BIRLA INSTITUTE OF TECHNOLOGY AND SCIENCE, Pilani
Pilani Campus
AUGS Division

FIRST SEMESTER, 2023-2024
COURSE HANDOUT

Date: 09-August-2023

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 : **PARITOSH SHUKLA**
Instructors : Drs. Ajay Kumar Sah, Anil Kumar, Inamur R. Laskar, Madhushree Sarkar, Partha Sarathi Addy, Prashant U. Manohar, Rajeev Sakhuja, Saumi Ray, S. C. Sivasubramanian, and Paritosh Shukla.

1. Course Description: Principles of thermodynamics, phase and chemical equilibrium, electrochemistry, kinetics; atomic structure, chemical bonding, solid state and structural chemistry, molecular spectroscopy; organic compounds, functional groups, structure and isomerism, stereochemistry, reactions and mechanisms, aromaticity, coordination chemistry, chemistry of representative elements.

2. Scope and Objective of the Course: The course is composed of two parts. The first part provides a comprehensive survey of various topics in electronic structure of atoms and molecules, spectroscopy, and bonding; and the second part focuses on understanding of the structure and reactivities of Organic and Coordination compounds. Organic structure identification by NMR spectroscopy will also be introduced.

Overall objective of the course is that the student should be exposed to some of the fundamental principles of stability of chemical structures and should be able to approach the chemical reactions in a systematic and logical way based on electronic structure theory.

3. Text Books:
T1: P.W. Atkins and Julio de Paula, Elements of Physical Chemistry: 6th Edition, Oxford University Press, Oxford, reprinted in 2015.
T2: T. W. Graham Solomons, Craig B. Fryhle, and Scott A. Snyder, Organic Chemistry, 12th Edition, John Wiley & Sons, Inc. New York, 2017

4. Reference Books:
R1: J. D. Lee, Concise Inorganic Chemistry, 5th Edition, Blackwell Science, Oxford, 1999.
R2: David Ball, Physical Chemistry, Brooks/Cole Thomson Learning, 2003.
R3: J. E. Huheey, E. A. Keiter et al., Inorganic Chemistry: Principles of Structure and Reactivity, 4th Edition, Pearson Education, 1993.
R4: R. T. Morrison and R. Boyd, 'Organic Chemistry', 6th Edition, PHI, New Delhi, 1992.

5. Course Plan[$]:

Module No. (LN)	**Lecture Session**	**Reference[#]**	**Learning outcomes**
1 (1-2)	Origin of Quantum Mechanics: Black body radiation, photoelectric effect, wave function, Schrodinger equation, Uncertainty principle, postulates of quantum mechanics.	T1: 12.1-12.6 R2: 9.7-9.8	• Recognize the need for quantum theory • Consolidate new concepts to be used in quantum mechanics
2 (3-5)	Quantum Theory Applications: Particle in a box, bound state, zero point energy, harmonic oscillator, molecular vibrations, dissociation energy, anharmonicity, angular momentum and rigid rotor.	T1: 12.7-12.9 (excluding 12.7b)	• Clarification on quantization of states, zero-point energy in simple systems.

3 (6-8)	Quantum Chemistry, Hydrogenic atom: Energy levels and wave functions, orbitals, spectral transitions.	T1: 13.1-13.7	• Translate the concepts of quantum mechanics in real molecular systems.
4 (9-10)	Quantum Chemistry, Many-electron Atoms: Pauli principle, many electron wave function, Orbital approximation, aufbau principle, term symbols, spin-orbit coupling.	T1: 13.8-13.12; 13.17-13.19	• Identify spin as another coordinate. • Interpret atomic transitions in terms of electronic states.
5 (11-12)	Chemical Bonding: MO theory: LCAO, bonding and antibonding orbitals, homonuclear diatomics	T1: 14.2, 14.8-14.10	• Chemical bond: stability by energy minimization • Distribution of electron in MO, bond order calculation
6 (13-16)	Rotational, Vibrational & Raman Spectroscopy: Absorption and Emission, different regions of electromagnetic spectrum; molecular rotation, Boltzmann population distribution; molecular vibrations, normal modes; Raman spectroscopy.	T1: 19.1-19.4, 19.7-19.11, 19.13	• Use the concepts of quantum mechanics to understand the molecular spectroscopy. • Concept of bond stretching, vibration of molecule. • Identify spectroscopy as an important tool in modern science.
7 (17-19)	Coordination Chemistry: Coordination compounds: effective atomic no. concept; chelates and isomerism; shapes of d-orbitals, crystal field theory, octahedral complexes, spectrochemical series, CFSE, effects of crystal field splitting	R1: p194-200 (SS); p202-214; p222-224, p232-235	• The concept of chelates and coordination compounds • Understanding structure and properties of coordination complexes in light of various theories
8 (20-22)	Distortion in Complexes: Tetrahedral, octahedral, and square planar arrangements, Jahn-Teller distortion, effect of geometrical distortions on stability, stability in other geometries	R1: p214-222	• Nature of ligand, idea of different orbitals and their effect in inorganic complexes • Idea of distortion in tetrahedral, octahedral, and square planar complexes
9 (23-25)	Electronic Spectroscopy and Stability of Coordination compounds: Electronic spectra of octahedral complexes, applications of term symbols, thermodynamic and kinetic aspects of inorganic complexes during reactions.	R1: p219-222 R1: p947-957 R3: p262-264, 380-381, 385-389	• Spectral nature of inorganic complexes • Effect of strength and the symmetry of ligand field on various energy levels • Identify the nature of stable and unstable complexes
10 (26-29)	Nuclear Magnetic Resonance: Principles, chemical shift, fine structure, ^{1}H and ^{13}CNMR of simple compounds	T1: 21.1-21.6 T2: 9.1-9.11C (for examples)	• Theoretical aspect of NMR spectroscopy, chemical shift and determination of organic molecular structure through ^{1}H, ^{13}C-NMR
11 (30-31)	Conformations: Conformational analysis of acyclic and cyclic alkanes (cyclohexane and di-substituted cyclohexane).	T2: 4.8-4.9,4.10 (SS?), 4.11-4.12,4.13	• Understanding conformation of acyclic and cyclic compounds.
12 (32-34)	Stereochemistry: Isomerism, chirality, origin of optical activity, stereochemistry of alkenes, acyclic & cyclic compounds bearing	T2: 5.1-5.14, 5.15-5.18, 7.2	• Concept of chirality and optical activity, learn stereochemistry for

	chiral centers, allenes and biphenyls; resolution.		compound having chiral carbon and resolution of enantiomers
13 (35-37)	Aromaticity & Pericyclic reactions: Huckel rule, aromatic compounds, electrocyclic and cycloaddition reactions	T2: 14.7, 14.8B; 15.11, 15.11 R4	• Concept of aromaticity and related rules. Different pericyclic reactions including cycloaddition
14 (38-40)	Reaction Mechanisms: Nucleophilic (S_N1, S_N2, S_NAr etc.) substitution, and elimination (E1, E2, Hoffmann and Cope elimination) reactions.	T2: 6.2-6.13;7.5-7.8, 20.12 T2: 8.1 (SS), 8.2-8.9, 8.11-8.14, 10.9	• Concept of nucleophilic substitution reactions • Concept of different elimination reactions

[$]The topics "principles of thermodynamics, phase and chemical equilibrium, electrochemistry, kinetics;" mentioned in course description are meant for self-study (SS). [#]Please refer the lecture slides for determining the depth of the content covered under each topic.

6. Evaluation Scheme:

Component	Duration	Weightage (%) (Total Marks 300)	Date & Time	Remarks
Mid-Semester Test	90 Minutes	30 (90 marks)		Closed Book
Continuous Evaluation[§] (Quiz)	-	30 (90 marks)	-	Closed Book
Comprehensive Examination	3 hour	40 (120 marks)		Partially Open Book[α]

[§]A total four quiz/assignment (each of 30 marks) will be conducted under continuous evaluation**. Best three** will be considered for final evaluation (i.e., one buffer). [α] Only text-books, reference books, class/tutorial hand-written notes, and course material (if any provided) will be allowed in the open book examination; only scientific non-programmable calculators are allowed during the tutorial, mid-semester, and comprehensive examinations.

7. Chamber consultancy hour: To be announced separately.

8. Notices: Notices, if any, will be uploaded/ displayed in **Nalanda / Chemistry Department Notice Board only**.

9. Make-up Policy: (Please also refer to the part I of handout given in the time-table booklet.)

Make-up for quiz/assignment will be considered for **genuine cases only** and only if a student misses two or more of these continuous evaluations; i.e., even in genuine cases the make-up will be arranged only for the number of components missed less one (buffer). Make-up for mid-semester test and comprehensive exam will be considered for **genuine cases** as per the Institute rules **against an application** by the student with documents.

Instructor-in-charge
CHEM F111