BIRLA INSTITUTE OF TECHNOLOGY AND SCIENCE, PILANI
INSTRUCTION DIVISION
Course Handout (II-SEM, 2017-18)

Course Number : CHEM F111
Course Title : General Chemistry
Instructor-in-charge : **Shamik Chakraborty**
Instructors :Ajay K. SahAnil Kumar, Bibhas RSarkar, Inamur R Laskar, Indresh Kumar, Madhushree Sarkar, Paritosh Shukla, Rajeev Sakhuja, Saumi Ray, Shamik Chakraborty, Subit Kumar Saha, and Surojit Pande.

Objectives:

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.

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

Reference Books:

R1: J. D. Lee, Concise Inorganic Chemistry, 5th Edition, Blackwell Science, Oxford, 1999.

R2: Physical Chemistry, David Ball

R3: Inorganic Chemistry: Principles of Structure and Reactivity, 4th Edition, Huheey, Keiter

R4: R. T. Morrison and R. Boyd, 'Organic Chemistry', 6th Edition, PHI, New Delhi, 1992.

Course Plan:

LN	Topic	Learning Objectives	Text[a]	Learning Outcome
1-3	Quantum Theory: Origins	Origin of quantum mechanics, photoelectric effect, black body radiation, wave function, Schrodinger equation, Uncertainty principle, few postulates of quantum mechanics	T1: 12.1-12.6	• Recognize the need for quantum theory • Consolidate new concepts to be used in quantum mechanics
4-5	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	• Clarification on quantization of states, zero-point energy in simple systems.
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.
9-10	Quantum Chemistry: Many-electron atoms	Pauli principle, many electron wavefunction, 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.
11-12	Chemical Bonding	Valence bond theory; MO theory: LCAO, bonding and antibonding orbitals	T1: 14.1-14.10	• Chemical bond: a need between atoms • Distribution of electron in MO, bond order calculation

13-16	Spectroscopy: Rotational and Vibrational Spectroscopy; Raman Spectroscopy, Electronic transitions	Absorption and Emission, different regions of electromagnetic spectrum, molecular rotation, molecular vibrations, normal modes, and rotational transitions accompany vibrational transitions, Boltzmann population distribution. Electronic spectroscopy, Lambert Beer's law	T1: 19.1-19.6, 19.7-19.13 20.1-20.8	• Use the concept of quantum mechanics to understand the molecular spectroscopy • Concept of bond stretching, vibration of molecule • Identify spectroscopy as an important tool in modern science
17-20	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 ^{1}H-NMR, Chemical shift and determination of organic molecular structure through ^{1}H, ^{13}C-NMR
21-23	Coordination Chemistry: Coordination compounds	Double salts and coordination compounds. Werner's work; effective atomic no. concept.; Chelates and isomerism; shapes of d orbitals, crystal field theory, octahedral complexes, spectrochemical series	R1: p194-200 (SS); p202-214; p222-224, p232-235	• The concept of chelates and coordination compounds • Development of coordination complexes in light of various theories
24-26	Distortion of Complexes; Tetrahedral, Octahedral, and Square planar arrangement	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
27-29	Coordination Chemistry: Octahedral complex, CFSE, and Electronic spectroscopy of Oh complexes	CFSE, effects of crystal field splitting, Electronic spectra of octahedral complexes, Applications of term symbols, Thermodynamic and kinetic aspects of Inorganic complexes, Latimar and Frost diagram	R1: p210-214, p219-222 R1: p947-960 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
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
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
35-37	Aromaticity & Pericyclic reactions	Huckel rule, aromatic compounds, electrocyclic and cycloaddition	T2: 14.7-14.8B; 15.1-	• Concept of aromaticity and related rules. Different

		reactions	15.11	pericyclic reactions including cycloaddition
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; 7.5-7.9, 20.12 T2: 8.1 (SS), 8.2-8.9, 8.12-8.15, 10.9	• Nucleophilic and electrophilic substitution reactions • Different addition and elimination reactions

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

Evaluation scheme:

Component	Duration	Weightage (%)	Date and Time	Remarks
Mid Semester test	90 min	30	10/3 4:00- 5:30 PM	Closed book
Continuous Evaluation[‡]	15 min	25	Continuous	(i) Assignment (Closed book) (ii) Quiz (Closed book)
Compre Exam.[$]	3 hours	45	14/5 AN	(i) 20% (Closed Book, MCQ) (ii) 25% (Open Book descriptive)

[‡]Tutorial hour will be used for a quick review of the highlights of the material covered in the lectures, clarification of doubts and problem solving. Overall **six** continuous evaluation component (15 Marks each) will be conducted throughout the semester. **Best Five** of the overall continuous evaluation components will be considered for final evaluation. Continuous evolution components would be two types, viz., Assignment and Quiz. Assignment (close book): a set of problems will be assigned periodically, of which the instructor will specify one to be solved by the students either in the tutorial hour or in a specified time beyond the class hours.Quiz (Close Book): a short quiz based on the lectures covered recently. Only scientific non-programmable calculators are allowed during the tutorial, mid-semester and comprehensive examinations.

[$]Comprehensive examination will have a close book quiz portion and an open-book section. **Only text-books, reference books, class/tutorial notes, and course material (if any provided) will be allowed in the open book examination.**

Chamber consultation hours: To be announced

Notices: Notices, if any, will be displayed on the **Nalanda&Department of Chemistry Notice Board only.**

Make up: Make up would be considered only for **genuine reasons.**Make-up for continuous evaluation (assignments/quizzes) will be considered (for genuine cases) only if more than one assignments/quizzes is missed by a student.

Instructor in-Charge
CHEM F111