Simple Applications	Relate the need for quantum theory. Define and consolidate new concepts to be used in quantum mechanics. Apply quantization of states and zero-point energy in simple systems.	**T1: 7A, 7B, 7C, 7E**
5-11	Atomic Structure and Spectra	Hydrogenic Atoms: Energy levels and Wavefunctions, Orbitals, spectral transitions, many-electron atoms: Pauli principle, orbital approximation, Aufbau principle, term symbols, (simple systems only), selection rule.	Identify the atomic orbital picture of the H-atom from quantum mechanics; spin-orbit coupling and atomic term symbols. Identify spin as another coordinate.	**T1: 8A, 8B, 8C, 8D**
12-14	Chemical Bonding: Valence Bond and Molecular Orbital Theories	VB Theory: electron pair bond, hybridization, resonance, MO theory: LCAO, bonding and antibonding orbitals, diatomic molecules	Demonstrate a successful description of the chemical bond; examine the application of molecular orbital theory to diatomic molecules. Recall Lewis's theory and the VSEPR model.	**T1: 9A, 9B, 9C**
15-16	Thermodynamics: The First Law, work, heat, internal energy, enthalpy, physical change	First Law and application of the first law to physical changes	The mathematical form of the First law of thermodynamics, various forms of first law statements, the definition of energy, heat, and work (system and surroundings, and sign convention), the definition of heat capacity, Internal energy, enthalpy, estimate the reaction enthalpy by variation of temperature.	**T1: 2A, 2B, 2C, 2D, 2E, 2F.5**
17-18	Thermodynamics: the Second Law, Entropy, Gibbs Energy	Natural and reversible processes, entropy and second Law, Calculation of entropy changes, absolute entropies, Gibbs energy	Alternative statements of the second law, Discuss Clausius inequality, differentiate between the entropy of system, surroundings, and universe, the irreversible nature of spontaneous and natural processes, evaluate entropy changes accompanying expansion, heating, and phase transition, define third law of thermodynamics, estimate the standard reaction entropy and statistical entropy, define the change in free energy.	**T1: 3A, 3B, 3C, 3D**

19-20	Spontaneity and Equilibrium	Applications of entropy and Gibbs free energy in chemical reactions	Calculate the change in free energy for a chemical change from tabulated thermodynamic data; predict the spontaneity of a reaction, determine how temperature affects the spontaneity of physical & chemical change based on ΔH and ΔS. Relate and apply the concept of chemical equilibrium and response of chemical equilibria to temperature and pressure.	**T1: 4A, 5A, 5B, 5C.1**
21 (partial portion is **SS**)	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, the remaining portions are self-study).**	Define the rate and order of reactions, write the general form of the rate law, and practical determination of order and rate constants from the available concentration values of reactants/products as a function of time. Usage of "methods of initial rates", "isolation method", half- life" concepts. Effect of temperature on the rates of reaction. Using steady-state approximation to derive rate law theoretically for a possible mechanism.	**T1: 6A, 6B, 6C, 6D.1, 6F**
22-23	Electronic Spectroscopy, Vibrational and	General features of molecular spectroscopy, electronic spectra: Franck-Condon principle, types of transitions, vibrational energy levels and spectra;	Relating the interaction between light and matter, detailed understanding of electronic states of atoms, molecules, Franck-Condon factors; predicting the possible vibrational frequencies, and electronic transitions, applying knowledge of detailed understanding of vibrational and electronic spectra of small molecules, isotope shifts.	**T1: 13A, 13D**, **13C.1-13C.3, 13C.5, 7E** **T2:** 2.15 – 2.16
24-26	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; apply the knowledge gained for the identification of organic molecules.	**T1:14A, 14B.1-14B.2** **T2:** 9.1-9.8
27-28	Conformations	Rotation around sigma bonds, conformational analysis of butane, cyclohexane, and substituted cyclohexanes.	Classify structural and constitutional isomers, and explain the terms torsional energy, torsional strain, and angle strain. Judge the stabilities, identify *cis* and *trans* relationship for the substituents on cyclohexanes, draw chair form of cyclohexane with the unambiguous representation of axial and equatorial substituents, and reason for the stability between the two isomers.	**T2:** 4.8-4.9, 4.10, 4.11-4.14
29-30	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

31-32	Substitution reactions	Nucleophilic substitution reactions (both S_N1 and S_N2) of alkyl halides.	List the types of substitution reactions (a mechanism). Analyze the role of substrate, solvent, and nucleophile.	**T2:** 6.2-6.13
33-34	Elimination reactions	Elimination reactions of alkyl halides; Hoffmann and Cope elimination.	Outline the types of elimination reactions. Explain the difference between Hoffman vs Zaitsev product. 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
35-36	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
37-39	Introduction to coordination compounds, VB theory and Crystal field theory for octahedral complexes	Double salts and coordination compounds. Werner's work; identification of structure by isomer counting. Effective atomic number. Explanation for the stability of complexes according to crystal field theory.	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 Explain and measure the stabilities of complexes using the crystal field splitting theory.	**T3:** p194-200, **T3:** p201-213
40-41	Jahn-Teller distortions; square planar and tetrahedral complexes	How do geometrical distortions stabilize the system? Stability in other geometries.	Interpret Jahn-Teller distortion. 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 co-ordination compounds.	**T3**: p223-225, 232-236, 307-308, 351-352, 389, 793, 807.

5. Evaluation Scheme:

Component	Duration	Weightage (%)	Date and Time	Nature of component
Midsem	90 min	30	05/01 9.00AM - 10.30AM	Closed Book
Class Tests (Assignments)#	-	30	To be announced	Open Book
Comprehensive Examination	180 min	40	13/02FN	Closed Book

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

Makeup is not permissible for the evaluation components (except in extreme situations), which would be decided by the Instructor in charge & the team.

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

7. **Notices**: Notices concerning the course will be displayed on the **Chemistry Department Notice Board / CMS or communicated through email**.

8. Academic Honesty and Integrity Policy: Academic honesty and integrity are to be maintained by all the students throughout the semester and **academic dishonesty is highly unacceptable**.

9. Make-up-policy: Make-up would be considered for very **genuine reasons only**.

Instructor-In charge
Jayanty Subbalakshmi