



Birla Institute of Technology & Science, Pilani
Hyderabad Campus

SECOND SEMESTER 2023-2024

Course Handout (Part - II)

Date: 09-01-2024

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 : **Amit Nag**

Instructors (Prof./Dr.) : **Balaji Gopalan, Manab Chakravarty, Himanshu Aggarwal, Chanchal Chakraborty, KVG Chandrasekhar, N Rajesh, Subit Kumar Saha, Sourav Bag and Amit Nag**

1. Scope and Objective of the Course: This course highlights the comprehensive study of electronic structure of atoms, molecules and chemical reaction via introducing quantum chemistry, spectroscopy, the study of interaction between the 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', 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).

The syllabus also includes lectures 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	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 12.1-12.7, 12.9 (7A, 7B, 7C, 7E)
4-8	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)
9-12	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. <i>Lewis theory and VSEPR model (self-study)</i>	Demonstrate successful description of chemical bond; examine the application of molecular orbital theory to diatomic molecules. Recall Lewis theory and VSEPR model.	T1 14.1-14.14 (9A, 9B, 9C)
13	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; compare reversible and irreversible processes (work done), classify and compare thermodynamic functions, influence of temperature and pressure on thermodynamic functions, illustrate bomb type calorimeter.	T1 2.1-2.9 (2A, 2B, 2C, 2D)
14-15	Thermodynamics: the Second Law, Entropy, Gibbs Energy	Natural and reversible processes, entropy and second Law, Calculation of entropy changes, absolute entropies, Gibbs energy.	Demonstrate understanding of key concepts related to the second law of thermodynamics, including alternative statements of the second law. Discuss energy transfer in the context of thermodynamics, differentiate between the entropy of system, surroundings and universe, calculate the changes. Compare reversible and irreversible processes (heat); evaluate entropy changes accompanying expansion, heating, phase transition, define third law of thermodynamics, estimate the standard reaction entropy and statistical entropy, spontaneity of a process in a closed system - concept of Gibbs free energy	T1 4.1-4.13 (3A, 3B, 3C, 3D)

16	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 effects spontaneity of physical & chemical change based on ΔH and ΔS . 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)
17 (partial portion is S.S.)	Chemical Kinetics: Experimental Methods, Reaction Rates, Temperature Dependence	<i>Rate laws, order, rate constants, Arrhenius equation; rate-determining step, reaction mechanisms</i> ; steady-state approximation. (except the steady-state approximation, remaining portions are self-study).	Define the rate and order of reactions, write the general form of the rate law, 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 10.1-10.9, T1 11.4-11.7 (6A, 6B, 6C, 6D-1, 6F)
18-20	Vibrational and Electronic Spectroscopy	General features, vibrational energy levels and spectra; electronic spectra: Franck-Condon principle, types of transitions	Relating the interaction between light and matter, apply knowledge of detailed understanding of vibrational and electronic spectra of small molecules, isotope shifts, detailed understanding of electronic states of atoms, molecules, Franck-Condon principle; predict the possible vibrational frequencies and electronic transitions	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
21-24	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 identification of organic molecules.	T1 21.1 – 21.4 (14A, 14B.1-14B.2) T2: 9.1-9.8
25-26	Conformations	Rotation around sigma bonds, conformational analysis of butane, cyclohexane, and substituted cyclohexanes.	Classify structural and constitutional isomers, explain the terms torsional energy, torsional strain, angle strain. Judge the stabilities, identify <i>cis</i> and <i>trans</i> relationship for the substituents on cyclohexanes, draw chair form of cyclohexane with unambiguous representation of axial and equatorial substituents, reason for the stability between the two isomers.	T2: 4.8-4.9, 4.10 (SS), 4.11-4.14

27-28	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
29-30	Substitution reactions	Nucleophilic substitution reactions (both S_N1 and S_N2) of alkyl halides.	List the types of substitution reactions (mechanism). Analyse the role of substrate, solvent and nucleophile.	T2: 6.2-6.13
31-32	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 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
33-34	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	<i>Double salts and coordination compounds. Werner's work; identification of structure by isomer counting. Effective atomic no. concept. (Self-study)</i>	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, deduce the effective atomic number.	T3: p194-201 (S.S.)
35-36	VB theory and Crystal field theory for octahedral complexes	Explanation for the stability of complexes according to crystal field theory.	Explain and measure the stabilities of complexes using the crystal field splitting theory.	T3: p203-213
37-39	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

40	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: p222-224, 307, 351-352, 389, 793, 807; p232-236
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5. Evaluation Scheme:

Component	Duration	Weightage (%)	Date and Time	Nature of component
Midsem	90 min	30	14/03 - 11.00 - 12.30PM	Closed Book
Class Tests [#]	-	20	To be announced	Open Book
Class Interaction ^{**}	-	10	Continuous	Open Book
Comprehensive Examination	180 min	40	13/05 AN	Closed Book

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

[#] **Two** announced tests will be conducted in the tutorial hour. **Make up is not permissible for this evaluation component.**

****This evaluation is based on the classroom interaction of the students with the instructor in respective tutorial section only. For the evaluation under this component, it is solely 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 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 **Chemistry Department Notice Board / CMS**.

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

Amit Nag

