BIRLA INSTITUTE OF TECHNOLOGY AND SCIENCE, PILANI
INSTRUCTION DIVISION
Course Handout

Course Number : CHEM F111
Course Title : General Chemistry
Instructor-in-charge : **RAJEEV SAKHUJA**
Instructors : Dalip Kumar, Subit K. Saha, Ram Kinkar Roy, Anil Kumar, Ajay K. Sah, Bharti Khungar, Inamur R. Laskar, Saumi Ray, Madhushree Sarkar, Paritosh Shukla, Prashant U. Manohar, Indresh Kumar, Surojit Pande, Shamik Chakraborty

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, chemical thermodynamics, kinetics and second part focuses on the applications of these topics in understanding the structure and properties of organic compounds and transition metal complexes.

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 and Craig B. Fryhle, Organic Chemistry, 10th Edition, John Wiley & Sons, Inc. New York, 2011

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]
1-3	Quantum Theory	Origins of quantum mechanics, atomis and molecular spectra, photoelectric effect, black body radiation, wave function, Schrodinger equation, Born interpretation, uncertainty principle	T1: 12.1-12.6
4-5	Quantum Theory	Simple applications of quantum mechanics	T1: 12.7-12.9
6-8	Quantum chemistry: atomic structure	Hydrogenic atom: spectra of hydrogenic atoms, permitted energy levels, quantum numbers and wavefunctions, orbitals, electron spin, Spectral transitions	T1: 13.1-13.7
9-10	Quantum chemistry: atomic structure	Many-electron atoms: Pauli principle, orbital approximation, aufbau principle, term symbols, spin-orbit coupling (term symbols of one electron system and Ground state determination of any p or d-system). (p^2 system in Tutorial class)	T1: 13.8-13.12, 13.17-13.19

11-13	Chemical Bonding: VB and MO Theories	VB theory: Diatomic molecules, hybridization, MO theory: LCAO, bonding and antibonding orbitals, diatomic molecules, Heteronuclear molecules (HF & CO)	T1: 14.1-14.5, 14.8-14.11
14-16	Spectroscopy: molecular vibrations and Electronic transitions	Introduction to spectroscopy, Vibrational spectroscopy: energy levels and vibrational transitions and applications of IR spectroscopy Electronic spectra: Franck-Condon principle, radioactive and non-radioactive decay transitions.	T1: 19.7-19.11, Lecture notes for application of IR spectroscopy, 20.1-20.6
17-19	Spectroscopy: Nuclear Magnetic Resonance	Principles, chemical Shift, fine Structure, spin relaxation & ^{1}H NMR of simple molecules	T1: 21.1-21.5 T2: 9.1-9.11C (for examples)
Self Study	Thermodynamics: The First Law	Thermodynamic systems, state functions, thermal equilibrium and temperature, work, internal energy and heat transfer, heat capacity, enthalpy, application of chemical change.	T1: Chapters 2-3
20-21	Thermodynamics: The second Law	Entropy and second Law, Direction of Spontaneous change, Absolute Entropies and the third Law, Standard Reaction Entropy, Spontaneity of Chemical Reactions, properties of Gibbs Energy	T1: 4.1-4.7, 4.10-4.13
22-23	Spontaneity and equilibrium	Thermodynamics of Transition, Condition of Stability, the Reaction Gibbs energy, Reactions at Equilibrium, standard reactions Gibbs energy	T1: 5.1-5.3, 7.1-7.4
Self Study	Chemical Kinetics	Reaction Rates, Rate laws, order, rate constants, determination of rate laws, half-lives, Arrhenius equation, Collision Theory, Transition State Theory	T1: chapter 10
24-25	Chemical Kinetics	Reaction Schemes: approach to Equilibrium, Consecutive reactions, Reaction Mechanisms, Formulation of Rate Laws, rate-determining step, steady-state approximation, rate- determining step	T1: 11.1-11.7
Self Study	Introduction to coordination compounds	Double salts and coordination compounds, Werner's work, Effective atomic no. concept, Chelates and Isomerism	R1: p194-200; p222-224, p232-235
26-28	Bonding in Transition metal Complexes	Valence Bond Theory; Shapes of d orbitals, Crystal Field Theory, Octahedral Complexes, Spectrochemical Series, Electronic Spectra of octahedral complexes, CFSE, Effects of Crystal Field Splitting	R1: p202-214
29-30	Jahn-Teller Distortion & Other geometries in Transition metal complexes	Tetragonal distortion of Octahedral Complexes: How do geometrical distortions stabilize the system? Stability in other geometries: Square planar arrangements, Tetrahedral complexes	R1: p214-222

31-32	Conformations	Rotation around sigma bonds, conformational analysis of butane, cyclohexane, and substituted cyclohexanes.	T2: 4.8-4.9, 4.10 (SS), 4.11-4.12
33-35	Stereochemistry	Isomerism, chirality, origin of optical activity, stereochemistry of cyclic & acyclic compounds, resolution.	T2: 5.1-5.13, 5.15-5.18, 7.2, 4.13, 5.14
36-38	Aromaticity, aromatic compounds & Pericyclic reactions	Huckel's Rule, Reactivity of aromatic compounds. Electrocyclic and cycloaddition reactions	T2: 14.7-14.8B, 15.1-15.11, Lecture slides for pericyclic reactions
39-42	Substitution, Elimination and Addition reactions	Nucleophilic substitution reactions (both S_N1 and S_N2) of alkyl halides and some inorganic compounds. (with emphasis on stereochemical aspect) Elimination reaction of alkyl halides; Hoffmann and Cope elimination. Addition reactions to C=C bond	T2: 6.2-6.13, 6.15-6.19, 7.5-7.8, 20.12; T2: 8.1 (Self study), 8.2-8.10, 8.12-8.15, 10.9 T2: F.1-F.3B

[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	5/10 4:00 - 5:30 PM	Closed book
Tutorials	10 min.	25	Continuous	Closed book[‡]
Compre Exam.	3 hours	45	2/12 AN	Partially open book[$]

[‡]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. There are two types of evaluation components that will be conducted in the tutorial. In the first type, a set of problems will be assigned periodically (on Nalanda Webpage), of which the instructor will specify one or two to be solved by the students in the tutorial hour of the following week. The second method of evaluation will be a short quiz based on the lectures covered recently. **Students must bring the tutorial problems sheets without fail**. Only scientific non-programmable calculators are allowed during the tutorials, tests and comprehensive examination. Sharing of calculators is not allowed in any examination.

[$]Comprehensive examination will have a closed 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 only.**

Make up: Make up would be considered only for **genuine reasons.**

Instructor in-Charge
CHEM F111