

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

Date: 02/08/2016

Course Number : CHEM F111
Course Title : General Chemistry
Instructor-in-charge : **MADHUSHREE SARKAR**
Instructors : Ram K. Roy, Dalip Kumar, Anil Kumar, Ajay K. Sah, Bharti Khungar, I. R. Laskar, Paritosh Shukla, Indresh Kumar, Surojit Pande, Rajeev Sakhuja, Shamik Chakraborty, Bibhas Ranjan Sarkar.

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: Physical Chemistry, David Ball

R2: J. D. Lee, Concise Inorganic Chemistry, 5th Edition, Blackwell Science, Oxford, 1999.

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 | Origins of quantum mechanics, photoelectric effect, black body radiation, wave function, Schrodinger equation, uncertainty | T1: 12.1-12.6 |
| 4-5 | Quantum Theory: Applications | Simple applications of quantum mechanics | T1: 12.7-12.9 |
| 6-8 | Quantum Chemistry: Hydrogenic atom | Energy levels and wavefunctions, orbitals, Spectral transitions, | T1: 13.1-13.7 |
| 9-10 | Quantum Chemistry: Many-electron atoms | Pauli principle, Orbital approximation, aufbau principle, term symbols, spin-orbit coupling. | T1: 13.8-13.12, 13.17-13.19 |
| 11-13 | Spectroscopy: Rotational and Vibrational Spectroscopy; Raman Spectroscopy | Rotational & vibrational energy levels, spectral analysis and applications | T1: 19.1-19.5, 19.6-19.13 |
| 14-16 | Spectroscopy: Nuclear Magnetic Resonance | Principles, chemical Shift, fine structure, ¹ H NMR of simple compounds | T1: 21.1-21.6 T2: 9.1-9.11C (for examples) |
| 17-19 | Thermodynamics: The | Thermodynamic systems, state functions, | T1: Chapters 2-3 |

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|-------|--|--|---|
| | First, second and third laws; Spontaneity and equilibrium | entropy, direction of spontaneous change, second law, absolute entropies and the third law, standard reaction entropy, spontaneity of chemical reactions, Gibbs energy thermodynamics of transition, conditions of stability, reaction Gibbs energy, reactions at equilibrium | (SS), 4.1-4.7 4.10-4.13; 5.1-5.8, 7.1-7.4 |
| 20-21 | Chemical Kinetics | Reaction schemes: approach to equilibrium, consecutive reactions, reaction mechanisms, formulation of rate laws, rate-determining step, steady-state approximation | T1: 10.1-10.9 (SS); 11.3-11.9 |
| 22-25 | Coordination Chemistry: Coordination compounds, Bonding | Double salts and coordination compounds. Werner's work; identification of structure by isomer counting; effective atomic no. concept.; Chelates and isomerism; valence bond theory; MO theory: LCAO, bonding and antibonding orbitals; shapes of d orbitals, crystal field theory, octahedral complexes, spectrochemical series, absorption spectroscopy, Lambert Beer's law, electronic spectra of octahedral complexes, CFSE, effects of crystal field splitting | R1: p194-200 (SS); p202-214; p222-224, p232-235 T1: 14.1-14.5, 14.8-14.10 |
| 26-28 | Tetragonal distortion of Octahedral Complexes; Square planar arrangements; Tetrahedral complexes | Jahn-Teller distortion: Effect of geometrical distortions on stability, stability in other geometries | R1: p214-222 |
| 29-30 | 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 |
| 31-33 | 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 |
| 34-36 | Aromaticity & Pericyclic reactions | Huckel rule, aromatic compounds, electrocyclic and cycloaddition reactions | T2: 14.7-14.8B; 15.1-15.11 |
| 37-40 | 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; 6.15-6.19, 7.5-7.8, 20.12 T2: 8.1 (SS), 8.2-8.10, 8.12-8.15, 10.9 |

^aPlease 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 | <TEST_1> | Close book |
| Continuous Evaluation [‡] | 15 min | 30 | Continuous | (i) Assignment (Open book) (ii) Quiz (Close book) |
| Compre Exam. [§] | 3 hours | 40 | <TEST_C> | (i) 20% Close Book MCQ; (ii) 20% Open Book Descriptive |

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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 will be two types of continuous evaluation components:

(i) Assignments (Open Book): A set of problems will be assigned periodically (on Nalanda Webpage). Based on the concepts of the assigned problems, different questions will be given for solving in the class. Students can refer to **text-books, reference books, class/tutorial notes and course material (if any provided)** for solving the problem(s). Overall **three** such assignments (each of 15 Marks) will be conducted throughout the semester. (ii) Quiz (Close Book): Short questions/numerical will be asked based on the lectures covered recently; Overall **four** such quizzes (each of 15 Marks) will be conducted throughout the semester. **Best six** of the overall continuous evaluation components will be considered for evaluation.

Only scientific **non-programmable calculators** are allowed during the tutorials, tests and comprehensive examination.

[§]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**