



Birla Institute of Technology & Science, Pilani
Hyderabad Campus

SECOND SEMESTER 2019-2020

Course Handout (Part - II)

Date: 06/01/2020

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 : **Balaji Gopalan**
Instructors : **Amit Nag, Chanchal Chakraborty, Himanshu Aggarwal, K. V. G. Chandrasekhar, Manab Chakravarty, Sounak Roy, Subit Kumar Saha, Tanmay Chatterjee**

1. Scope and Objective of the Course: This course highlights the comprehensive study of electronic structure of atoms, molecules and chemical reaction via introducing quantum chemistry, spectroscopy, the study of interaction between the matter and electromagnetic radiation, thermodynamics, chemical equilibrium, and chemical kinetics as a part of general physical chemistry. It also provides a comprehensive survey of the concepts involved in the study of conformations, stereochemistry, functional groups, reaction mechanisms and coordination chemistry as a part of organic and inorganic chemistry.

2. Text Books:

T1: P.W. Atkins & Julio de Paula, 'The Elements of Physical Chemistry', Fifth/Sixth/International edition (Oxford University Press, Oxford 2009/2013/2017).

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

(R2) D. W. Ball, 'Physical Chemistry', First Edition, India Edition (Thomson, 2007).

The syllabus also includes lectures and tutorial class notes.

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

Note: The sections of the Chapters in the Text book are given below based on **the 5th Edition (and international edition in bracket) of P.W. Atkins & Julio de Paula.**

Lec. No.	Learning Objectives	Topics to be Covered	Learning Outcomes of the Lectures	Chapter in the Text Book
1-3	Quantum Theory	Origin of quantum mechanics; Black body radiation, Wave function, Schrodinger equation, Uncertainty principle - Simple Applications	Relate the need for quantum theory. Define and consolidate new concepts to be used in quantum mechanics. Apply quantization of states and zero-point energy in simple systems.	T1: 12.1-12.7 (7A, 7B, 7C)
4-8	Atomic Structure and Spectra	Hydrogenic Atoms: Energy levels and Wave functions, Orbitals, spectral transitions, many-electron atoms: Pauli principle, orbital approximation, Aufbau principle, term symbols, (simple systems only), selection rule.	Identify the atomic orbital picture of H-atom from quantum mechanics; spin orbit coupling and atomic term symbols. Identify spin as another coordinate.	T1: 13.1-13.11, 13.17-13.19. (8A, 8B, 8D) (SS): 13.15-13.16 (8C)
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)	Demonstrate successful description of chemical bond; examine the application of molecular orbital theory to diatomic molecules. Recall Lewis theory and VSEPR model.	T1: 14.1-14.14 (9A, 9B, 9C)
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.	Comprehend the concept of energy; compare reversible and irreversible processes (work done), classify and compare thermodynamic functions, influence of temperature and pressure on thermodynamic functions, illustrate bomb type calorimeter.	T1: 2.1-2.9 (2A, 2B, 2C, 2D)
Self Study	Thermochemistry	Application of the first law to physical and chemical changes	Define formation reaction of a compound, calculate the change in enthalpy based on tabulated data (Hess's law, formation data, bond energy data), calculate the change in the enthalpy for physical change (both change in temperature and phase change) adopt the first law of thermodynamics and apply to the chemical reactions to calculate the enthalpy of phase transition, ionizations, combustions, reactions, product formations, estimate the reaction enthalpy by variation of temperature.	T1: 3.1-3.7, 7.6 (2E, 2F)
14-15	Thermodynamics: the Second Law, Entropy,	Natural and reversible processes, entropy and second Law,	Demonstrate understanding of key concepts related to the second law of thermodynamics, including	T1: 4.1-4.13 (3A, 3B, 3C, 3D)

	Gibbs Energy	Calculation of entropy changes, absolute entropies, Gibbs energy.	alternative statements of the second law. Discuss energy transfer in the context of thermodynamics, differentiate between the entropy of system, surroundings and universe, calculate the changes. Compare reversible and irreversible processes (heat); evaluate entropy changes accompanying expansion, heating, phase transition, define third law of thermodynamics, estimate the standard reaction entropy and statistical entropy, define the change in free energy.	
16	Spontaneity and Equilibrium	Applications of entropy and Gibbs free energy in chemical reactions	Calculate the change in free energy for a chemical change from tabulated thermodynamic data; predict the spontaneity of a reaction, determine how temperature effects spontaneity of physical & chemical change based on ΔH and ΔS . Relate and apply concept of chemical equilibrium and response of chemical equilibria to temperature and pressure.	T1: 5.1 – 5.3, 7.1-7.4 (4A, 5A) SS: 7.6 (5B, 5C)
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.	Define the rate and order of reactions, write the general form of the rate law, practical determination of order and rate constants from the available concentration values of reactants/products as a function of time. Usage of "methods of initial rates", "isolation method", half-life concepts. Effect of temperature on the rates of reaction. Using steady state approximation to derive rate law theoretically for a possible mechanism.	T1: 10.1-10.9, T1: 11.4-11.7 (6A, 6B, 6C, 6D-1, 6F)
19-21	Vibrational and Electronic Spectroscopy	General features, vibrational energy levels and spectra; electronic spectra: Franck-Condon principle, types of transitions	Relating the interaction between light and matter, apply knowledge of detailed understanding of vibrational and electronic spectra of small molecules, isotope shifts, detailed understanding of electronic states of atoms, molecules, Franck-Condon factors; predict the possible vibrational frequencies and electronic transitions.	T1: 12.9, 19.6 – 19.8; 19.11; 20.1 – 20.4 (7E, 13A, 13C.1-13C.3, 13C.5, 13D) T2: 2.15 – 2.16
22-25	Nuclear Magnetic Resonance Spectroscopy	Principles, chemical shift, fine structure, spin relaxation, applications (identification of organic compounds).	Understand the basic principles and techniques of nuclear magnetic resonance spectroscopy; apply the knowledge gained for identification of organic molecules.	T1: 21.1 – 21.4 (14A, 14B) T2: 9.1-9.8
26-27	Conformations	Rotation around sigma bonds, conformational analysis of butane, cyclohexane, and substituted	Classify structural and constitutional isomers, explain the terms torsional energy, torsional strain, angle strain. Judge the stabilities, identify <i>cis</i> and	T2: 4.8-4.9, 4.10 (SS) , 4.11-4.14

		cyclohexanes.	<i>trans</i> relationship for the substituents on cyclohexanes, draw chair form of cyclohexane with unambiguous representation of axial and equatorial substituents, reason for the stability between the two isomers.	
28-29	Stereochemistry	Isomerism, chirality, origin of optical activity, stereochemistry of cyclic compounds, resolution.	Define stereochemistry, outline different types of isomerism, differentiate between configurational and conformational isomers, enantiomers, chirality, specific rotation, optical activity, diastereomers, meso compounds and racemic mixtures, designate the R and S configurations, explain geometrical isomerism, optical resolution.	T2: 5.1-5.13, 5.15-5.18, 7.2
30-31	Substitution reactions	Nucleophilic substitution reactions (both S _N 1 and S _N 2) of alkyl halides.	List the types of substitution reactions (mechanism). Analyse the role of substrate, solvent and nucleophile.	T2: 6.2-6.13
32-33	Elimination reactions	Elimination reactions of alkyl halides; Hoffmann and Cope elimination.	Outline the types of elimination reactions. Explain the difference between Hoffman vs Zaitsev product. Identify the importance of substrate, solvent and base. Examine difference between nucleophile and base; Hoffman and Cope elimination mechanism. Compare substitution and elimination reactions.	T2: 6.15-6.19, 7.5-7.8, 20.13
34-35	Addition reactions	Addition reactions to >C=C< bond	Infer the fundamental mechanism of an addition reaction; choose Markovnikov's and anti-Markovnikov reaction. Analyse the mechanism of oxymercuration / demercuration and hydroboration – oxidation.	T2: 8.1 (SS), 8.2-8.14, 10.9
36	Aromaticity and aromatic compounds	Structure and reactivity of benzene and other aromatic compounds.	Distinguish aromatic, non-aromatic and anti-aromatic systems. Spell the mechanism of electrophilic aromatic substitution and the effect of directing groups.	T2: 14.3-14.7, 15.1-15.2, 15.6-15.11 (SS)
37	Introduction to coordination compounds	Double salts and coordination compounds. Werner's work; identification of structure by isomer counting. Effective atomic no. concept.	Demonstrate comprehensive and well-founded knowledge of structure and bonding theories relevant to inorganic molecular compounds. Interpret Werner's theory, coordination compound, ligand and valency, describe coordination compounds, deduct the effective atomic number.	T3: p194-201
38-39	VB theory and Crystal field theory for octahedral complexes	Explanation for the stability of complexes according to crystal field theory.	Explain and measure the stabilities of complexes using the crystal field splitting theory.	T3: p203-212
40-41	Jahn-Teller distortions;	How do geometrical distortions	Interpret Jahn-Teller distortion. Formulate the	T3: p214-222

	square planar and tetrahedral complexes	stabilize the system? Stability in other geometries.	crystal field theory to understand square planar and tetrahedral complexes.	
42	Chelates & Isomerism	Different types of ligands and stabilization due to entropy factors and electron delocalization in the rings.	Distinguish various types of ligands and isomerism in co-ordination compounds.	T3: p222-224, 307, 351-352, 389, 793, 807; p232-235

5. Evaluation Scheme:

Component	Duration	Weightage (%)	Date and Time	Nature of component
Midsem Test	90 mins	35	5/3 1.30 -3.00 PM	
Class Tests [#]	-	20	Continuous	Open Book [#]
Comprehensive Examination*	3 hrs	45	11/05 AN	

Tutorials: The tutorial hour are engaged used for quick review of the material covered in the lectures, clarification of doubts, and problem solving.

[#] Make up is not permissible for this evaluation component (except for extreme situation) which would be decided by the Instructor in charge & team.

* The **Comprehensive Examination** will be a **closed book** exam, with **quiz portion** and **descriptive section**.

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

7. Notices: Notices concerning the course will be displayed on the **Chemistry Department Notice Board / CMS**.

8. Academic Honesty and Integrity Policy: Academic honesty and integrity are to be maintained by all the students throughout the semester and no type of academic dishonesty is acceptable.

9. Make-up-policy: Make up would be considered only for very **genuine reasons** (*such as institute deputation outside for sports/cultural fest, hospitalization (with appropriate documentary proof), marriage ceremony of siblings (not cousins)*) and any other extreme emergency situations which would be decided by the team of instructors.

Instructor-In charge

Balaji Gopalan

