

BIRLA INSTITUTE OF TECHNOLOGY & SCIENCE, PILANI
HYDERABAD CAMPUS
FIRST SEMESTER 2016-2017
Course Handout (Part - II)

Date: 01/08/2016

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 : **Dr. Durba Roy**

Instructors: Prof. Anupam Bhattacharya, Prof. J. Subbalakshmi, Prof. R. Krishnan,
Prof. Manab Chakravarty, Dr. Sounak Roy, Dr. Subhas Ghosal and Dr. Durba Roy.

1. Scope and Objective of the Course: This course provides a comprehensive survey of the concepts involved in the study of the electronic structure of atoms and molecules (part of quantum chemistry), spectroscopy, chemical equilibrium, and chemical kinetics, concepts of organic stereochemistry, functional groups, reaction mechanisms and coordination chemistry.

2. Text Books:

T1: P.W. Atkins & Julio de Paula, 'The Elements of Physical Chemistry', Fifth/Sixth edition (Oxford University Press, Oxford 2009).

T2: T. W. Graham Solomons and Craig B. Fryhle, 'Organic Chemistry', 10th Edition, John Wiley & Sons, Inc. New York, 2011.

T3: J. D. Lee, 'Concise Inorganic Chemistry', 5th Edition, Blackwell Science, Oxford, 1999.

3. Reference Books:

(R1) D. W. Ball, 'Physical Chemistry', First Edition, India Edition (Thomson, 2007).

(R2) L. G. Wade, Jr. and M. S. Singh, 'Organic Chemistry', 6th Edition, Pearson Education Inc., 2006.

❖ *The syllabus also includes lecture and tutorial notes*

4. Course Plan (SS stands for 'self study'):

L N	Learning Objectives	Topics to be covered	Chapter in the Text Book
1-3	Quantum Theory	Origins of Quantum Mechanics, Black body radiation, Wave function, Schrodinger Equation, Uncertainty, Simple Applications.	T1: 12.1-12.7
4-8	Atomic Structure and Spectra	Hydrogenic Atoms: Energy Levels and Wavefunctions, Orbitals, Spectral Transitions, Many-electron Atoms: Pauli Principle, Orbital Approximation, Aufbau Principle, Term symbols, (Simple systems only) Selection rule	T1: 13.1-13.11, 13.17, 13.19 (SS): 13.15-13.16
9-12	Chemical Bonding: Valence Bond and Molecular Orbital Theories	VB Theory: Electron Pair Bond, Hybridization, Resonance, MO Theory: LCAO, Bonding and Antibonding Orbitals, Diatomic Molecules. Lewis theory and VSEPR model (self study)	T1: 14.1-14.14
13	Thermodynamics: the First Law, Internal Energy and Enthalpy	Thermodynamic Systems, State Functions, Thermal Equilibrium and Temperature, Work, Internal Energy and Heat Transfer, Heat Capacity.	T1: 2.1-2.9

Self Study	Thermochemistry	Application of the First Law to physical and chemical changes.	T1: 3.1-3.7 17.6
14-15	Thermodynamics: the Second Law, Entropy, Gibbs Energy	Natural and Reversible Processes, Entropy and Second Law, Calculation of Entropy Changes, Absolute Entropies, Gibbs Energy.	T1: 4.1-4.13
16	Spontaneity and Equilibrium,	Applications of entropy and Gibb's free energy in Chemical reactions	T1: 5.1 – 5.3, 7.1-7.4
17-18	Chemical Kinetics: Experimental Methods, Reaction Rates, Temperature Dependence	Rate Laws, Order, Rate Constants, Arrhenius Equation, Rate-determining step, Reaction mechanisms. Steady-state Approximation.	T1: 10.1-10.9, T1: 11.4-11.7
19-20	Vibrational and Electronic Spectroscopy	General Features, Vibrational Energy Levels and Spectra; Electronic Spectra: Franck-Condon Principle, Types of Transitions	T1: 12.9,19.6 – 19.8; 19.11 T1: 20.1 – 20.4 T2: 2.16
21-23	Nuclear Magnetic Resonance Spectroscopy	Principles, Chemical Shift, Fine Structure, Spin Relaxation, Applications (Identification of organic compounds).	T1: 21.1 – 21.4 T2: 9.1-9.8
24-25	Conformations	Rotation around sigma bonds, conformational analysis of butane, cyclohexane, and substituted cyclohexanes.	T2: 4.8-4.9, 4.10 (SS), 4.11-4.14
26-27	Stereochemistry	Isomerism, chirality, origin of optical activity, stereochemistry of cyclic compounds, resolution.	T2: 5.1-5.13, 5.15-5.18, 7.2
28-29	Substitution reactions	Nucleophilic substitution reactions (both S _N 1 and S _N 2) of alkyl halides.	T2: 6.2-6.13
30-31	Elimination reactions	Elimination reaction of alkyl halides; Hoffmann and Cope Elimination.	T2: 6.15-6.19, 7.5-7.8, 20.13
32	Addition reactions	Addition reactions to >C=C< bond	T2: 8.1 (SS), 8.2-8.14, 10.9
33	Aromaticity and aromatic compounds	Structure and reactivity of benzene and other aromatic compounds.	T2: 14.3-14.7, 15.1-15.2, 15.6-15.11 (SS)
34	Introduction to coordination compounds	Double salts and coordination compounds. Werner's work; Identification of structure by isomer counting. Effective Atomic No. concept.	T3: p194-201
35-36	VB theory and Crystal field theory for octahedral complexes	Explanation for the stability of complexes according to crystal field theory	T3: p203-212
37-38	Jahn-Teller distortions; Square planar and tetrahedral complexes	How do geometrical distortions stabilize the system? Stability in other geometries	T3: p214-222

39-40	Chelates & Isomerism	Different types of ligands and stabilization due to entropy factors and electron delocalization in the rings.	T3: p222-224, 307,351-352, 389, 793, 807. p232-235
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5. Evaluation Scheme:

Component	Duration	Weightage%	Date Time	Remarks
Test – I	60 min	20%	8/9, 4.00--5.00 PM	Closed Book
Test – II	60 min	20%	25/10, 4.00--5.00 PM	Closed Book
Class Tests [#]	-	20%	Continuous	Open Book [#]
Comprehensive Examination [*]	3 hr	40%	09/12 FN	Closed Book [*]

Tutorials: The 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.

[#] No makeup would be given for this evaluation component.

^{*} The **Comprehensive Examination** will be a **closed book** exam, with **quiz portion having 16% weightage** and **descriptive section having 24% weightage**.

6. **Chamber Consultation Hours:** To be announced through a notice.

7. **Notices:** Notices, if any, concerning the course will be displayed on the **Chemistry Department Notice Board as well as in CMS**.

8. **Make-up-policy:** Make up would be considered only for very **genuine reasons**.

Instructor-in-charge
CHEM F111