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

FIRST SEMESTER, 2020-21
COURSE HANDOUT

Date: 03.11.2020

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 : **INAMUR RAHAMAN LASKAR**
Instructor(s) : **Ram Kinkar Roy, Indresh Kumar**
Tutorial/Practical Instructors: Saumi Ray, Ajay Kumar Sah, Bharti Khungar, Paritosh Shukla, Rajeev Sakhuja and Bibhas Ranjan Sarkar

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, bonding, Coordination Chemistry and second part focuses on understanding of the structure and properties of organic compounds and NMR.

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[a]	Learning outcomes
1 (1-2)	Origin of quantum mechanics: black body radiation, 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, zeropoint 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-	Quantum Chemistry, Many-electron	T1: 13.8-	• Identify spin as another

10)	atoms:Pauli principle, many electron wavefunction, Orbital approximation, aufbau principle, term symbols, spin-orbit coupling.	13.12; 13.17-13.19	coordinate. • Interpret atomic transitions in terms of electronic states.
5 (11-12)	Chemical Bonding:Valence bond theory; MO theory: LCAO, bonding and antibonding orbitals, homonucleardiatomics	T1: 14.1-14.10	• Chemical bond: stability by energy minimization • Distribution of electron inMO, bond order calculation
6 (13-16)	Spectroscopy: (Rotational, Vibrational, Raman and Electronic):Absorption and Emission, different regions of electromagnetic spectrum, molecular rotation, molecular vibrations, Raman spectroscopy, normal modes, Boltzmann population distribution. Electronic spectroscopy, Lambert Beer's law	T1: 19.1-19.4, 19.6-19.11, 19.13 20.1-20.6	• 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 of 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)	Coordination Chemistry, Electronic spectroscopy and stability aspects: 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 unstablecomplexes
10 (26-29)	Spectroscopy, 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 1H-NMR, Chemical shift and determination of organic molecular structure through 1H, 13C-NMR
11 (30-31)	Conformations: Rotation around sigma bonds, conformational analysis of butane, cyclohexane, and di-substituted cyclohexanes	T2: 4.8-4.9,4.10 (SS), 4.11-4.12,4.13	• Conformation and configuration of acyclic and cyclic i.e. substituted cyclohexane
12 (32-34)	Stereochemistry: Isomerism, chirality, origin of optical activity, stereochemistry of cyclic & acyclic saturated and unsaturated, resolution.	T2: 5.1-5.14, 5.15-5.18, 7.2	• Concept of chirality and optical activity, learn to stereochemistry for 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 (38-41)	Reaction Mechanisms:Nucleophilic (S_N1, S_N2, S_NAr etc.) and electrophilic substitution reactions; electrophilic addition reactions; Elimination reactions (E1, E2 and Hoffmann and Cope elimination)	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 and electrophilic substitution reactions • Concept of Different addition and elimination reactions

[a]Please refer the lecture slides for determining the depth of the content covered under each topic.

6. Evaluation Scheme:

Component	Weightage (%)
MIDSEM Examination	30
Continuous Evaluation	30
Comprehensive Examination	40

All the tests will be conducted by online platform.

- **A total four tutorial evaluations will be conducted under continuous evaluation. Best three** will be considered for final evaluation.

7. Prescribed Hour (equivalent to chamber consultancy hour): To be announced separately.

8. Notices: Notices, if any, will be uploaded in **Nalanda only**.

9. Make-up Policy: Make-ups are not encouraged as one buffer will be provided.

Instructor-in-charge