# GURU NANAK COLLEGE (AUTONOMOUS)

**VELACHERY ROAD, CHENNAI – 600042** 

(Re-accredited at 'A-Grade' by NAAC) Affiliated to University of Madras



## M.Sc. (CHEMISTRY)

(SEMESTER PATTERN WITH CHOICE BASED CREDIT SYSTEM)

## **SYLLABUS**

(For the candidates admitted for the Academic year 2022-23 and thereafter)

## **PREAMBLE**

The purpose of post-graduate education in Chemistry is to create highly skilled man power in specific areas, which leads to greater knowledge and creation of wealth of the nation. Chemistry is a fundamental science and has contributed immensely to the improvement of the life of people by providing many requirements and essentialities. The developments in chemistry during last few decades are phenomenal and it is also seen that more inclination is towards biological sciences. New branches of chemistry are emerging and gaining importance, such as bioorganic chemistry, bioinorganic chemistry, chemistry, materials chemistry, computational nano chemistry, etc. Chemistry at industrial scale is also undergoing radical changes and is based on deep understanding the chemical phenomena. The aid of computers has also accelerated the growth in the practice of Chemistry. Chemists cannot isolate themselves from other disciplines. So, inter disciplinary courses /extra disciplinary courses have also been included which will help the students to have wider knowledge of other disciplines. Green chemistry has emerged as a new approach to the practice of Chemistry. Chemical industry is now under pressure from both the Government and the Society to develop eco-friendly processes and products which will reduce waste and prevent toxic substances from entering the environment. Efforts are taken to minimize polluting the environment and at the same time not compromising with the gain of knowledge which will enable the students to accept any challenge in chemistry and to move towards research.

## LEARNING OUTCOME BASED CURRICULUM

## **FRAMEWORK**

## From the Academic Year 2022- 23 and there after

## Vision

- To enhance the quality of education beyond the text book / syllabi based exam-oriented system to research and analytical based learning.
- To produce quality graduates and post graduates to excel in the field of education / research / industry.
- To encourage the learners of exceptional quality to take up research and motivate them to contribute to the needs of the society.
- To encourage the faculty to constantly involve themselves in research in addition to the regular work, which would enable them to develop research-oriented learning skills.

## **Mission**

- To inculcate the scientific methodology of learning chemistry by focusing more on practical.
- To enhance the creativity in learning chemistry among the learners using visual aids.
- To produce and to modernize the infra structure to impart and understand the importance of practical skill accuracy and data interpretation.
- To encourage the learners to participate in the teaching learning process to enhance their analytical and problem-solving skill and to develop leadership qualities.
- To motivate the students by conducting seminars/workshops with the inputs of eminent scientists, distinguished alumni and industrialist.
- Visit to Industries and scientific centres to have exposure on sophisticated instruments and recent developments in chemistry.

## **PROGRAMME OUTCOME**

At the completion of M. Sc. in Chemistry the students are able to:

**PO 1:** acquire a broad learning in advances in chemistry that stresses scientific reasoning and analytical problem solving with a molecular perspective and develop the ability to communicate scientific information in written and oral formats.

**PO 2:** expose broader experimentation in chemistry on applied aspect and also using modern instrumentation to understand the importance of the chemical transformation for high throughput applications.

**PO 3 :** investigate the interdisciplinary nature of chemistry in biology, medicine, materials science to excel in R&D for the benefit of societal needs and have extra acquaintance in humanities other than chemistry.

**PO 4:** execute the laboratory skills needed to design, interpret chemical research; acquire a foundation of research in chemistry

**PO 5:** develop the skills required to succeed in higher learning in chemistry, in the chemical industry and in academic profession.

## PROGRAMME SPECIFIC OUTCOME

The students at the time of graduation will be able to

**PSO 1:** adopt to the major scientific and technological challenges in research, industry as they are welltrained in experimental techniques like synthesis, separation, distillation, crystallization *etc*.

**PSO 2**: compete in the international, National, state level assessments.

## M.Sc., - CHEMISTRY COURSE STRUCTURE (2022– 23) Batch

Semester	Course Component	Subject Name		Hours	CIA	ESE	Total
	Core Theory-I	Organic Chemistry - I	4	4	50	50	100
	Core Theory-II	Inorganic Chemistry - I	4	4	50	50	100
<b>-</b>	Core Theory-III	Physical Chemistry I	4	4	50	50	100
Semester –	Core Elective-I##	##	3	4	50	50	100
me	Core Practical-I*	Organic Chemistry Practical	-	4	50	50	100
Se	Core Practical-II*	Inorganic Chemistry Practical	-	4	50	50	100
	Core Practical-III*	Physical Chemistry Practical	-	4	50	50	100
	Soft Skill –1	Personality Enrichment	2	2	50	50	100
	Total C	redits: 17 / Total Hours per week: 3	30				
	Core Theory- IV	Organic Chemistry - II	4	4	50	50	100
	Core Theory-V	Inorganic Chemistry - II	4	4	50	50	100
=	Core Theory-VI	Physical Chemistry - II	4	4	50	50	100
	Core Practical-I *	Organic Chemistry Practical	4	4	50	50	100
ste	Core Practical-II *	Inorganic Chemistry Practical	4	4	50	50	100
Semester –	Core Practical-III *	Physical Chemistry Practical	4	4	50	50	100
Se	EDE 1#	#	3	4	50	50	100
	Soft Skill – 2	Workplace Communication Skills	2	2	50	50	100
	Total Credits: 29 / Total Hours per week: 30						

Semester	Course Component	Subject Name		Hours	CIA	ESE	Total
	Core Theory-VII	Organic Chemistry - III	4	4	50	50	100
	Core Theory-VIII Inorganic Chemistry - III		4	4	50	50	100
	Core Theory-IX	Physical Chemistry - III	4	4	50	50	100
Semester – III	Core Elective-II##	Research Methodology and Research Ethics	3	4	50	50	100
Seme	Core Practical-IV *	Electroanalytical Chemistry Practical	-	4	50	50	100
	Core Practical-V *	Analytical Chemistry Practical	-	4	50	50	100
	EDE II#	#	3	4	50	50	100
	Soft Skill-3	Self and Time Management Skills	2	2	50	50	100
	Summer Internship** Summer Internship **		2				
	Total	Credits: 22 / Total Hours per week	: 30				
	Core Theory – X Organic Chemistry - IV		4	4	50	50	100
	Core Theory – XI	Physical Chemistry - IV	4	4	50	50	100
IV	Core Elective – III##	##	3	4	50	50	100
Semester – IV	Core Practical-IV *	Electroanalytical Chemistry Practical	4	4	50	50	100
Sen	Core Practical-V *	Analytical Chemistry Practical	4	4	50	50	100
	Core –XII	Project	6	8	50	50	100
	Soft Skill-4	Spoken and Presentation Skills	2	2	50	50	100
	Total Credits: 27 / Total Hours per week: 30						
	Grand Total Credits: 95 / Total Hours : 120						

<sup>\*</sup> Practical Examinations are conducted once in an academic year – at the end of semester II and semester IV.

<sup>\*\*</sup>The students must undergo summer internship for three weeks after the second semester and the reports to be submitted.

The following elective courses are offered to the students of Chemistry department.

Elective –1: Analytical Chemistry

Elective –2: Research Methodology and Research Ethics

Elective –3: Chemistry of Natural Products

Elective –4: Nanochemistry and its applications

\*Any one EDE (Extra Disciplinary Elective) offered by other departments to be opted by the chemistry students in semester II and semester III.

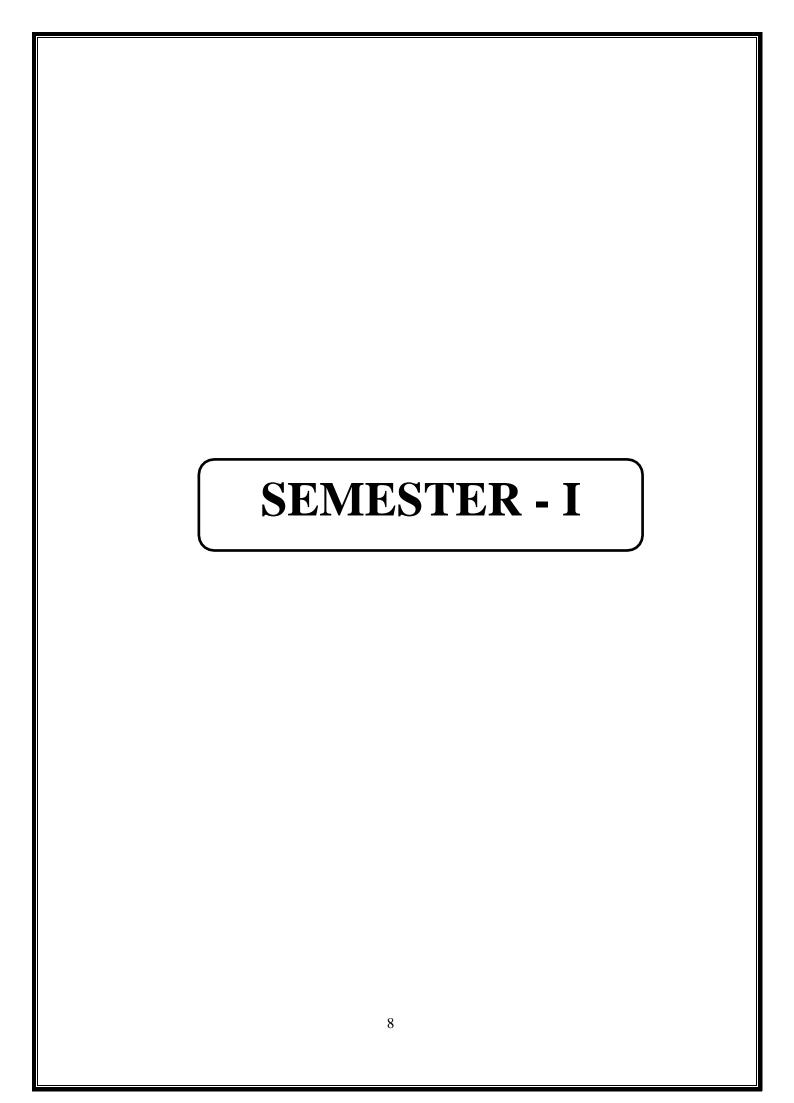
The following EDE courses are offered to other departments.

EDE - 1: Nutrition and Dietetics

EDE - 2: Applied Chemistry

EDE – 3 : Environmental Chemistry

EDE – 4 : Forensic Science



## GURU NANAK COLLEGE (AUTONOMOUS) CHENNAI-600042

# (Effective for the batch of candidates admitted from 2022–23) CORE THEORY-I ORGANIC CHEMISTRY-I

SUBJECT CODE:	THEORY	<b>MARKS: 100</b>
SEMESTER: I	CREDITS: 4	<b>TOTAL HOURS: 60</b>

#### **COURSE FRAMEWORK:**

- This course aims to explain basic concepts in stereochemistry and methods of determining reaction mechanisms.
- To explain synthetic application of aliphatic nucleophilic substitution, elimination reactions in organic syntheses.

#### **COURSE OUTCOME:**

On completion of the course the students will be able to

- 1. identify the absolute configuration of molecules–D/L, R/S, erythro /threo, meso/dl, E-Z, Pro R, Pro S, Re and Si face.
- 2. apply the concept to conformational analysis for cyclic and acyclic systems.
- 3. determine the reaction mechanism by kinetic and non-kinetic methods, mechanism and applications of aliphatic nucleophilic substitution reactions.
- 4. get a detailed picture of electrophilic, nucleophilic and free radical addition reaction mechanisms with stereo chemical aspects. Mechanism of carbene, nitrene intermediates and application in name reactions.
- 5. explain the reaction mechanism and stereo chemistry of E1, E2 and E1CB and to predict its regioselectivity

## **UNIT-I:** Stereochemistry–I

(15 hrs)

Optical activity - chirality- conditions for optical activity-asymmetry and dissymmetry - dissymmetry of allenes, biphenyls, para cyclophanes, ansa compounds and molecules with helical structures – absolute configuration – D/L and R/S notation of acyclic chiral molecules, allenes, biphenyls and spiro compounds – molecules with more than one asymmetric centre – erythro/threo and meso/dl configuration – Fisher-Projection – Newmann and Sawhorse projection- interconversion of projection formulae – prochiral centre - Crams rule and Prelogs rule-opticalpurity—enantiomeric excess—stereo specific and stereoselective reactions.

Geometrical isomerism: E-Z nomenclature of olefins and oximes- geometrical and optical isomerism of mono and disubstituted cyclopropane, cyclobutane, cyclopentane and cyclohexane derivatives - homotopic, enantiotopic and diastereotopic hydrogen - prochiral carbon (up to 10 carbons only)-pro R and pro S & Re and Si face-determination of configuration.

## **UNIT-II:** Stereochemistry–II

(10 hrs)

Conformation and conformational analysis - conformation of simple 1,2-disubstituted ethane derivatives- cyclopropane, cyclobutane, cyclopentane and cyclohexane derivatives-conformational freeenergy— conformational analysis of mono and disubstituted cyclohexanes and their streochemical feature (geometrical and optical isomerism) — conformation and stereochemistry of decalin and 9-methyldecalin-conformation of glucose.

Conformation and reactivity: steric and product development control – reduction of tertiary butyl cyclohexanone by hydride – stereo chemistry of oxidation of cis and trans tertiary butyl cyclohexanols by Cr (VI) – stereochemistry of the reaction between nitrous acid and  $\alpha$ -amino cyclohexanols. Asymmetric synthesis: Evans and Enders methods.

## UNIT-III: Methods of determining reaction mechanisms (15 hrs)

Kinetic and non-kinetic methods of determining reaction mechanisms-Thermodynamic and kinetic aspects - spectroscopic studies - Hammond's postulate - isotope effects – energy profile diagrams – intermediate *vs* transition state – product analysis and its importance – cross over experiments. Quantitative treatment of structure and reactivity – Hammett and Taft equations. Classification of solvents, solvent effects in organic chemistry–solute–solvent interactions–specific and non-specifics elective solvation.

 $S_N1$ ,  $S_N2$  and  $S_Ni$  mechanism-neighbouring group participation- reactivity, structural and solvent effects-substitution in norbornyl and bridge head systems-substitution by ambident nucleophiles such as cyano, nitro, phenoxide and ambident dianions-substitution at carbon doubly bonded to oxygen and nitrogen – alkylation and acylation ofamines, halogen exchange, von-Braun reaction, alkylation and acylation of active methylenecarboncompounds, hydrolysis ofesters, Claisen and Dieckmann condensations.

## UNIT-IV: Organic reaction mechanisms - Addition to carbon-carbon

## and carbon-hetero multiple bonds

(10hrs)

Mechanism - Electrophilic, nucleophilic and free radical addition. Addition of halogen, nitrosyl chloride to olefins, Hydration of olefins and acetylenes. Hydroboration, Hydroxylations and Michael addition. Diels-Alder reaction, 1,3 -dipolar additions. Carbene and their addition to double bond- Simmon –Smith reaction, Mannich, Stobbe, Darzen, Wittig, Wittig-Horner and Benzoin reactions. Nitrene: Methods for generating nitrenes and their reactions. (Stereochemical aspects be studied wherever applicable).

## **UNIT-V: Elimination Reactions**

(10 hrs)

E<sub>1</sub>, E<sub>2</sub> and E<sub>1</sub>CB mechanism – spectrum, orientation of the double bond – Hoffman and Saytzeff rule – competition, elimination and substitution. Typical eliminations to be studied – dehydration, dehydro-halogenation and similar reactions. Stereochemistry of E<sub>2</sub> eliminations in cyclohexanes and bicyclic systems. Mechanism of pyrolytic elimination. Examples: Chugaev and Cope elimination.

## **TEXTBOOKS:**

- 1. D.Nasipuri, Stereochemistry of Organic Compounds, 2<sup>nd</sup> edition, New Age Publishers, 2005.
- 2. March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure, 8<sup>th</sup> Edition, Michael B. Smith, 2019.

- 3. E.L.Eliel., S.H.Wilen, Stereochemistry of Organic Compounds, John Wiley & Sons, 2008.
- 4. Sachin Kumar Ghosh, Advanced General Organic Chemistry-A Modern Approach, Part I, 3<sup>rd</sup> Edition, 2010.
- 5. V.K.Ahluwalia, Rakesh Kumar Parashar, Organic Reaction Mechanisms, 4<sup>th</sup> edition, 2010.
- 6. R.T.Morrison, R.N.Boyd and S.K.Bhattacharjee, Organic Chemistry, Pearson Prentice hall, seventh edition, 2012.
- 7. Dr.Anup Pathak, Dr. Anupa Saha, Organic Chemistry, Volume I, 2<sup>nd</sup> Edition,2012.
- 8. P.S.Kalsi, Stereochemistry and Mechanism Through Solved Problems, New Age International Ltd, 5<sup>th</sup> edition, 2019.
- 9. P.S.Kalsi, Stereochemistry, Conformation and Mechanism, New Age New Academic Sciences, 10<sup>th</sup> edition,2020.
- 10. P.S.Kalsi, Organic reactions and their Mechanism, New Age International Ltd,5<sup>th</sup> edition,2021.

#### **REFERENCES:**

- 1. K.Mackie, M.Smith, P.Aitken, Guide Book to Organic Synthesis, ELBS, England, 3<sup>rd</sup> edition, 2000.
- 2. R.Bruckner, Advanced Organic Chemistry Reaction Mechanism, Elsevier, New Delhi, 2002.
- 3. J.Clayden, N. Greeves, S. Warren and P. Wothers, Organic Chemistry, Oxford University Press, 2<sup>nd</sup> edition, 2014.
- 4. F.A.Carey and R.J.Sundberg, Advanced Organic Chemistry, Parts A and B. Springer, 5<sup>th</sup> edition, 2015.

## **WEBLINKS**

- 1. www.epgpathshala.nic.in
- 2. <a href="https://nptel.ac.in/">https://nptel.ac.in/</a>
- 3. https://swayam.gov.in/
- 4. https://www2.chemistry.msu.edu/faculty/reusch/VirtTxtJml/intro1.htm

## **Question Paper Pattern**

Section	<b>Question Component</b>	Numbers	Marks	Total
Section- A	MCQ:1-10, Fill in: 11-15, T/F:16-20 Answer all questions	1 – 20	1	20
Section-B	Short Answer/Problems Answer any 5 out of 8 questions	21–28	7	35
Section-C	Essay Answer any 3 out of 5 questions	29-33	15	45
	100			

## **Distribution of Questions**

C4:	T T *4	No.o	f Questions
Section	Unit	Theory	Problem
	Unit– 1	4	
	Unit– 2	4	
Section-A	Unit–3	4	
	Unit–4	4	
	Unit–5	4	
	Unit– 1	1	1
	Unit– 2	2	
Section- B	Unit–3	1	1
	Unit–4	1	
	Unit–5	1	
	Unit- 1	1	
	Unit-2	1	
Section- C	Unit-3	1	
	Unit-4	1	
	Unit– 5	1	

## CORE THEORY-II INORGANIC CHEMISTRY-I

SUBJECT CODE:	THEORY	<b>MARKS: 100</b>
SEMESTER: I	CREDITS: 4	<b>TOTAL HOURS: 60</b>

## **COURSE FRAMEWORK:**

- To impart the knowledge about the theories on bonding, structure, properties and reactions of various coordination complexes.
- To impart the basics of reaction mechanisms and substitution reactions of coordination complexes
- To introduce the rings, cages and cluster type of inorganic compounds.
- To enunciate nuclear chemistry for higher learning.

## **COURSE OUTCOME:**

On completion of the course the students will be able to

- 1. discuss and compare the various theories of bonding in coordination complexes.
- 2. evaluate and apply the reaction mechanisms, stability constant, and the various methods of determination of stability constant and the stereochemistry of the inorganic complexes.
- 3. outline the mechanism of electron transfer reactions and Marcus -Hush theory and predict the substitution reaction of complexes.
- 4. explain and interpret the various models of nucleus and various nuclear reactions.
- 5. explain about the inorganic cages, clusters and rings which are very much useful for leading current research area of materials science.

## UNIT-I: Bonding and properties of coordination complexes (15 hrs)

Stereo isomerism of coordination complexes. Stability of metal complexes and determination of stability constants by Job's and Bjerrum's method. Introduction to CFT, CFSE, spectrochemical series and applications. High spin and low spin complexes-Magnetic properties of coordination compounds. Calculation of  $\Delta o$  and  $\Delta \tau$  and their relationship. Jahn-Teller tetrahedral distortion. Nephelauxetic effect, Molecular orbital theory-based on group theoretical approach, Symmetry of molecular orbitals formed from atomic orbital overlap, LCAO-MO model, TASO, LUMO and HOMO concepts inbonding. M.O. diagrams of octahedral, tetrahedral and square planar complexes.

## **UNIT-II: Reactions in coordination compounds**

(15hrs)

Labile and Inert complexes. Substitution reaction in octahedral complexes – general mechanism, general rate law for A, D and I - distinction between D, Id, IA pathways, replacement of coordinated water, mechanism of acid hydrolysis, base hydrolysis – DCB mechanism –direct and indirect evidences in favor of the mechanism. Stereochemical changes in dissociation (S<sub>N</sub>2) and displacement (S<sub>N</sub>2) mechanism through various geometries of coordination compounds. Ligand substitution reactions without cleavage of M-L bond. Anation reactions. Substitution in square planar complexes – general mechanism, Trans effect, influences of entering and leaving groups. Application of trans effect – synthesis of isomers of Pt(II) and Co(III) complexes – theories of trans effect.

Stereoisomerism in inorganic complexes, Optical rotatory dispersion (ORD) and circular dichroism (CD). Isomerization and racemization reactions in octahedral complexes.

## **UNIT –III:** Coordination chemistry - Reaction mechanisms

Electron transfer reactions – Inner sphere (ISET) and outer sphere (OSET) electron transfer processes. Key ideas concerning electron transfer between transition metals. Chemical activation and electron transfer, role of bridging ligand with ISET reaction – tunneling transfer – multiple bridging in the activated complex in the ISET process. Complimentary and non- complimentary ET reactions. Cross reactions and Marcus-Hush theory.

## **UNIT-IV: Nuclear Chemistry**

(10 hrs)

(10 hrs)

Nuclear structure: Composition of the nucleus, nuclear size, shape and density, nuclear models: shell model-salient features, filling of orbitals, nuclear configuration, Liquid drop model, theories of nuclear forces – pi-meson theory. Nuclear reactions: types of nuclear reactions, nuclear fission, fission products, theory of nuclear fission. Orbital electron capture, kinetics of nuclear reactions (t<sub>1/2</sub> and decay constant) - applications of carbon dating and rock dating. Discovery of artificial radioactivity, synthesis of transuranium elements, importance and applications of artificial radioactivity, production and separation of radioactive isotopes.

## **UNIT-V: Inorganic Rings, Cages and Clusters**

(10hrs)

Clusters: Boranes, carboranes, metallo boranes and metallo carboranes- synthesis and structure of neutral boron hydrides, polyhedral borane anions and dianions, capping rules, PSEPT (Wade's rules). Low nuclearity metal-carbonyl clusters and 14 n+2 rule, high nuclearity metal-carbonyl and other clusters (Rhenium cluster complexes) with internal atoms.

Boron-nitrogen compounds: Borazines and B-N clusters. P-N and P-S compounds: polyphosphazene and cyclic aminophosphanes, phosphorus-oxide and phosphorus-sulfide cages. Sulfur-nitrogen compounds.

Isopoly and heteropoly acids and salts (Mo, W, V, Nb and Ta), Heteropoly anions-structure and reactivity; heteropoly blues. Macrocyclic ligands; types- Schiff bases; crown ethers and cryptands and porphyrins.

#### **TEXTBOOKS:**

- P.W. Atkins, T. Overton, J. Rourke, M. Weller and F. Armstrong; Shriver and Atkins: Inorganic Chemistry, 5<sup>th</sup> Edition, Oxford University Press, 2013.
- 2. J. E. Huheey, E. A. Keiter, R.L. Keiter and O. K. Medhi, Inorganic Chemistry Principles of structure and reactivity, 4<sup>th</sup> Edition, Pearson, 2013.
- 3. C. E. Housecroft and A. G. Sharpe, Inorganic Chemistry, 4<sup>th</sup> edition, Prentice-Hall, 2012.
- 4. K.F. Purcell and J.C. Kotz, Inorganic Chemistry, Sengage Learning India Pvt. Ltd, 1<sup>st</sup> edition, 2010.
- Karl H. Lieser, Nuclear and Radiochemistry: Fundamentals and Applications, 2<sup>nd</sup> edition, 2001, Wiley, NY.
- 6. H. J. Arnikar, Essentials of Nuclear Chemistry, 4<sup>th</sup> edition, New Age Publishers, 1995.
- 7. D. M. P. Mingos, David J. Wales, Cluster Chemistry, Prentice Hall, 1990.

## **REFERENCES:**

- 1. M.C. Day and J. Selbin, Theoretical Inorganic Chemistry, Literary Licensing, LLC, 2012.
- 2. I. Kaplan, Nuclear Physics, 2<sup>nd</sup> edition, Narosa Book Distributors Pvt. Ltd.
- **3.** G. . Friedlander, J. W. Kennedy, E. S. Macias and J. M.Miller, Nuclear and Radiochemistry, John Wiley & Sons, 1985.
- 4. D. Banerjea, Coordination Chemistry, 2<sup>nd</sup> edition, Asian Books Pvt. Ltd. ,2007.

## **WEBLINKS:**

- 1. https://www.chemicalforums.com/
- 2. https://nptel.ac.in/
- 3. https://chem.libretexts.org/
- 4. http://www.ilpi.com/genchem/web.html#12

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Section- C	Essay Answer any 3 out 5 questions	29–33	15	45
TOTAL MARKS				100

## **Distribution of Questions**

G	TT .*4	No.of	<b>Questions</b>
Section	Unit	Theory	Problem
	Unit-1	4	
	Unit–2	4	
Section -A	Unit–3	4	
	Unit-4	4	
	Unit–5	4	
	Unit-1	2	
	Unit–2	1	
Section-B	Unit-3	1	
	Unit-4	2	
	Unit–5	2	
	Unit-1	1	
	Unit–2	1	
Section- C	Unit-3	1	
	Unit-4	1	
	Unit–5	1	

## CORE THEORY-III PHYSICAL CHEMISTRY-I

SUBJECT CODE:	THEORY	<b>MARKS: 100</b>
SEMESTER: I	CREDITS: 4	<b>TOTAL HOURS: 60</b>

#### **COURSE FRAMEWORK:**

- To learn the basic concepts in group theory and the need for quantum mechanics and appreciate their significance.
- To learn the basic concepts in chemical kinetics.

## **COURSE OUTCOME:**

On completion of the course the students will be able to

- 1. analyze the need for quantum mechanics, relate quantum mechanical operators to observables and the use of operator algebra to solve simple eigen value equations, relate molecular phenomena viz. translational, rotational and vibrational motion to model systems and solve Schrodinger equation to arrive at the eigen values.
- 2. distinguish molecular and crystallographic symmetry, to assign point group for molecules, apply multi symmetry operations to derive character tables.
- 3. gain knowledge of symmetry-based selection rules for vibration land electronic spectroscopy and predict the IR and Raman activity of a molecule.
- 4. acquire in depth knowledge about theories of chemical kinetics and to calculate specific rate, activation energy and frequency factor.
- 5. calculate Michaelis-Menten constant for enzyme—substrate binding by Lineweaver-Burk plot.

## UNIT-I: Quantum Chemistry-I

(12hrs)

Inadequacy of classical theory-blackbody radiation-photo electric effect-Compton effect- Bohr's Quantum theory and subsequent developments-wave particle duality-deBroglie equation- Heisenberg's uncertainty principle. Quantum mechanical postulates - Schrodinger wave equation- elementary applications of Schrodinger equation- the particle in a box(one, two and three dimensional cases) –particle in aring.

## **UNIT-II:** Group Theory-I

(12hrs)

Symmetry elements and symmetry operations-point groups-identification and determination. Reducible and irreducible representations- direct product rep resentation-Orthogonality theorem-its consequences-character table.

## **UNIT-III: Group Theory-II**

(12 hrs)

Hybrid orbitals in non-linear molecules-(CH<sub>4</sub>, XeF<sub>4</sub>, BF<sub>3</sub>, SF<sub>6</sub> and NH<sub>3</sub>). Symmetry based selection rules for infrared, Raman and electronic spectra of ethylene and formaldehyde.

#### UNIT-IV: Chemical Kinetics-I

(12 hrs)

Effect of temperature on reaction rates-collision theory of reaction rates-molecular beams- collision cross sections-effectiveness of collisions-probability factors-potential energy surfaces-partition functions-and activated complex. Eyring equation-estimation of free energy and entropy of activation and their significance.

## **UNIT-V: Chemical Kinetics-II**

(12 hrs)

Reactions in solutions-effect of pressure, dielectric constant and ionic strength on reactions in solutions- kinetic isotope effects —linear free energy relationships-Hammett and Taft equations.

## **TEXTBOOKS:**

- D.A. McQuarrie, Quantum Chemistry, University Science books, viva books Pvt.Ltd.,
  - 2<sup>nd</sup> edition, reprint, 2016.
- 2. I.N.Levine, Quantum Chemistry, Pearson Education Pvt.Ltd.,7<sup>th</sup> edition, 2016.
- 3. R.Anantharaman, Fundamentals of Quantum Chemistry, Macmillan India Limited, 2<sup>nd</sup> edition, 2004.
- 4. R.K.Prasad, Quantum Chemistry, New Age India, 4<sup>th</sup> edition, 2020.
- V.Ramakrishnan and M.S.Gopinathan, Group theory in Chemistry, Vishal Publication,
  - 2<sup>nd</sup> edition, Reprint 2013.
- K.V.Raman, Group theory and applications in Chemistry, Tata McGraw Hill, 3<sup>rd</sup> Edition 1994.
- 7. S. Swarnakakshmi, T.Saroja, R.M.Ezhilarasi, A Simple approach to group theory in Chemistry, Universities Press, Kindle edition, 2019.
- R.K.Prasad, Quantum Chemistry-theory solved problems and solutions, NewAge International publishers, Reprint 2017.

- J.Rajaram and J.C.Kuriacose, Kinetics and Mechanism of Chemical Transformations, McMillan India Ltd., 3<sup>rd</sup> edition,reprint,2009.
- 10. K.J.Laidler, Chemical Kinetics, Harper and Row, Pearson Pvt. Ltd., New York, 3<sup>rd</sup> edition, 2011.
- 11. K.L. Kapoor, A text book of Physical Chemistry, Macmillan India Ltd, reprint, 2010.

## **REFERENCES:**

- F.A.Cotton, Chemical application of group theory, John Wiley & Sons Inc., New Delhi, 3<sup>rd</sup> edition, 2009.
- Alan Vincent, Molecular Symmetry and Group theory-Programmed Introduction to chemical applications, Wiley, NewDelhi, 2<sup>nd</sup> Edition, 2013.
- 3. H.Eyring, J.Walter and G.Gimball, Quantum Chemistry, John Wiley & Sons Inc., New York, 1944.
- 4. L.S.Pauling and F.B.Wilson, Introduction to quantum mechanics with to a application chemistry, McGraw Hill Book Company, NewYork, 2015
- 5. Peter Atkins and Ronald Friedman Molecular quantum mechanics, Oxford University Press,Oxford, 5<sup>th</sup> edition, 2011.
- 6. David J.Griffiths, Introduction to Quantum mechanics, Cambridge University Press,3<sup>rd</sup> edition, fifth reprint,2018.
- 7. G.M.Barrow, Physical Chemistry, TataMcGraw Hill, 5<sup>th</sup> edition, 2008.
- 8. R.G.Frost and Pearson, Kinetics and Mechanism, Wiley, New York, 3<sup>rd</sup> edition, 1981.
- 9. W.J.Moore and R.G. Pearson, Kinetics and Mechanism, Wiley, New York,3<sup>rd</sup> edition,1981.

## WebLinks:

- 1. www.chemguide.co.uk>physical>basicrates>energyprofiles
- 2. iopscience.iop.org
- 3. http://nptel.ac.in
- 4. mooc.org
- 5. http://www.ch.ic.ac.uk/achemlab/symmetry/
- 6. http://www.reciprocalnet.org/edumodules/symmetry/intro.html

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TOTAL MARKS				100

## **Distribution of Questions**

Castion	TT:4	No. o	of Questions	
Section	Unit	Theory	ory Problem	
	Unit-1	4		
	Unit-2	4		
Section- A	Unit–3	4		
	Unit-4	4		
	Unit-5	4		
	Unit-1	1	1	
	Unit-2	1		
Section -B	Unit-3	2		
	Unit-4	1		
	Unit–5	2		
	Unit-1	1		
	Unit-2	1		
Section -C	Unit-3	1		
	Unit-4	1		
	Unit5	1		

## CORE ELECTIVE-I ANALYTICAL CHEMISTRY

SUBJECT CODE:	THEORY	<b>MARKS: 100</b>
SEMESTER: I	CREDITS: 3	<b>TOTAL HOURS: 60</b>

#### **COURSE FRAMEWORK:**

- To create the better understanding of "Analytical Chemistry" to evolve proper analytical data and practice to report the result with uncertainty.
- To enhance the competency in the analysis of complex materials and also the finished products of chemical manufacturing sectors; to enable the instrumental based chemical analysis in all the arena of chemical processes.
- To establish the competency of chemical analysis in applied research, chemical processes and testing/quality control laboratories with a view to eliminate the gap between academics and industry and also between basic and applied sciences.

## **COURSE OUTCOME:**

On completion of the course the students will be able to

- 1. develop analytical skill in chemistry; to evolve proper analytical data and practice to report the results with uncertainty component.
- 2. explore the analysis of complex chemical materials / manufactured chemical matrices very systematically with suitable analytical methods.
- 3. demonstrate the instrumental based chemical analysis in all the arena of chemical processes and products through separations, quantifications and structural determination of chemicals.
- 4. establish the competency of chemical analysis in the applied research, chemical processes and testing / quality control laboratories with regulatory compliances.
- 5. design new analytical routes for the day-to-day evolution of newly discovered chemical products.

## UNIT-I: Fundamentals in chemical analysis and analytical laboratory functioning (10hrs)

Statistical treatment of analytical data: regression analysis, standard deviation-comparison of results- F, T and Q tests. Calibrations – general idea of calibration, calibration of glassware, balance, instruments and other equipment. Uncertainty in chemical analysis: theory, significance, sources of uncertainty for simple volumetric analysis. Sampling of solid, liquid and gases – primary sample, laboratory sample, analytical sample, handling, collection, transport, storage.

Details on method development and method validation in chemical analysis, essentials of quality control and quality assurance systems in chemical processes; Basic idea and necessity of accreditations/certification such as GLP, ISO(NABL),FDA and FSSAI. Role of ISI and Agmark certification on the consumer products.

## **UNIT- II: Analysis of complex materials and atomic spectroscopy** (15 hrs)

Physico-chemical analysis of medicines (formulated), ores, fertilizers, alloys, packed foods, water and air. [Note: Any one representative example in each category and testing of important parameters only.]

Theory, instrumentation and applications of atomic absorption, spectroscopy ICP-MS; Flame emission spectrometry and ICP-OES. Application of these techniques in water and food analysis. Moisture analyser (KFRmethod) and C,H,N analysis (instrumental methods).

## **UNIT-III:** Separation techniques

(15 hrs)

Chromatographic techniques: classification, principle, instrumentation (if applicable) and applications of column ,ion-exchange, electrophoresis, TLC, paper chromatography, GLC and HPLC (with different detectors) and GPC. Special emphasis on GC- MS, GC-MS/MS, LC-MS, LC-MS/MS. Role of chromatographic techniques in R&D and quality control laboratories.

## **UNIT-IV:** Electroanalytical methods

(12hrs)

Polarography – Theory and instrumentation. Type sof current- includes kinetic & catalytic current and advantages and disadvantages of DME. Significance of Ilkovic equation and its significance. Qualitative and quantitative applications to the analysis of inorganic compounds and determination of dissolved oxygen. Cyclic voltammetry – theory, instrumentation and applications to inorganic and organic compounds. Application of CV in applied research viz.,prediction of reaction mechanism, redox behavior of chemical compounds and identification of number of electrons in the electrochemical processes. Amperometry and biamperometry-theory, instrumentation and applications. EIS Technique in Chemical Analysis

## **UNIT-V:** Thermal and radioanalytical techniques

(8 hrs)

Principle, instrumentation and applications of TGA, DTA and DSC. Radio isotopes, Radio analytical methods-principle, instrumentation and applications of neutron activation

and isotopic dilution analysis. Radiometric titrations, radiometric methods in diagnosis of diseases.

## **TEXTBOOKS:**

- 1. David Harvey; Modern Analytical Chemistry; McGraw-Hill, 1st edition, 2000.
- 2. J.Mendham, R.C.Denney, J.D.Barnes and M.Thomas, Vogel's Text book of quantitative Chemical Analysis; Pearson Education Pvt.Ltd.6<sup>th</sup> edition,2004.

## **REFERENCES:**

- 1. E.Prichard, Quality in the analytical chemistry aboratory, John Wiley and sons, 1997.
- 2. W.Funk, V.Dammann, G.Donnevert, Quality assurance in analytical, VCH Weinheim, 1995.
- 3. Douglas A. Skoog, Donald M. West and F. James Holler, Fundamentals of Analytical Chemistry; 9<sup>th</sup> edition, Harcourt Asia Pvt., Ltd., 2014.
- 4. Douglas A. Skoog, Donald M. Westand F. James Holler, Analytical Chemistry:
  An Introduction; 7<sup>th</sup> edition, Saunders College Publishers, 2000.
- 5. Dean, John A. Merritt, Lynne L., Jr. Settle, Frank A., Jr. Willard, Hobart H;Instrumental Methods of Analysis, Wadsworth Publishing, seventh Edition,1988.
- 6. D.A. Skoog, Principles of Instrumental Analysis, 5th ed., Saunders College Publishing, Philadelphia, London, 1998.
- 7. A.J.Bard and L.R.Faulkner, Electro chemical methods, JohnWiley,1980.
- 8. S.M.Khopkar, Environmental Pollution Analysis, New Age International publication, 2011.
- 9. Seonard'l Ciacere, Water and water pollution (hand book), Vol I to IV, Marcel Dekkerinc.N.Y,1972.
- 10. Guidelines for drinking-water quality, 3<sup>rd</sup> edition, (incorporating first and second addenda), WHO report.
- 11. Martin Hocking, Handbook of chemical technology and pollution control, AP Publication, 3<sup>rd</sup> edition, 2005.
- 12. Chemical analysis of metals; Sampling and analysis of metal bearing ores: American Society for Testing and Materials Technology & Engineering, 1980.
- 13. Manual of Procedures for Chemical and Instrumental Analysis of Ores, Minerals, and Ore Dressing Products. Government of India, Ministry of Steel & Mines, Indian Bureau of Mines, 1979.

- 14. Yeshajahu Pomeranz, Clifton E. Meloan, Food Analysis: Theory and practice, Springer, 3<sup>rd</sup> edition, 2002.
- 15. George Charalanbous, Analysis of food and beverages, Academic press, 1978.
- 16. Connor's Text book of Pharmaceuticals Analysis, John Wiley, 3<sup>rd</sup> edition, 2001.
- 17. Encyclopaedia of industria lchemical analysis, Snelletal; Interscience, 1966.

## Weblinks:

- 1. https://chem.libretexts.org/
- 2. https://nptel.ac.in/course.html
- 3. https://www.lcresources.com/resources/reslinks.html
- 4. https://www.chemicalforums.com/index.php?PHPSESSID=kj kh7lljum5hebhscma2hhlsp7&board=8.0
- 5. Refer websites of ISO, NABL, FDA, USEPA, ASTM, ICH, FSSAI and BIS

## Visits to:

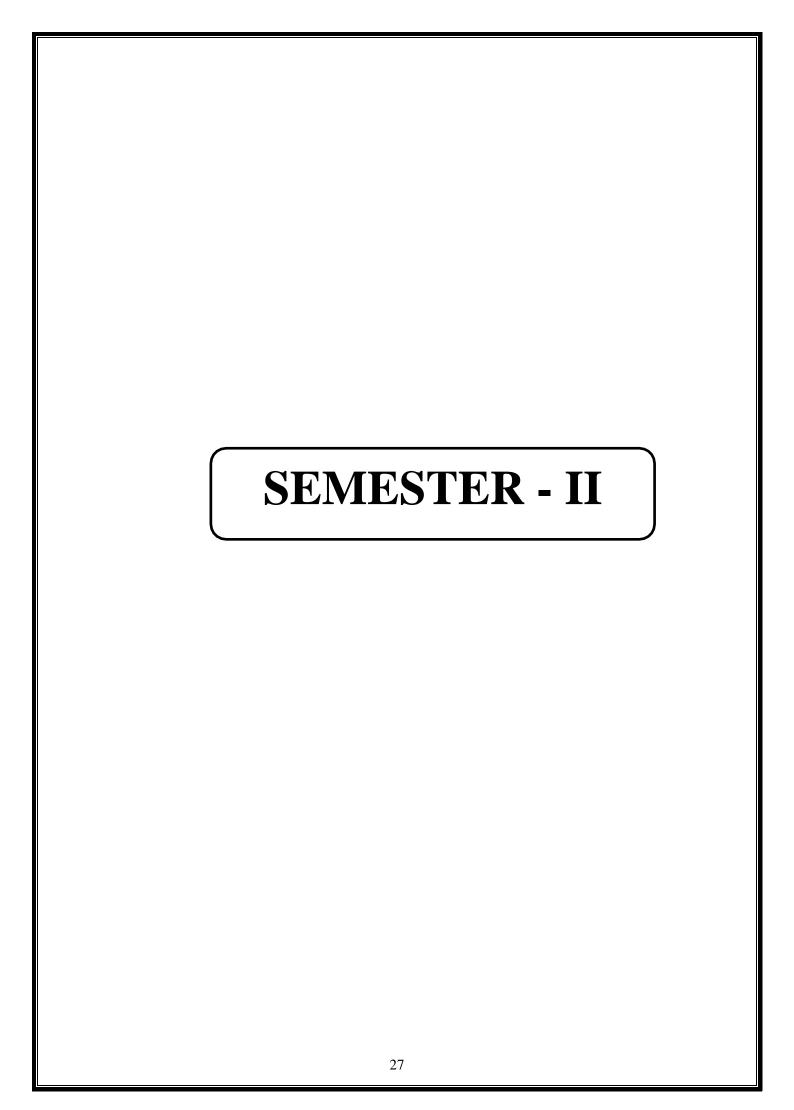
- 1. GLP, ISO and FDA certified R&D and QC laboratories.
- 2. BIS & FSSAI approved establishments.
- 3. Various chemical industries with established analytical laboratories.

## **Question Paper Pattern**

Section	Question Component	Numbers	Marks	Total
Section- A	MCQ:1-10, Fillup: 11-15, T/F:16-20 Answer all questions	1 – 20	1	20
Section- B	Short Answer /Problems Answer any 5 out of 8questions.	21–28	7	35
Section -C	Essay Answer any 3 out of 5 questions	29–33	15	45
TOTAL MARKS				100

## **Distribution of Questions**

Section	Unit	No. of Questions		
		Theory	Problem	
	Unit-1	4		
	Unit-2	4		
Section -A	Unit-3	4		
	Unit-4	4		
	Unit-5	4		
	Unit- 1	1	1	
	Unit-2	1		
Section –B	Unit–3	1	1	
	Unit-4	2		
	Unit–5	1		
	Unit– 1	1		
	Unit-2	1		
Section –C	Unit-3	1		
	Unit-4	1		
	Unit-5	1		



## CORE THEORY-IV ORGANIC CHEMISTRY- II

SUBJECT CODE:	THEORY	<b>MARKS: 100</b>
SEMESTER: II	CREDITS: 4	<b>TOTAL HOURS: 60</b>

#### **COURSE FRAMEWORK:**

- This paper explains the concepts of aromatic compounds, their electrophilic and nucleophilic substitution reactions.
- In addition, mechanism of some of the important rearrangements and pericyclic reactions in organic chemistry will be discussed.
- The first part of the course brings forth the salient features of oxidation and reduction reactions in organic synthesis.

## **COURSE OUTCOME**

On completion of the course the students will be able to

- 1. use oxidation and reduction reagent for preparing a new synthetic compound.
- 2. apply the concept of aromaticity to identify aromatic, anti-aromatic and non-aromatic compounds.
- 3. apply logically the concept of direction for both electrophilic and nucleophilic reactions in aromatic compounds.
- 4. identify the different types of rearrangement reactions and predict the mechanisms involved.
- 5. use the Woodward-Hoffmann rule to predict the stereochemistry of product under thermal and photochemical conditions for different types of pericyclic reaction.

## **UNIT-I: Oxidation and Reduction**

(15 hrs.)

Mechanism – study of the following oxidation reactions – use of chromium(VI),MnO<sub>4</sub>-, MnO<sub>2</sub>, TPAP, Moffatt, Oppenauer and Swern oxidation of alcohol–oxidative cleavage of glycols and their related compounds, Oxidative cleavage of ketones, aldehydes and alcohols, ozonolysis- oxidation of methylene to carbonyl, oxidation of aryl methane – allylic oxidation of olefins. Reductions: catalytic hydrogenation – hydrides – nucleophilic and electrophilic -MPV reduction- selectivity in reduction of 4-t-butyl cyclohexanones using selectrides-synthetic importance of Clemmensen and Wolf-Kishner reductions-Modifications of Wolf-Kishner reduction-Birch reduction.

## UNIT-II:Aromatic electrophilic and nucleophilic substitutions (15 hrs)

Aromatic electrophilic substitution: The arenium ion mechanism. Orientation and reactivity of mononuclear, polynuclear aromatic hydrocarbons (Naphthalene, Anthracene) and Heterocyclic compounds (Quinoline and Isoquinoline) nitration, halogenations, sulphonation, alkylation, acylation and diazonium coupling. Formylation reactions (Gattermann, Gattermann-Koch, Vilsmeyer-Haack and Riemer-Tiemann reaction)-synthesis of di and tri substituted benzenes (symmetrical tribromobenzene, 2-Amino-5-methylphenol, 3-nitro-4-bromobenzoicacid, 3,4-dibromonitrobenzene,1,2,3-trimethylbenzene) starting from benzene or any monosubstituted benzene.

Aromatic nucleophilic substitution: Methods for the generation of benzyne intermediate and reactions of aryne intermediate- nucleophilic substitution involving diazonium ions. Aromatic nucleophilic substitution of activated halides. Ziegler alkylation. Chichibabin reaction and von-Richter rearrangement.

## **UNIT-III: Aromaticity**

(10 hrs)

Concept of aromaticity, Huckel's rule, Craig's rule – Huckel MO theory of aromaticity frost cycle Alternant and Non-alternant hydrocarbons –Aromaticity of benzenoid, heterocyclic and non-benzenoid compounds systems with 2, 4, 8 and 10 electrons – Annulenes (up to C18) compounds, azulene, ferrocene, tropolone and sydnones. Concept of homo aromatic and hetero aromatic molecules.

## **UNIT-IV: Pericyclic Reactions**

(10 hrs)

Introduction-construction of  $\pi$  molecular orbitals of ethylene and 1,3-butadiene, symmetry in  $\pi$  molecular orbitals. Classification- electrocyclic reactions – Woodward Hoffmann rule- (4n)  $\pi$  and (4n+2)  $\pi$  systems- Ring opening and ring closing reactions - interconversion of cyclobutene-butadiene system and interconversion of cyclohexadiene-hexatriene, FMO analysis, Correlation diagram method.

Cycloaddition-Woodward Hoffmann rule in  $(\pi 2s+\pi 2s)$  and  $(\pi 4s+\pi 2s)$  cycloaddition reactions-FMO analysis and Correlation diagram method. Diels-Alder reaction-Retro Diels-Alder reactions. Cheleotropic Reactions-[2+2]Cheleotropic cycloaddition, Cheleotropic Elimination (Basic idea only) Sigmatropic rearrangements – Classification- Woodward-Hoffmann rule– FMO analysis of [1,3], [1,5] and [1,7] hydrogen shift reactions – carbon shift reactions. [3,3] sigmatropic shifts–Cope and Claisen Rearrangement, Degenerate Cope reaction. Fluxional isomerism semibullyalene and bullyalene.

## **UNIT-V:** Molecular rearrangements

(10 hrs)

A study of mechanism of the following rearrangements: Beckmann, Curtius, Hofmann, Schmidt, Lossen, Wolff, Pinacol, Wagner Meerwin, Demjanov, Dienone-Phenol, Favorski, Benzidine, Claisen, Cope, Sommlet-Hauser, Pummerer and Von-Richter rearrangements. A study of the following name reactions: Dieckmann cyclization, Hofmann-Loffler Freytag reaction, Shapiro reaction, Eschenmoser-Tanabe and Ramburg-Backlund reactions.

#### **TEXTBOOKS:**

- 1. R.Bruckner, Advanced Organic Chemistry, Reaction Mechanism, Elsevier, NewDelhi,2002.
- 2. J. March, Advanced Organic Chemistry; Reactions, Mechanisms and Structure, Wiley interscience,6<sup>th</sup> edition,2007.
- 3. Sachin Kumar Ghosh, Advanced General Organic Chemistry-A Modern Approach, Part I, 3<sup>rd</sup> Edition, 2009.
- 4. V.K.Ahluwalia, Rakesh Kumar Parashar, Organic Reaction Mechanisms, 4th edition, 2009
- 5. T.L.Gilchrist and C.W.Rees, Carbenes, Nitrenes and Arynes, Thomas Nelson and Sons Ltd.,London,1969.
- 6. Jagdamba Singh and Jaya Singh, Photochemistry and Pericyclic reaction, New Academic Sciences Limited ,3<sup>rd</sup> edition,2012.
- 7. Ratan Kuma rKaur, Frontier Orbital and Symmetry Controlled Pericyclic reaction ,Books & allied Pvt.Ltd.,1<sup>st</sup> Edition,2010.
- 8. P.S.Kalsi,Organic reactions and their Mechanism, New Age International Ltd, 5<sup>th</sup> edition, 2021.

## **REFERENCES:**

- 1. F.A.Carey and R.J.Sundberg, Advanced Organic Chemistry, Part A and Part-B, Springer (INc), 5<sup>th</sup> edition,2015.
- 2. J.Clayden, N. Greeves, S. Warren and P. Wothers, Organic Chemistry, Oxford University Press, 2<sup>nd</sup> edition, 2014.
- 3. R.O.C.Norman and J.M.Coxon, Principles of organic synthesis, CRC Press, 3<sup>rd</sup> edition,2012.
- 4. W.Carruthers and Goldham, Some Modern Methods of Organic Synthesis,

- Cambridge University Press, 4th edition,2012.
- 5. H.O.House, Modern Synthetic Reactions, The Benjamin Cummings Publishing Company, London,1972.

## **WEBLINKS**

- 1. www.epgpathshala.nic.in
- 2. https://nptel.ac.in/
- 3. https://swayam.gov.in/
- 4. https://www2.chemistry.msu.edu/faculty/reusch/VirtTxtJml/intro1.htm

## **Question Paper Pattern**

Section	<b>Question Component</b>	Number s	Mark s	To tal
Section-A	MCQ:1-10, Fill in: 11-15, T/F:16-20 Answer all questions	1 – 20	1	20
Section- B	Short Answer /Problems Answer any 5 out of 8questions	21–28	7	35
Section- C	Essay Answer any 3 out of 5 questions	29–33	15	45
TOTAL MARKS			100	

## **Distribution of Questions**

C4:	Unit	No. of Questions		
Section		Theory	Problem	
	Unit– 1	4		
	Unit–2	4		
Section A	Unit–3	4		
	Unit–4	4		
	Unit–5	4		
	Unit– 1	2		
	Unit– 2	1		
Section B	Unit–3	1	1	
	Unit–4	1		
	Unit–5	1	1	
	Unit– 1	1		
	Unit-2	1		
Section C	Unit–3	1		
	Unit–4	1		
	Unit–5	1		

## CORE THEORY-V INORGANIC CHEMISTRY - II

SUBJECT CODE:	THEORY	MARKS: 100
SEMESTER: II	CREDITS: 4	<b>TOTAL HOURS: 60</b>

## **COURSE FRAMEWORK:**

- To expose the student to the basics of organometallic chemistry, reactions of organometallic complexes and their industrial applications.
- To educate the bioinorganic compounds to understand their functions and applications in biological systems
- To empower a thorough learning of solid-state chemistry and magnetic properties of solids and to introduce the recent advancements in the field of materials science.

## **COURSE OUTCOME:**

On completion of the course the students will be able to

- 1. analyze the structure, bonding and reactivity of organometallic compounds, assess about synthetically useful transformations and gain information on the mechanism of the catalytic processes of organo metallic complexes that is useful for the current synthetic organic chemistry field.
- 2. identify elaborately on the content of biological inorganic processes that helps the students in the future research of biomimetics and computational chemistry.
- 3. utilize the complete knowledge on the oxygen carriers and iron sulphur proteins and able to analyze how metal ions take part in biological system and their physiological effect on biological system and to compile photosynthesis and photosystem1 and photosystem 2, vitamin B12 model system and their reaction.
- 4. explain the complete description of chemistry behind the solids and to analyze the preparation, characterization of solids and describe the principles concerning solid state structures and to describe specific crystal structures by applying basic crystallographic concepts.
- 5. explore the magnetic properties of solids and its recent applications in various field.

## **UNIT – I: Organometallic compounds**

(15 hrs)

Synthesis, structure, bonding and reactivity of metal alkyls, carbenes, alkenes, alkynes, DCD model, arene complexes - metallocenes and bent metallocenes (Ferrocenes, Zirconium and Titanium complexes). Organometallic reactions: association, substitution, addition, oxidative addition, reductive elimination, insertion and deinsertion, electrophilic and nucleophilic attack on ligands and fluxional isomerism. Catalytic applications of organometallics: Hydrogenation of olefins, Wacker-Smidt synthesis, oxo process, Repp's catalyst, Monsanto acetic acid process, Zeigler-Natta polymerization of alkenes and oligomerisation, Enantioselective functional group interconversions. Transmetallation and cyclization reaction of organometallics.

## UNIT-II:Bio-inorganic chemistry -I

(10 hrs)

Introduction to Bio-inorganic chemistry. Metal Storage, Transport and Bio mineralization; ferritin, transferrin and siderophores, sodium and potassium ion balance. Essential and trace metal ions. Metalloenzymes - Zinc enzymes - carboxypeptidase and carbonic anhydrase, Vitamin B12, catalase, peroxidase, superoxide dismutase and copper proteins. Medicinal applications of coordination compounds— anti rheumatoid - gold compound—anti diabetic - anti cancer agents— role of metal ions in diagnosis and treatment-Cisplatin.

## **UNIT-III: Bio-inorganic chemistry -II**

(10hrs)

Oxygen Carriers — Haemoglobin, myoglobin — structure — function — Oxygenation and stereochemistry — Bohr effect, Non — heme oxygen carriers — Hemerythrin and Haemocyanin. Biological redox systems: cytochromes — classification, cytochrome a, b and c. Cytochrome P-450, Iron — sulphur proteins — rubredoxin and ferridoxin. Chlorophylls and photosynthesis — structure, function and mechanism. Nitrogen fixation — introduction — types of nitrogen fixing microorganisms, Nitrogenase enzyme — Metal clusters in nitrogenase — redox property — Dinitrogen complexes — nitrogen fixation via nitride formation and reduction of dinitrogen to ammonia.

## **UNIT-IV: Solid State Chemistry - I**

(13 hrs)

Glide plane and screw axis, point group and space group. Structural aspects of rock salt, rutile, fluorite, antifluorite, zinc blende, wurtzite, crystobalite, spinels, inverse spinels. Single crystal analysis and its applications. Powder diffraction - refinement and structure solution of some compounds, indexing with JCPDS and its application. Band theory of solids – band gap, conduction mechanism, temperature dependence of conductivity, intrinsic and extrinsic semiconductors.

## **UNIT – V:** Solid State Chemistry - II

(10hrs)

Crystal defect, lattice defects - stoichiometric and non-stoichiometric defects, defect formation. Determination of defects, thermodynamics of Schottky and Frenkel defect and incorporation of stoichiometric excess defects (structural and thermodynamic aspects). Phase transitions, diffusion, diffusion coefficient, diffusion mechanisms, vacancy and interstitial diffusion. Inorganic phosphors- synthesis and applications. LED, FED – an introduction, Lasers- introduction and types, Inorganic laser - instrument and principle, Ruby, Nd: YAG laser – working and mechanism. Domain theory – Hysteresis Loop – applications. Properties of pervoskites and magneto-plumbites- Hard and Soft magnetic materials- superconductivity in metals, alloys and ceramics materials (mixed oxides)- BCS theory, Meissner effect.

#### **TEXT BOOKS:**

- 1. J. E. Huheey, E. A. Keiter, R.L. Keiter and O. K. Medhi Inorganic Chemistry Principles of structure and reactivity, 4<sup>th</sup> Edition, Pearson, 2013.
- 2. C. E. Housecroft and A. G. Sharpe, Inorganic Chemistry, 4<sup>th</sup> edition, Prentice-Hall, 2012.
- 3. K.F. Purcell and J.C. Kotz, Inorganic Chemistry, Sengage Learning India Pvt. Ltd,1<sup>st</sup> edition, 2010.
- 4. Dr. B.D. Gupta, Dr. Anil J. Elias, Basic Organometallic Chemistry: Concepts, Syntheses and applications, 2<sup>nd</sup> Edition, University Press, 2013.
- 5. Rossette M. Roat Malone, Bio-inorganic Chemistry: A short course, 2<sup>nd</sup> edition, Wiley, NY, 2007.
- 6. A. R. West, Solid State Chemistry and its applications, Wiley, 1<sup>st</sup> edition, 2001.

## **REFERENCES:**

- 1. R. C. Mehrotra and A. Singh, Organometallic Chemistry, A Unified Approach, New Age International, 2009.
- 2.R. B. Jordan, Reaction Mechanism of Inorganic and Organometallic Systems, 2<sup>nd</sup> edition, Oxford University Press, 1998.
- 3. Ivano Bertini, Harry B. Gray, Stephen J. Lippard, Joan Selverstone Valentine, Bioinorganic Chemistry, University Science Books, 1994.
- 4. Stephen J. Lippard, Jeremy M. Berg, Principles of Bioinorganic Chemistry, University Science Books, 1994.
- 5. D. K. Chakraborty, Solid State Chemistry, New Age Science, 2<sup>nd</sup> edition, 2010.
- 6. H. V. Keer, Principles of the Solid State, 1<sup>st</sup> Edition, New Age International Publishers, 2005.

## WebLinks:

- 1. https://www.chemicalforums.com/
- 2. https://nptel.ac.in/
- 3. https://chem.libretexts.org/
- 4. http://www.ilpi.com/genchem/web.html#12

## **Question Paper Pattern**

Section	Question Component	Numbers	Marks	Total
Section-A	MCQ:1-10, Fill in: 11-15, T/F:16-20 Answer all questions	1 – 20	1	20
Section- B	Short Answer /Problems Answer any 5 out of 8questions	21–28	7	35
Section- C	Essay Answer any 3 out of 5 questions	29–33	15	45
TOTAL MARKS				100

## **Distribution of Questions**

Castian	Unit	No. of Questions		
Section		Theory	Problem	
	Unit- 1	4		
	Unit– 2	4		
Section- A	Unit–3	4		
	Unit–4	4		
	Unit– 5	4		
	Unit– 1	2		
	Unit– 2	2		
Section -B	Unit–3	2		
	Unit–4	1		
	Unit–5	1		
	Unit– 1	1		
	Unit–2	1		
Section -C	Unit-3	1		
	Unit-4	1		
	Unit–5	1	_	

# CORE THEORY-VI PHYSICAL CHEMISTRY - II

SUBJECT CODE:	THEORY	<b>MARKS: 100</b>
SEMESTER: II	CREDITS: 4	TOTAL HOURS: 60

#### **COURSE FRAMEWORK:**

- To learn enzyme kinetics, surface reactions and fast reactions.
- To learn the need for quantum mechanics and appreciate its significance.

#### **COURSE OUTCOME:**

On completion of the course the students will be able to

- 1. analyse the mechanism of acid–base and enzyme catalyzed reactions.
- 2. distinguish various adsorption isotherms and heterogeneous catalyst reactions.
- 3. gain knowledge about kinetics of complex reactions and fast reactions.
- 4. derive eigen values and wave functions of H and He atoms using approximation methods.,concept of antisymmetric wave function and to solve Hartree and Hartree Fock equation for helium atom.
- 5. apply molecular orbital and valence bond treatment to simple homonuclear diatomic molecules- H2<sup>+</sup> and H2, MOT of higher diatomic molecules, HMO treatment of simple conjugated systems.

#### UNIT-I: Catalysis

(10hrs)

Acid base catalysis-mechanism of acid base catalyzed reactions-Bronsted catalysis law. Catalysis by enzymes-rate of enzyme catalyzed reactions-effect of substrate concentration, pH and temperature on enzyme catalyzed reactions-Inhibition of enzyme catalyzed reactions.

#### **UNIT-II:** Adsorption

(10 hrs)

Langmuir and BET adsorption isotherms-adsorption coefficient and its significance. Kinetics and mechanism of surface reactions-surface reactions catalyzed by metals, semi-conductor oxides.

#### **UNIT-III:** Kinetics of complex reactions

(15 hrs)

Reversible reactions-consecutive reactions-parallel reactions-Chain reactions - general treatment of chain reactions-Rice-Herzfeld mechanism and explosions limits. Study of fast reactions-relaxation methods-temperature and pressure jump methods-stopped flow and flash photolysis method.

### **UNIT-IV:** Quantum Chemistry-II

(10 hrs)

The harmonic oscillator- the rigid rotor-the hydrogen atom-the Schrodinger equation for hydrogen atom- the solution – the origin of quantum numbers (angular momentum and spin)-their physical significance.

#### UNIT-V: Quantum Chemistry-III

(15 hrs)

Approximation methods – perturbation and variation method- Application to hydrogen, helium atoms- R-S coupling, j-j coupling and term symbols for atoms in ground state- Slater rules, Slater orbital and HF-SCF methods- Born – Oppenheimer approximation-Valence Bond theory for hydrogen molecule–LCAO–MO theory for di and poly atomic orbitals - concepts of hybridization- Huckel theory for conjugated molecules (ethylene, butadiene, benzene and pyridine \*) semi empirical methods.

\* not for ESE.

#### **TEXT BOOKS:**

- D.A. McQuarrie, Quantum Chemistry, University Science books, viva books Pvt. Ltd, 2<sup>nd</sup> edition, reprint, 2016.
- 2. I.N. Levine, Quantum Chemistry, Pearson Education Pvt. Ltd, 7<sup>th</sup> edition, 2016.
- 3. R. Anantharaman, Fundamentals of Quantum Chemistry, Macmillan India Limited, 2<sup>nd</sup> edition, 2004.
- 4. R.K. Prasad, Quantum Chemistry, New Age India, 4<sup>th</sup> edition, 2020.
- R.K. Prasad Quantum Chemistry-theory solved problems and solutions, New Age International publishers, Reprint 2017.
- J.Rajaram and J.C.Kuriacose, Kinetics and Mechanism of Chemical Transformations, McMillan India Ltd., 3<sup>rd</sup> edition, reprint, 2009.
- 7. K.J.Laidler, Chemical Kinetics. Harper and Row, Pearson Pvt. Ltd., New York, 3<sup>rd</sup> edition, 2011.
- 8. K. L. Kapoor, A text book of Physical Chemistry, Macmillan India Ltd, reprint, 2010.

#### **REFERENCES:**

- 1. H.Eyring, J.Walter and G.Gimball, Quantum Chemistry, John Wiley & Sons Inc., NewYork, 1944.
- 2. L.S. Pauling and F.B. Wilson, Introduction to quantum mechanics With Application to chemistry McGraw Hill Book Company, New York, 2015.

- 3. Peter Atkins and Ronald Friedman, Molecular quantum mechanics,Oxford University Press, Oxford, 5<sup>th</sup> edition, 2011 .
- 4. David J. Griffiths, Introduction to Quantum mechanics, Cambridge University Press ,3<sup>rd</sup> edition, fifth reprint, 2018.
- 5. G.M. Barrow, Physical Chemistry, Tata McGraw Hill, 5<sup>th</sup> edition, 2008.
- 6. R.G. Frost and Pearson, Kinetics and Mechanism, Wiley, New York, 3<sup>rd</sup> edition, 1981.
- 7. W.J. Moore and R.G. Pearson, Kinetics and Mechanism, Wiley New York, 3<sup>rd</sup> edition, 1981

#### WebLinks:

- 1. http://swayam.gov.in
- 2. <a href="http://search.ebscohost.com">http://search.ebscohost.com</a>
- 3. MATLAB
- 4. www.virtlab.com
- 5. nptel.ac.in
- 6. http://antoine.frostburg.edu/chem/senese/101/quantum/index.shtm

# **Question Paper Pattern**

Section	Question Component	Numbers	Marks	Total
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TOTAL MARKS			100	

G. A.	TT . •4	No. o	f Questions
Section	Unit	Theory	Problem
	Unit-1	4	
	Unit-2	4	
Section- A	Unit-3	4	
	Unit-4	4	
	Unit-5	4	
	Unit-1	1	1
	Unit-2	1	
Section -B	Unit-3	1	
	Unit-4	1	1
	Unit-5	2	
	Unit-1	1	
	Unit-2	1	
Section -C	Unit-3	1	
	Unit-4	1	
	Unit–5	1	

# CORE PRACTICAL-I ORGANIC CHEMISTRY PRACTICAL

SUBJECT CODE:	PRACTICAL	<b>MARKS: 100</b>
SEMESTER: I &II	CREDITS: 3	<b>TOTAL HOURS: 60</b>

#### **COURSE FRAMEWORK:**

- The practical is designed to give an exposure to lab techniques in analysis of organic molecules and synthesis of simple organic compounds.
- To provide the basic training for extraction of compounds from natural products and chromatographic separation.

#### COURSE OUTCOME

On completion of the course the students will be able to

- gain hands-on experience in the separation of two component mixture, purification and identification of the functional groups present.
- 2. expertise in the preparatory methods of organic compounds by single and double stage methods.
- 3. use various purification techniques and extraction methods involving natural products.

#### Unit – I Analysis of mixture of organic compounds.

Identification of components in a two-component mixture and preparation of their derivatives. Determination of b.p./m.p. for components and m.p. for the derivatives.

#### **Unit- II** Preparation of organic compounds

### (a) Single stage any five)

- 1. Preparation of o-benzyl benzoicacid
- 2. p-nitrobenzoic acid from p-nitrotoluene
- 3. Anthroquinone from anthracene
- 4. Benzhydrol from benzophenone
- 5. m-nitroaniline from m-dinitrobenzene
- 6. 1,2,3,4-tetrahydrocarbozole from cyclohexanone
- 7. Methylorange from sulphanilicacid

#### (b) Two stage\* (any three)

- 1. Sym-tribromobenzene from aniline.
- 2. p-nitroaniline from acetanilide
- 3. m-nitrobenzoicacid from methyl benzoate.

- 4. 2,4-dinitrobenzoicacid from p-nitrotoluene.
- 5. m-nitrobenzoicacid from benzaldehyde
- 6. p-bromoaniline from acetanilide

#### **Unit-III**

## (a)Extraction of natura lproducts\* (any two)

- 1. Caffeine from tea leaves
- 2. Lactose from milk
- 3. Citric acid from lemon
- 4. Pipierine from black pepper

## (B) Chromatographic Separations:\*

- 1. Column chromatography-separation of anthracene and acid from anthracene picrate.
- 2. Thin layer chromatography separation of green leaf pigments.
- 3. Paper chromatography
- 4. Identification of amino acids

## (C) Quantitative estimation of common drugs\*

- 1. Estimation of vitamin C in tablets by Iodimetry.
- 2. Estimation of Aspirin by spectrophotometry
  - \*Only for Internal Assessment

# CORE PRACTICAL - II INORGANIC CHEMISTRY PRACTICAL

SUBJECT CODE:	PRACTICAL	MARKS: 100
SEMESTER: I &II	CREDITS:3	TOTAL HOURS: 60

#### **COURSE FRAMEWORK:**

 To train the candidate in inorganic compound preparation, separation of the two metal ions by chromatographic method and deduction identification of cations by semi micro method.

#### **COURSE OUTCOME**

On completion of the course the students will be able to

- 1. analyse the given inorganic mixture containing both common and rare cations.
- 2. explore their knowledge in the volumetric analysis of metal ions.
- 3. prepare the metal complexes in good yield.
- 4. separate the metal ions through chromatography techniques.

#### **EXPERIMENTS**

#### Unit- I.

**Semi micro qualitative analysis:** A mixtures containing two common and two rare cations.

The following are the rare cations to be included: W, Mo, Ti, Te, Se, Ce, Th, Zr, V, UandLi.

## Unit -II. Complexometric titrations (EDTA) - Estimation of Ca, Mg and Zn.

## Unit-III. Preparation of the following complexes (anyseven):

- 1. Potassiumtris(oxalato)aluminate(III)trihydrate.
- 2. Tris(thiourea)copper(I)chloride
- 3. Potassiumtris(oxalato)chromate(III)trihydrate
- 4. Sodiumbis(thiosulphato)cuprate(I)
- 5. Tris(thiourea)copper(I)sulphate
- 6. Sodiumhexanitrocobaltate(III)
- 7. Chloropentamminecobalt(III)chloride
- 8. Bis(acetylacetanato)copper(II)
- 9. Hexaminenickel(II)chloride
- 10. Bis(thiocynato)pyridinemanganese,(ll)

## **Unit -IV. (Only for internal assessment)**

Separation of a mixture of two metalions by paper chromatography.

Separation of zinc and magnesium on a cation exchanger.

#### **TEXTBOOKS:**

- 1. A.L. Vogel, Textbook of Inorganic quantitative analysis, ELBS, 3<sup>rd</sup> edition,1976.
- 2. G.S.Vehla,Vogel's text book of Macro and Semi micro Qualitative Inorganic Analysis, 5<sup>th</sup> edition, Revised, 1979.
- 3. Dougles A.Skoog, F.James Holler. Stanley R Crouch, Principles of Instrumental Analysis, 3<sup>rd</sup> edition2007.

# CORE PRACTICAL - III PHYSICAL CHEMISTRY PRACTICAL

SUBJECT CODE:	PRACTICAL	<b>MARKS: 100</b>
SEMESTER: I &II	CREDITS:3	<b>TOTAL HOURS: 60</b>

#### **COURSE FRAMEWORK:**

- To understand and verify the concepts and equations in physical chemistry by carrying out suitable experiments.
- Typical list of possible experiments are given. A minimum of 10 12 experiments have to be performed.

#### **COURSE OUTCOME:**

On completion of the course the students will be able to

- 1. determine the order and calculate the rate constant for the reaction
- 2. draw and interpret the phase diagram of two component systems
- 3. apply distribution law to find the partition coefficient and equilibrium constant.
- 4. to verify Freundlich adsorption isotherm.

#### **UNIT-I**

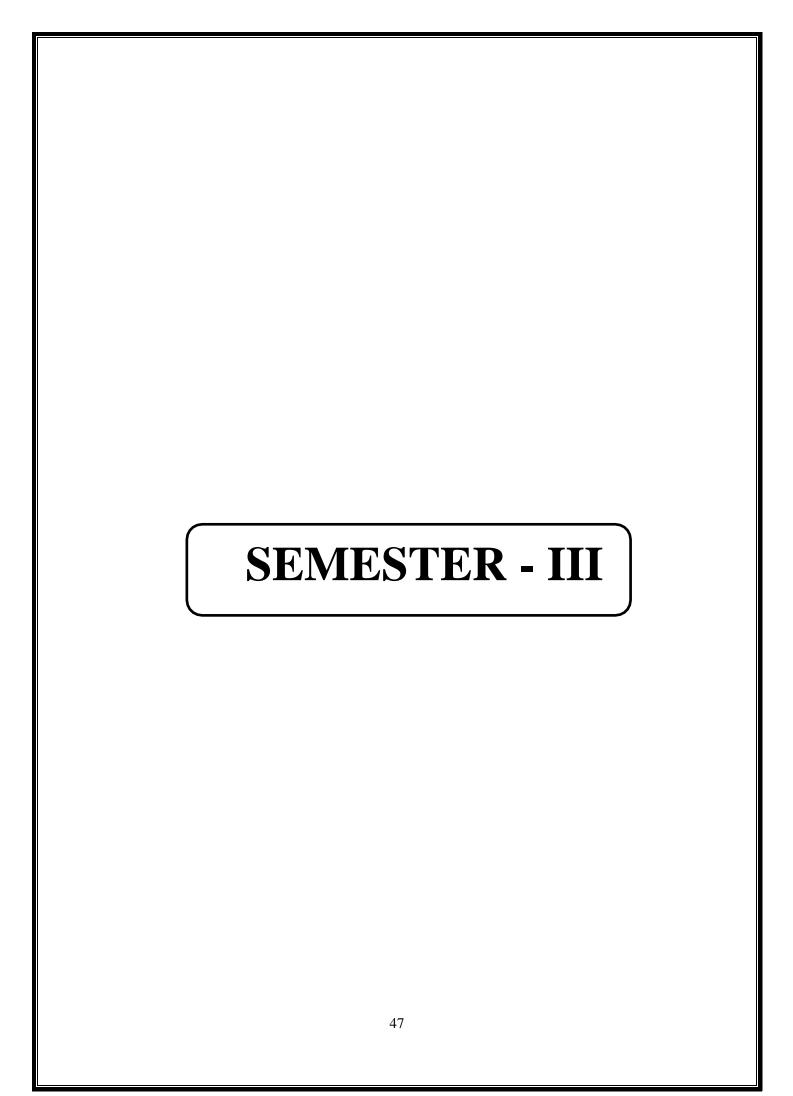
- Study of the adsorption of acetic acid or oxalic acid on charcoal, verification of Freundlich isotherm and determination of concentration of given acetic acid or oxalic acid.
- 2. Construction of phase diagram for a simple binary system; naphthalene—biphenyl, naphthalene—p-dichlorobenzene, naphthalene-diphenylamine.
- 3. Construction of phase diagram for the three-component system (partially miscible liquid system) acetone –chloroform –water; chloroform–acetic acid–water.
- 4. Determination of the equilibrium constant of the reaction between iodine and potassium iodide by partition method.
- 5. Determination of the concentration of given potassium iodide solutions by partition method.
- 6. Determination of molecular weight of benzoic acid and the degree of association of benzoic acid in benzene using partition method.

#### **UNIT-II**

- 1. Kinetic study and comparison of rate constant for the inversion of cane sugar in presence of acid using polarimeter.
- 2. Kinetic study of the reaction between acetone and iodine in acidic medium and determination of the order with respect to iodine and acetone.
- 3. Kinetic study of saponification of ethylacetate by sodium hydroxide conducto metrically and determination of order of the reaction.
- 4. Kinetic study and comparison of acid strengths using acid catalyzed hydrolysis of methyl acetate.
- 5. Determination of temperature coefficient and energy of activation for the acid catalyzed hydrolysis of methyl acetate.
- 6. Determination of the rate constant and order for the reaction between potassium persulphate and potassium iodide.
- 7. Study of the primary salt effect on the kinetics of oxidation of iodide by persulphate
- 8. Kinetic study of the decomposition of sodium thiosulphate by mineral acid.

#### **REFERENCES:**

- 1. B.Viswanathan and P.S.Raghavan, Practical Physical Chemistry, Published by viva books, 2012.
- 2. B.D.Khosla, V.C.Garg and A.Khosla, Senior Practical Physical chemistry, R.Chand & Co New Delhi, 2011.
- 3. P.S.Sindu, Practical Physical chemistry- A modern Approach, MacMillan IndiaLtd, first edition, 2006.
- 4. C.W. Garland, J.W.Nibler and D.P. Shoemaker Experiments in Physical Chemistry, Tata McGraw-Hill, NewYork, eighth edition, 2003.
- 5. A.M.Halpern,G.C.McBane,ExperimentsinPhysicalChemistry,W.H.Freeman&Co, NewYork. Third edition, 2003.



# CORE THEORY-VII ORGANIC CHEMISTRY-III

SUBJECT CODE:	THEORY	MARKS: 100
SEMESTER: III	CREDITS: 4	TOTAL HOURS: 60

#### **COURSE FRAMEWORK:**

- The first part of the paper explains about electronic and vibrational spectroscopy through problem solving approach.
- The instrumentation methods and the applications of NMR spectroscopy, Mass spectrometry in the determination of structure of organic molecules are given.
- Photochemical reactions involving carbonyl, alkene are discussed in detail.

#### **COURSE OUTCOME**

On completion of the course the students will be able to

- 1. predict the structure based on electronic and vibrational transitions.
- 2. identify different techniques and judicially use them as per requirements.
- 3. Interpret spectra based on UV, IR, Mass and NMR to predict the structure of the target molecule.
- 4. select the proper ionization method and interpretation of mass spectra to arrive at the structure of the target molecule.
- 5. synthesize new molecules based on different types of photo chemical reactions

#### **UNIT-I: UV-Vis and IR spectroscopy**

(10 hrs)

Principles and applications of ultraviolet and infrared spectroscopy in organic molecular structure determination. Optical rotator dispersion and its applications. Cotton effect, Octant rule and axial haloketone rule. Woodward-Fisher rule for conjugate systems and unsaturated ketones – Scott rules for aromatic ketones with problem solving approach. (for molecules with a maximum 10 carbon atoms)

#### UNIT-II: Nuclear Magnetic Resonance Spectroscopy (10hrs)

Nuclear magnetic resonance spectra: Theory- the nuclear spin, Larmor frequency, NMR isotopes, population of nuclear spin levels - relaxation processes. Chemical shift-shielding constant, diamagnetic anisotropic influence - ring currents — diatropy and paratropy. Spin-spin interaction-low- and high-resolution spectra. Nuclear magnetic decoupling-double resonance—nuclear overhauser effect - Fourier transform technique-<sup>13</sup>C NMR spectroscopy.

### **UNIT-III: Applications of NMR Spectroscopy to Organic Compounds** (15 hrs)

Proton NMR applications to structure elucidation of simple organic molecules – chemical shift values of various chemically non-equivalent protons and correlation to protons bonded to carbon and protons bonded to other nuclei-chemical exchange, effect of deuteration. First order PMR spectra-complex spin-spin interaction between two, three, four and interacting nuclei, virtual coupling, simplification of complex spectra using shift reagents-coupling constant-variation of coupling constant with dihedral angle, Karplus curve. <sup>13</sup>C-NMR applications to structure elucidation of simple organic molecules—complete decoupled CMR—off resonance spectra-chemical shift values. Elementary treatment of two-dimensional NMR spectroscopy, NOESY, COSY and DEPT.

# **UNIT-IV:** Mass Spectrometry

(15 hrs)

Fragmentation process, even and odd electron ions, scission with rearrangement. Retro Diels Alder reaction, McLafferty rearrangement, double bond and / or ring equivalent simplied from a formula. Fragmentation associated with functional groups aliphatic compounds, aldehydes, ketones, carboxylic acids, esters, amides, alcohols, thiols, amines, ethers, sulphides and halides, aromatic compounds, elimination due to ortho groups. Identification of organic compounds using mass spectrometry problems. Conjunct problems based on UV-Vis, IR, NMR and Mass data. Determination of molecular formula using analytical data.

#### **UNIT-V: Organic Photochemistry**

(10 hrs)

Photochemistry of ketones –Norrish Type-I, Norrish type–II Photoreduction, photochemistry of olefins-cis–trans isomerization. Photocycloaddition, Paterno–Buchi reaction photo chemistry of aromatic compounds photorearrangements. Di- $\pi$  methane rearrangement, Barton reaction and Photo Fries reaction. Photochemistry of cyclohexadienones- photochemistry of santonin- synthesis of Vitamin D from cholesterol.

#### **TEXT BOOKS:**

- 1. Y RSharma, Elementary Organic Spectroscopy-Principles and Chemical Applications, revised edition, S.Chand& Company Pvt. Ltd., 2010.
- 2. P.S. Kalsi, Spectroscopy of Organic Compounds, 6<sup>th</sup> edition, New Age International, 2007.
- 3. Jagdamba Singh and Jaya Singh, Photochemistry and Pericyclic reaction, New Academic Sciences Limited, 3<sup>rd</sup> edition, 2012.
- 4. V.K.Ahluwalia, Rakesh Kumar Parashar, Organic Reaction Mechanisms, 4th edition, 2009.

#### **REFERENCES:**

- 1. Donald L. Pavia, Gary M. Lampman, George S. Kriz, James A. Vyvyan, Introduction to Spectroscopy, 5th Edition, 2015.
- 2. Jag Mohan, Organic Spectroscopy: Principles & Applications, Paper back edition 2<sup>nd</sup> edition, 2004.

#### **WEBLINKS**

- 1. www.epgpathshala.nic.in
- 2. https://nptel.ac.in/
- 3. https://swayam.gov.in/
- 4. https://www2.chemistry.msu.edu/faculty/reusch/VirtTxtJml/intro1.htm

# **Question Paper Pattern**

Section	Question Component	Numbers	Marks	Total
Section- A	MCQ:1-10, Fill in:11-15 T/F:16-20 Answer all questions	1 – 20	1	20
Section-B	Short Answer /Problems Answer any 5 out of 8 questions	21–28	7	35
Section- C Essay Answer any 3 out 5 questions 29–33 15		45		
TOTAL MARKS			100	

C4:	TT *4	No. o	of Questions
Section	Unit	Theory	Problem
	Unit-1	4	
	Unit-2	4	
Section-A	Unit–3	4	
	Unit-4	4	
	Unit–5	4	
	Unit-1	1	
	Unit-2	1	
Section-B	Unit-3	1	1
	Unit-4	1	1
	Unit–5	1	1
	Unit– 1	1	
	Unit-2	1	
Section-C	Unit–3	1	
	Unit-4	1	
	Unit–5	1	

# CORE THEORY-VIII INORGANIC CHEMISTRY-III

SUBJECT CODE:	THEORY	<b>MARKS: 100</b>
SEMESTER: III	CREDITS: 4	<b>TOTAL HOURS: 60</b>

#### **COURSE FRAMEWORK:**

- To introduce the concept of interaction of matter with electromagnetic radiations leading to structural determination of inorganic and organometallic compounds.
- To understand the basic concepts of UV- VIS, IR, Raman, ESR, Mossbauer, Photoelectron, NQR and NMR spectra, to determine the structure of unknown compounds and to develop problem solving skills.
- To educate the photochemistry of inorganic compounds for applied research.

#### **COURSE OUTCOME**

On completion of the course the students will be able to

- 1. demonstrate the bonding properties related structural identification of coordination complexes and to compute magnetic properties
- 2. to learn about UV -Visible spectroscopy and to predict the term symbols, interpret the Orgel diagram, Tanabe- Sugano diagram, electronic spectra of inorganic and organometallic compounds.
- 3. compare the principles, chemical shifts, coupling constants, application of Mossbauer and NQR spectroscopy and applications of <sup>1</sup>H, <sup>19</sup>F, <sup>31</sup>P NMR to simple inorganic molecules.
- 4. discuss the principle and instrumentation of Electron Spin Resonance spectroscopy and its applications, to apply to the free electron character available in a molecular entity to predict structure of complexes and to discuss the principle and instrumentation of photoelectron spectroscopy, Interpretation of Vibrational spectral data for ionized (M<sup>+</sup>) species.
- 5. explain the various types of inorganic photochemical reactions, mechanism of solar energy conversion using ruthenium bipyridyl complexes, predict the photo processes in inorganic and apply in the development of sensitized solar cells photo catalysis

### UNIT – I: Electronic spectroscopy and its applications (15hrs)

Electronic spectra of diatomic and polyatomic molecules- Term states of d<sup>n</sup> ions - Term Symbols-characteristics of d-d transitions - electronic spectra of coordination compounds - selection rules - band intensities and band widths – energy level diagrams of Orgel and Tanabe – Sugano diagrams - spectra of Ti<sup>3+</sup>, V<sup>3+</sup>, Ni<sup>2+</sup>,Cr<sup>3+</sup>, Co<sup>2+</sup>, Cr<sup>2+</sup> and Fe<sup>2+</sup> calculation

of 10Dq and B for  $V^{3+}$ (oct) and  $Ni^{2+}$ (oct) complexes. Charge transfer spectra - classification, mechanisms and interpretation with suitable examples. Magnetism in coordination complexes using A, E and T terms.

# UNIT – II: Applications of IR and Raman Spectroscopy (8 hrs)

Introduction to IR and Raman spectroscopy. Applications of Infrared and Raman, electronic spectroscopy to inorganic systems-metal complexes, organometallic and simple inorganic compounds with special references to coordination sites, isomerism etc., inorganic structure determination. Vibrational spectra of metal carbonyls.

# UNIT – III: Mossbauer and NQR Spectroscopy and applications of NMR Spectroscopy to Inorganic molecules (12hrs)

Mossbauer spectroscopy-principle, instrumentation – recoil energy, Doppler effect-number of MB signals isomer shift quadrupole splitting – magnetic splitting. Applications of <sup>57</sup>Fe, <sup>119</sup>Sn and <sup>129</sup>I Mossbauer spectroscopy. NQR spectroscopy theory and instrumentation nuclear quadrupole coupling constants-applications. Applications of <sup>11</sup>B, <sup>31</sup>P, <sup>19</sup>F, <sup>119</sup>Sn and <sup>195</sup>Pt NMR spectroscopy in the structural assessment of simple inorganic compounds. Applications of NMR in the study of co-ordination complexes, organometallic derivatives and trans effect. Inter and intramolecular exchange studies using NMR-Fluxional behavior of inorganic molecules.

### UNIT - IV: ESR Spectroscopy and Photoelectron Spectroscopy (15 hrs)

ESR spectra of transition metal complex - copper, manganese and vanadyl complexes. Applications of ESR spectroscopy based on multiplicity, anisotropy, magnitude of g values and A values covalency of complexes. Photoelectron spectroscopy—basic principles of UPS and XPS — photoelectron spectra- Koopmann's theorem—fine structure in PES, applications of UPS. ESCA—Introduction—chemical shift and correlation with electronic charges—satellite peaks, spectral splitting, instrumentation, applications—Auger electron spectroscopy—determination of dipole moment.

#### **UNIT V: Photochemistry of Co-ordination Compounds** (10 hrs)

Types of photochemical reaction – photo isomerization, photo substitution and photo redox reactions of cobalt, chromium, platinum and ruthenium complexes. Excitons, polarons, solitons, semiconductor junctions, photocurrent and photo voltage,

photoconductors, photovoltaic cells and photo galvanic cells, solar batteries. Solar energy conversion- photo electro chemistry-photo catalysis- role of ruthenium bipyridyl [Ru(bpy)<sub>3</sub>]<sup>2+</sup>complexes in solar energy conversion.

#### **TEXT BOOKS:**

- 1. Drago R.S, Physical Methods for Chemists, Saunders, (W.B), Co.Ltd, 2<sup>nd</sup> edition, 1992.
- 2. Ebsworth E.A.V, DWA Rankin and C. Craddock, Structural methods in inorganic chemistry, Blackwell Science Inc., 2<sup>nd</sup> edition, 1987.
- 3. Jagdamba Singh, Spectroscopy of Inorganic Compounds: Principles, Problems, and their solutions, 1<sup>st</sup> edition, 2020.
- 4. V. Balzani and, V. Carassiti, Photochemistry of coordination compounds,. Academic Press, 1970.

#### **REFERENCES:**

- 1. Bodie E. Douglas, Darl H. McDaniel and John J. Alexander, Concepts and Models of Inorganic Chemistry, 3<sup>rd</sup> edition, John Wiley and Sons, 1994.
- 2. J. E. Huheey, E. A. Keiter, R.L. Keiter and O. K. Medhi, Inorganic Chemistry Principles of structure and reactivity, 4<sup>th</sup> edition, Pearson, 2013.
- 3. Gary L. Miessler, Donald A. Tarr, Inorganic Chemistry, 3<sup>rd</sup> edition, Pearson, 2004.

### WebLinks:

- 1. https://www.chemicalforums.com/
- 2. https://nptel.ac.in/
- 3. https://chem.libretexts.org/
- 4. <a href="http://www.ilpi.com/genchem/web.html#12">http://www.ilpi.com/genchem/web.html#12</a>

# **Question Paper Pattern**

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Section- C Essay Answer any 3 out 5 questions 29–33 15		45		
TOTAL MARKS			100	

Continu	T I 24	No.of	f Questions
Section	Unit	Theory	Problem
	Unit– 1	4	
	Unit–2	4	
Section-A	Unit–3	4	
	Unit–4	4	
	Unit–5	4	
	Unit– 1	1	
	Unit-2	2	
Section-B	Unit-3	2	
	Unit–4	2	
	Unit– 5	1	
	Unit– 1	1	
	Unit-2	1	
Section-C	Unit–3	1	
	Unit–4	1	
	Unit–5	1	

# CORE THEORY-IX PHYSICAL CHEMISTRY-III

SUBJECT CODE:	THEORY	MARKS: 100
SEMESTER: III	CREDITS: 4	<b>TOTAL HOURS: 60</b>

#### **COURSE FRAMEWORK:**

- To learn the principles of rotational, vibrational, Raman, electronic and mass spectroscopy and their applications.
- To understand the significance and applications of classical thermodynamics and solution electrochemistry.

#### **COURSE OUTCOME**

On completion of the course the students will be able to

- 1. discuss knowledge about the principle of microwave, Infrared spectroscopy.
- 2. apply the knowledge gained to calculate  $\lambda$ max values for a molecule using UV Visible spectroscopy and apply mass spectroscopy to find the fragmentation pattern of molecules.
- 3. understand partial molar properties and its significance, fugacity, thermodynamics of ideal and non-ideal binary solution.
- 4. analyze about Debye Huckle theory of strong electrolytes, ion-ion interaction, limiting law, Onsager equation, Bjerrum ion association concept.
- 5. explain the models of electrical double, mechanism of one electron transfer electrode reaction, theories of corrosion.

#### UNIT-I: Spectroscopy-I

(15 hrs)

Interaction of radiation with matter- rotational spectroscopy of rigid rotor-derivation of Jmax- non-rigid rotor- diatomic and polyatomic molecules – Stark effect. Vibrational spectroscopy-harmonic oscillator-anharmonicity-vibrational spectra of polyatomic molecules-overtones, combination of bonds-vibrational coupling-Fermi resonance. Vibrational rotational lines-PQR branches-Determination of bond length, force constant, vibrational frequency. Applications involving isotopic substitution. Raman spectra-Stokes and anti-stokes lines. Classical and quantum theory-Rotational and vibrational Raman spectra.

### **UNIT-II:** Spectroscopy-II

(10 hrs)

Electronic spectra of diatomic and polyatomic molecules- Franck-Condon principle – determination of dissociation energy – pre dissociation spectra – selection rules-types of electronic transitions–effect of conjugation and solvent-chromophores, auxochromers, Bathochromic and Hypsochromic shifts. Term symbols for electronic states of H<sub>2</sub> molecule. NMR spectroscopy-principle – instrumentation - equation of motion of spin in magnetic fields, chemical shift, spin-spin coupling-relaxation effects.

Mass spectrometry-principle—instrumentation—isolation techniques-EI, CI, FD - LD, LIMA, PD, FAB, SIMS - presentation of spectral data – molecular ions-determination of molecular mass-Isotopic peaks-determination of molecular formula- Metastable peaks. Fragmentation—nitrogen rule.

### UNIT-III: Thermodynamics-I

(10 hrs)

Partial molar properties—Partial molar freeenergy (chemical potential)-Partial molar volume-partial molar heat content-their significance and determination of these quantities-variation of chemical potential with temperature and pressure. Thermodynamics of real gases- gas mixture-fugacity definition-determination of fugacity—variation of fugacity with temperature and pressure- thermodynamics of ideal and non-ideal binary solutions-dilute solutions-excess functions for non-ideal solutions and their determination-the concepts of activity and activity co-efficient-determination of standard free energies-choice of standard states-determination of activity and activity coefficient for non-electrolytes.

### **UNIT-IV:** Electrochemistry of Solutions

(10hrs)

Ion-solvent interaction-Born's treatment (structureless continuum model only, no derivation); ion- ion interaction-Mean ionic activity and activity coefficient-concept of ionic strength-Debye - Huckel theory of strong electrolytes- derivation of Debye-Huckel limiting law-validity of the equation-Debye-Huckel limiting law at low and appreciable concentration of the electrolytes-qualitative and quantitative verification-Debye-Huckel-Bronsted equation.

Ion transport-theory of strong electrolytes for electrolytic conductance-derivation of Onsager equation-validity of the equation-modification of Onsager equation. Ion association- Bjerrum treatment of association-Bjerrum ion association constant-factors influencing ion association-effect of ion association on conductivity and activity coefficient of electrolytes in solution.

UNIT-V: Electrodics (15 hrs)

The electrode-electrolyte interface-electrical double layer-IHP-OHP-contact adsorption-surface excess and its importance-Thermodynamics of electrified interface-electro capillary phenomenon - Lippmann equation, Lippmann potential-polarizable and non-polarizable interface. Structure of double layer-Helmholtz-Perrin, Guoy-Chapmann and Stern models of electrical double layer. Electrokinetic phenomena (Electrophoresis, electro osmosis, sedimentation potential and streaming potential – concepts only) derivation of Butler-Volmer equation for one step electron transfer reactions, Tafel equation- significance of exchange current density and symmetry factor Polarization and over potential- A brief account of Hydrogen overpotential-factors affecting Hydrogen overpotential-mechanism of hydrogen evolution and oxygen evolution-concentration polarization.

Corrosion: Theories, types, prevention of corrosions. Fuel Cells-hydrogen-oxygen fuelcell, construction and applications.

#### **TEXTBOOKS:**

- 1. Sharma B. K., Instrumental methods of analysis, Goel Publication, 24<sup>th</sup> edition, 2014.
- 2. Pavia D. L. and Lampman, G.M., Introduction to Spectroscopy, Cengage Learning India Private Limited, 5<sup>th</sup> edition, 2015.
- 3. K.L.Kapoor, Physical chemistry, MacMillan India Ltd, 3<sup>rd</sup> edition, 2009.
- 4. S.Glasstone, Introduction to Electrochemistry, Liton educational Publishing INC, reprint 2010.

#### **REFERENCES:**

- 1. R.S.Drago, Physical Methods in Chemistry, Thomson learning, 1977.
- 2. DragoR.S, Physical Methods for Chemists, Saunders, (W.B), Co.Ltd, 2<sup>nd</sup> edition, 1992.
- 3. ChristianG.D., Analytical Chemistry, Wiley, 7<sup>th</sup> edition, 2014.
- 4. Skoog, D.A.,Instrumental methods of analysis- Saunders College Publication, 3<sup>rd</sup> edition,2007.
- 5. J.O.M.Bokris and A.K.N.Reddy, Electrochemistry, Vol. 1&2, Kluwer academic /Plenum publishers, New York, 2<sup>nd</sup> edition,2002.
- 6. D.R.Crow, Principles and Applications of Electrochemistry, Chapman and Hall, 4<sup>th</sup> edition, 1994.
- 7. M.C.Gupta, Statistical thermodynamics, Wiley, Eastern, New Delhi, reprint, 2009.
- 8. Nester Perez, Electrochemistry and corrosion science, Springer London, reprint, 2010.

## WebLinks:

- 1. http://ccl.osc.edu/ccl.cca.html
- 2. http://www.chem.swin.esu.au/chem\_ref.html
- 3. http://www.colby.edu/chemistry/PChem/Lecture1.html
- 4. http://hyperphysics.phy-astr.gsu.edu/hbase/chemical/electrode.html#c3
- 5. www.spectro.com

# **Question Paper Pattern**

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TOTAL MARKS			100	

C4:	T I • 4	No.o	f Questions
Section	Unit	Theory	Problem
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	Unit– 2	4	
Section-A	Unit–3	4	
	Unit-4	4	
	Unit–5	4	
	Unit– 1	1	1
	Unit–2	1	
Section-B	Unit–3	1	1
	Unit-4	1	
	Unit–5	1	1
	Unit-1	1	
	Unit-2	1	
Section-C	Unit–3	1	
	Unit-4	1	
	Unit–5	1	

# CORE ELECTIVE -II RESEARCH METHODOLOGY AND RESEARCH ETHICS

SUBJECT CODE:	THEORY	MARKS:100
SEMESTER: III	CREDITS: 3	TOTAL HOURS: 60

#### **COURSE FRAMEWORK:**

- To explain various aspects of research methodology like Literature, planning, data analysis and report writing.
- To inculcate the ethics to be followed while pursuing research.

#### **COURSE OUTCOME**

On completion of the course the students will be able to

- 1. gain knowledge about problem selection, literature search and metrics involved in research.
- 2. acquire theoretical knowledge about planning, method development and data analysis involved in research.
- 3. demonstrate skill in report writing in the expected format and to select the appropriate journal for publication
- 4. show integrity in research and aware of scientific ethics to be followed.
- 5. follow publication ethics and identify predatory journal with the help of plagiarism software

#### **UNIT I: Research Problem**

(15hrs)

Objectives of research, types of research – basic, applied, and other types-Problem selection. Innovative and Sustainable research, literature survey –primary, secondary and tertiary sources. Chemical abstract and its importance, Journals – International and National, reviews, monographs, data books. Research metrics- Impact factor, citation index , hindexand i-10 index. Indexing – Web of Science and Scopus.

#### UNIT II: Research planning, methods and data analysis (10hrs)

Planning and conducting experiments-Methods development- Product, process and analytical method and validation. Case study: Organic, Inorganic and Analytical methods Presentation of data-Types of errors-Gross, systematic and random errors- types of data and data analysis - measures of mean, standard deviation and measures of variability- correlation, and method of least squares, regression analysis.

### **UNIT III: Scientific Report writing and publication**

(10hrs)

Scientific Report writing-manuscript. Thesis, books and patent–Procedure for presenting tables, graphs and figures, foot-notes, bibliography and appendices-Abbreviations, symbols and SI units-Journal finder / journal suggestion tools viz. JANE, Elsevier journal finder, Springer Journal Suggester. Publishers: ACS, RSC, Elsevier, Taylor & Francis, Wiley and Springer-Patent, IPR, copy right. Proposal writing and funding agencies in India.

#### **UNIT IV: Scientific Conduct**

(10hrs)

Ethics with respect to science and research-Intellectual honesty and research integrity-Scientific misconducts: Falsification, Fabrication and Plagiarism (FFP)-Redundant publications: duplicate and overlapping publications-Selective reporting and misrepresentation of data.

#### **UNIT V: Publication Ethics**

(15 hrs)

Publication ethics: definition, introduction and importance-Best Practices / standard setting initiatives and guidelines: COPE, WAME, etc.-Conflicts of interest-Publication misconduct: definition, concept, problems that lead to unethical behavior -Violation of publication ethics, authorship and contributorship- Identification of publication misconduct, complaints and appeals Predatory publishers and journals-Use of plagiarism software like Turnitin, Urkund and other open source software tools.

#### **REFERENCES:**

- 1. Thesis and Assignment Writing J Anderson, B.H. Dursten and M. Poole, Wiley Eastern (1977).
- 2. Statistical Method, Gupta S. P, Sultan Chand and Sons, New Delhi, 2004
- 3. Hand Book for Authors Journal of the American Chemical Society Publications
- 4. Chemical publications Their nature and uses
- 5. Scientific Integrity and Research Ethics: An Approach from the Ethos of Science (Springer Briefs in Ethics) by <u>David Koepsell</u>, Springer publications.
- 6. Textbook of Research Ethics: Theory and Practice by Sana Loue, Springer publications.

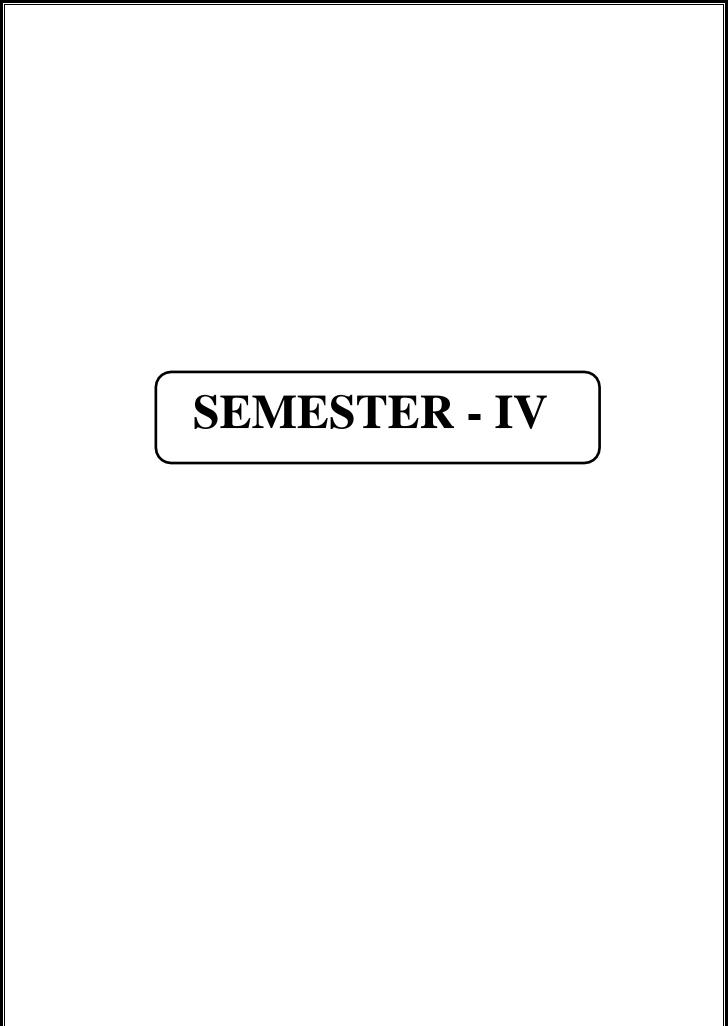
#### **WEBLINKS:**

- $\underline{1.}\ https://www.publichealthnotes.com/research-ethics-definition-principles-and-advantages/$
- 2. https://www.niehs.nih.gov/research/resources/bioethics/whatis/index.cfm
- 3. https://www.ccmb.res.in/newsfiles/year-2020/csir\_ethics\_2020.pdf
- <u>4.</u> https://www.insaindia.res.in/pdf/Ethics\_Book.pdf

# **Question Paper Pattern**

Section	Question Component	Numbers	Marks	Total
Section- A	MCQ:1-10, Fill in:11-15 T/F:16-20 Answer all questions	1 – 20	1	20
Section-B	Short Answer /Problems Answer any 5 out of 8 questions	21–28	7	35
Section- C Essay Answer any 3 out 5 questions 29–33		15	45	
TOTAL MARKS			100	

Continu	T I 24	No. o	f Questions
Section	Unit	Theory	Problem
	Unit– 1	4	
	Unit–2	4	
Section-A	Unit–3	4	
	Unit–4	4	
	Unit–5	4	
	Unit– 1	2	
	Unit–2	1	
Section-B	Unit–3	2	
	Unit–4	1	
	Unit–5	2	
	Unit– 1	1	
	Unit-2	1	
Section-C	Unit–3	1	
	Unit–4	1	
	Unit–5	1	



# CORE THEORY–X ORGANIC CHEMISTRY–IV

SUBJECT CODE:	THEORY	MARKS:100
SEMESTER: IV	CREDITS: 4	<b>TOTAL HOURS: 60</b>

#### **COURSE FRAMEWORK:**

 To introduce the basic methodology for the synthesis of organic compounds using dissection method, various reagents, name reactions and also to acquire knowledge about green synthetic methods.

#### **COURSE OUTCOME**

On completion of the course the students will be able to

- 1. apply the retro synthetic approach to develop methodology for synthesising new compounds involving C-C and C=C.
- 2. logically approach the usage of various reagents for organic synthesis.
- 3. apply the methodology involved in advanced name reactions for synthesizing new compounds.
- 4. approach synthesis of complex organic compounds in a logical manner.
- 5. apply green chemistry principle for synthesis of organic compounds.

#### **UNIT-I:** Modern Synthetic Methodology

(15 hrs)

Retro synthetic analysis- disconnections - Synthons: Donors and acceptor and their synthetic equivalent- FGI-FGA-UMPOLUNG. Formation of C-C bond using alkylation and acylation of enamines, enolates, active methylene compounds and organometallic compounds-RMgX, R<sub>2</sub>LiCu, RLi with special references to synthesis of 1,2-1,3-1,4-1,5-and1,6-dicarbonyl compounds. Synthesis of unsaturated carbonyl compounds using aldol condensation, Claisen reaction and Michael reaction - Cyclisation methods- Robinson annulations. Formation of C=C bond using Wittig, modified Wittig reactions, Peterson olefination and Julia olefination. Role of sulphur ylides and rearrangements (Pinacol-Pinacolone and Favorski rearrangement) in organic synthesis. Protection and deprotection of functional groups (-OH, -NH<sub>2</sub>,C=O,-COOH).

### **UNIT-II: Synthetic Reagents**

(15 hrs)

Reagents used for oxidation- TPAP, Dess-martin, silver carbonate / molecular seives and CAN. Reagents used for reductions-(PPh<sub>3</sub>)<sub>3</sub>RhCl, Lindlar catalyst, 9-BBN, chiral boranes, NaBH<sub>3</sub>CN, DIBAL and selectrides - Birch reduction (Hetero cyclic compound). Role of Bu<sub>3</sub>SnH, trimethylsilylchloride, LDA and dithiane inorganic synthesis. Ring closing metathesis.

#### **UNIT-III: Synthetic Applications of Name Reaction**

(10 hrs)

Sandmeyer reaction, Ullmann reaction, Gomberg reaction, Pschorr reaction, Huns dicker reaction. Heck reaction, Suzuki coupling, McMurry olefination, Prins reaction, Ritter reaction, Mitsunobu reaction, Sharpless asymmetric epoxidation, Kumada coupling, Negishi coupling, Stille coupling Buchwald-Hartwig Cross Coupling and Sonogashira coupling.

#### **UNIT-IV: Retero Synthesis of Target Molecules**

(10 hrs)

Retero synthetic analysis, donor and acceptor synthons- examples and synthesis of target molecules - 5-hexenoic acid, bicyclo (4, 1, 0) heptane-2-one, trans-9-methyl-1-decalone, Cubane, longifolene, cis – jasmone and onocerin.

# **UNIT-V:** Green Chemistry

(10 hrs)

Introduction to green chemistry; efficiency/atom economy - definition, needs and goals. Twelve principles of green chemistry with detailed descriptions. Comparison of conventional chemical methods with green chemical methods. Organic synthesis in aqueous medium (highlight of requirements) - Diels-Alder reaction, Knoevenagel reaction and Heck reactions. Ionic liquids as solvent-preparation, merits of ionic liquid as solvent and application to Suzuki coupling, Henry reaction and hydrogenations. Polymer supported phase transfer catalysts – principle of catalysis and applications to C, N, O and S alkylations. Microwave and Ultrasound assisted synthesis –principle behind these techniques and application to esterification, reduction and coupling reactions.

#### **TEXTBOOKS:**

- 1. R.O.C Norman and J.M.Coxon, Principles of organic synthesis, CRC press, 3<sup>rd</sup> edition, 2017.
- 2. Ratan Kumar Kar, Fundamentals of organic synthesis—the retro synthetic analysis vol-2, New central book agencies, first reprint, 2014.
- 3. Timothy K. Dickens, Stuart Warren, Chemistry of the Carbonyl Group: A Step-by-Step Approach to Understanding Organic Reaction Mechanisms, Revised edition, 2018.
- 4. Michael B. Smith, March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure, 8<sup>th</sup> Edition, 2019.
- 5. V.K.Ahluwalia, Green Chemistry-Greener alternative to synthetic organic transformation, Narosa Publishing House Pvt. Ltd, 1<sup>st</sup> edition, 2012.
- 6. William Caruthers and Coldham, Modern methods of organic synthesis, Cambridge Univ. Press, 4<sup>th</sup> edition, 2016.
- 7. I.L.Finar,Organic chemistry Vol-II, Pearson Education Pvt. Ltd, 5<sup>th</sup> edition,2006.

#### **REFERENCES:**

- 1. Ratan Kumar Kar, Frontier Orbital and Symmetry Controlled Pericyclic reaction, Books & allied Pvt. Ltd, 1<sup>st</sup> edition,2012.
- 2. Stuart Warren, Organic synthesis-The Dissconnection approach, John Wiley(P) Ltd, Reprint, 2011.
- 3. F.A.Carey and R.J.Sundberg, Advanced Organic Chemistry, Part-A and Part-B. Plenum Press, New York, 5<sup>th</sup> edition, 2015.
- 4. J. Clayden, N. Greeves and S. Warren, Organic Chemistry, Oxford University Press,  $2^{nd}$  edition, 2014.
- 5. Rashmi Sanghi and M.M.Srivastava, Green Chemistry, Narosa Publishing House Pvt. Ltd, 5<sup>th</sup> edition, 2012.
- 6. J.P.Tierney and P. Lidstrom, Microwave Assisted Organic Synthesis, Wiley India Pvt. Ltd, 1<sup>st</sup> edition, reprint, 2016.

#### **WEBLINKS**

- 1. www.epgpathshala.nic.in
- 2. https://nptel.ac.in/
- 3. https://swayam.gov.in/
- 4. <a href="https://www2.chemistry.msu.edu/faculty/reusch/VirtTxtJml/intro1.htm">https://www2.chemistry.msu.edu/faculty/reusch/VirtTxtJml/intro1.htm</a>

# **Question Paper Pattern**

Section	Question Component	Numbers	Marks	Total
Section- A $MCQ:1-10$ , Fill in: 11-15 $T/F:16-20$ $1-20$ Answer all questions		1 – 20	1	20
Section-B	Short Answer /Problems Answer any 5 out of 8 questions	21–28	7	35
Section- C Essay Answer any 3 out 5 questions		29–33	15	45
TOTAL MARKS			100	

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Section	Unit	Theory	Problem
	Unit- 1	4	
	Unit–2	4	
Section-A	Unit–3	4	
	Unit-4	4	
	Unit–5	4	
	Unit– 1	1	1
	Unit-2	1	
Section-B	Unit–3	1	1
	Unit-4	1	1
	Unit–5	1	
	Unit– 1	1	
	Unit-2	1	
Section-C	Unit–3	1	
	Unit-4	1	
	Unit–5	1	

# CORE THEORY–XI PHYSICAL CHEMISTRY–IV

SUBJECT CODE:	THEORY	MARKS: 100
SEMESTER: IV	CREDITS: 4	<b>TOTAL HOURS: 60</b>

#### **COURSE FRAMEWORK:**

- To understand and appreciate the significance of statistical thermodynamics.
- To learn the theory and applications of photochemistry.
- To learn the basics of computational chemistry.

#### **COURSE OUTCOME**

On completion of the course the students will be able to

- 1. analyze and apply concepts of partition function to heat capacities of solids and gases, black body radiation, electron gas in metals.
- 2. gain knowledge on basic concepts of ensembles, statistical probabilities in the filling of atomic and molecular energy levels, partition functions and their derivation.
- 3. explain the fundamentals of photochemistry, Absorption and Emission of radiation, Stern Volmer analysis, Quantum efficiency and Molecular structure and photophysical and photo che mical reactivity.
- 4. demonstrate the fast reaction techniques such as flash photolysis and fluorescence and lifetime measurements.
- 5. design molecular structure, bond angle, bond length and electron density, calculate bond energy enthalpy, entropy and free energy of constructed molecules, draw and visualize both small and big molecules using online tools and to perform online molecular docking analysis

# **UNIT-I: Thermodynamics-II**

(12 hrs)

Concept of thermodynamic probability-distribution of distinguishable and indistinguishable particles. Maxwell-Boltzmann,Fermi-Dirac and Bose-Einsteinstatistics-Modes of contribution to energy. Partition function—Translational,vibrational and rotational partition functions for mono, diatomic and polyatomic ideal gases.

# **UNIT-II: Thermodynamics–III**

(12 hrs)

Thermodynamic functions in terms of partition functions —equilibrium constant for isotope exchange and dissociation of diatomic molecules- heat capacity of solids (Einstein and Debye models) -ortho and para hydrogen- Planck's radiation law —electron in metals.

## **UNIT-III: Fundamentals of photochemistry**

(12 hrs)

Absorption and emission of radiation-Frank-Condon principle-Physical properties of electronic excited molecules - Spin multiplicity - Singlet and triplet excited states - decay of electronically excited states - radiative and non radiative processes-fluorescence and phosphorescence-Spin forbidden non-radiative transitions-internal conversion and intersystem crossing-energy transfer process-excimers and exciplexes-delayed fluorescence and phosphorescence - Triplet-Triplet annihilation-static and dynamic quenching-Stern-Volmer analysis.Quantum efficiency-quantum yield - sensitization and sensitizer - allowed- forbidden process -(Molecular structure and photophysical and photochemical reactivity)

## **UNIT-IV: Techniques and Photochemical Reactions**

(12 hrs)

Quantum yield measurements-Flash photolysis techniques-Actinometry-quantum yield of photophysical process and photochemical reactions. Life time measurements-Steady state and non steady state methods. Fluorescence spectroscopy-principle-instrumentation and applications—fluorescence-based sensors

# **UNIT-V: Computational Chemistry**

 $(12hrs)^*$ 

Introduction to Cheminformatics - History of Cheminformatics - data storage, retrieval and presentation -Types of Databases - Cambridge structural database –different file formats (SMILES, .cif,. mol,. xyz,. Pdb etc.,) -Online property calculators with examples. Introduction to Online resources- online 2D and 3D chemical structure drawing-designing of molecules and demonstrating experiments—Protein data bank - Protein structure visualization tools –PyMol, and Swiss PDB Viewer. Introduction to drug design - Structured-based drug design - Ligand based drug design – difference between drugs and inhibitors - Molecular Docking – Types (Rigid and flexible docking)-Online docking servers. (Definitions only-Pharmacophore, pharmacokinetics, lead molecule, search algorithm and scoring function)

<sup>\*</sup>Not for End Semester Examination, only for Continuous Internal Assessment

#### **TEXT BOOKS:**

- 1. K.L.Kapoor, Physical chemistry, Mac Millan India Ltd, 3<sup>rd</sup> edition, 2009.
- 2. K.K. Rohatgi Mukherjee, Fundamentals of photochemistry, New Age International Pvt. Ltd, 3<sup>rd</sup> edition,2014.
- 3. M.C.Gupta, Statistical thermodynamics, New Age International Private Limited 3<sup>rd</sup> edition, 2021.

# **REFERENCES:**

- 1. B.C McClelland ,Statistical thermodynamics, Chapman and Hall, London, 1973.
- 2. N.J.Turro, Modern Molecular Photochemistry (MMP), University Press, MenloPark, CA,1978.
- 3.A. Gilbertand J. Baggott, Essentials of Molecular Photochemistry, CRC Press, London, UK,1991.
- 4. Andrew R.Leach, Molecular Modelling: Principles and Applications, 2<sup>nd</sup> edition, Pearson Education; 2009.

#### WebLinks:

- 1. www.docsity.com
- 2. www.acdlabs.com
- 3. www.studocu.com
- 4. mooc.org
- 5. nptel.ac.in
- 6. www.gaussian.com
- 7. MOLPRO

# **Question Paper Pattern**

Section	Question Component	Numbers	Marks	Total
Section- A	MCQ:1-10, Fill in:11-15 T/F:16-20 Answer all questions	1 – 20	1	20
Section-B	Short Answer /Problems Answer any 5 out of 8 questions	21–28	7	35
Section- C Essay Answer any 3 out 5 questions		29–33	15	45
TOTAL MARKS			100	

G. A.	TT .*4	No. o	f Questions
Section	Unit	Theory	Problem
	Unit-1	5	
	Unit-2	5	
Section-A	Unit–3	5	
	Unit-4	5	
	Unit-5	-	
	Unit-1	1	1
	Unit-2	2	
Section-B	Unit-3	2	
	Unit-4	2	
	Unit–5	-	
	Unit-1	2	
	Unit-2	1	
Section-C	Unit–3	1	
	Unit-4	1	
	Unit–5	-	

# CORE ELECTIVE –III CHEMISTRY OF NATURAL PRODUCTS

SUBJECT CODE:	THEORY	<b>MARKS: 100</b>
SEMESTER: IV	CREDITS:3	<b>TOTAL HOURS: 60</b>

#### **COURSE FRAMEWORK:**

• To create awareness about the chemistry of biomolecules and their reactions.

#### **COURSE OUTCOME**

On completion of the course the students will be able to

- 1. explain the fundamental concept to nucleic acids and its functioning.
- 2. propose the total synthesis of peptide and to elucidate the structure of various steroids.
- 3. write the synthesis of camphor  $\alpha,\beta$ -carotenoids and lycopene.
- 4. outline the synthesis of complex organic compounds like morphine, cocaine,
- 5. reserpine and synthesis of flavones isoflavones and anthocyanin. gain expertise in the bio synthesis of cholesterol terpenoids alkaloids amino acids and bile acid.

#### UNIT- I: Nucleic acids

(10 hrs)

Pyrimidine and purine bases-synthesis of Adenine, Guanine, Thymine, Cytosine and Uracil. Structure and role of nucleic acid – nucleoside, nucleotide and poly nucleotides –DNA and RNA–structure, types–biological functions–genetic code.

#### **UNIT-II: Proteins and Steroids**

(15 hrs)

Proteins-classification, Merrifield synthesis, end group analysis, structure and biological functions. Steroids-Diel's hydrocarbon, synthesis of bile acid. Structural elucidation of cholesterol-conversion of cholesterol into estrone, testosterone and progesterone. Synthesis of equilenin.

#### **UNIT-III:** Terpenoids and Carotenoids

(15 hrs)

Classification, occurrence, general methods of determining structure - isoprene rule. Synthesis of the following molecules –  $\alpha$  and  $\beta$ - Carotene, lycopene, zingiberin, eudesmol and santonin.

## UNIT-IV: Alkaloids and Anthocyanins

(10 hrs)

Total synthesis of cocaine, morphine, reserpine and quinine. Flavones, isoflavones, anthocyanins (Synthesis only). Structural elucidation of lysergic acid and

# **UNIT-V: Biosynthesis**

(10 hrs)

General principles involved in the biosynthesis of amino acids, alkaloids, steroids and terpenoids. Biosynthesis of cholestrol, prostaglandin, phenanthrene alkaloids and bile acids.

#### **TEXTBOOKS:**

- 1. I.L. Finar, Organic chemistry, Vol-II, ELBS Publication, 5<sup>th</sup> edition, 1986.
- 2. O.P.Agarwal, Organic Chemistry of Natural Products, Krishna Prakashan Media Pvt. Ltd, 42<sup>nd</sup> edition, 2011.
- 3. Gurdeep R.Chatwal, Organic chemistry of Natural products, Himalaya Publishing House, 2005.
- 4. L.A.Pacquette, Principles of Modern Heterocyclic Chemistry, Benjamin Cummings Publishing Co,London, 1978.

#### **WEBLINKS**

- 1. www.epathshala.nic.in
- 2. www.nptel.ac.in
- 3. http://swayam.gov.in

# **Question Paper Pattern**

Section	Question Component	Numbers	Marks	Total
Section- A	MCQ:1-10, Fill in:11-15 T/F:16-20 Answer all questions	1 – 20	1	20
Section-B	Short Answer /Problems Answer any 5 out of 8 questions	21–28	7	35
Section- C	Essay Answer any 3 out 5 questions	29–33	15	45
TOTAL MARKS			100	

Continu	T T 34	No. o	f Questions
Section	Unit	Theory	Problem
	Unit– 1	4	
	Unit–2	4	
Section-A	Unit–3	4	
	Unit–4	4	
	Unit– 5	4	
	Unit– 1	2	
	Unit-2	1	
Section-B	Unit–3	2	
	Unit-4	2	
	Unit–5	1	
	Unit– 1	1	
	Unit–2	1	
Section-C	Unit-3	1	
	Unit–4	1	
	Unit–5	1	

#### **CORE ELECTIVE-III**

#### NANOCHEMISTRY AND ITS APPLICATIONS

<b>SUBJECT CODE:</b>	THEORY	MARKS: 100
SEMESTER-IV	CREDITS: 3	TOTAL HOURS: 60

#### **COURSE FRAMEWORK:**

- To introduce the recent advancements in the field of materials science viz. nanochemistry.
- To enable the students to know about the various syntheses and properties of nano materials and to learn the applications of nanoparticles in modern technology.

#### **COURSE OUTCOME**

On completion of the course the students will be able to

- 1. explain the basics of nano chemistry.
- 2. describe the synthetic methods of nanomaterials.
- 3. demonstrate the characterization methods of various nanomaterials
- 4. investigate the chemistry of metal and carbon based nanomaterials.
- 5. demonstrate the various applications of nanomaterials and utilize their knowledge to develop novel nanomaterials during their research in the future.

# UNIT - I: Nanomaterials - Introduction, classification and properties (12 hrs)

Nanomaterials- Classification based on dimensions -1D, 2D, 3D and 0D. Shell structures, metal oxides, semiconductors, composites. Size dependent properties of nanomaterials. Mechanical, physical and chemical properties. Host-Guest Complexation: Introduction, Nature of supramolecular interactions, Type of host - guest complexes, Structure of complexes.

#### **Unit II: Synthesis of nanomaterials**

(10 hrs)

Bottom up (physical and chemical techniques) and top down methods (mechanical methods and lithography). Wet and dry method, Self- Assembly-Self Assembled Monolayers (SAM) - Vapour deposition method – Laser ablation method, Chemical Vapour Deposition (CVD), Sol-gel pyrolysis method, combustion method and Microwave assisted synthesis.

#### **Unit III: Metal, Carbon and Polymer based Nanomaterials**

(12 hrs)

Metal based nanomaterials: Noble metals – Ag, Au, Pd, Pt, metal oxide nanomaterials – ZnO, TiO<sub>2</sub>, CeO<sub>2</sub> and iron oxides. Carbon based nanomaterials: Fullerenes, graphene, carbon nanotube (CNT), and carbon quantum dots. Functionalization of CNT, electronic, vibrational, mechanical and optical properties of carbon nanomaterials. Synthesis of nanomaterials – Carbon, Metal, polymer based materials and dendrimer composites.

#### **Unit IV: Characterization of Nanomaterials**

(12 hrs)

XRD - Debye Scherer method (determination of structure and crystallite size); Structural characterization – morphology - Scanning Electron Microscopy (SEM/ FESEM), Transmission Electron Microscopy (TEM/HRTEM) – Crystallite size and SAED pattern. Scanning probe microscopy (SPM)- Atomic Force Microscopy (AFM), Scanning Tunneling microscopy (STM). Optical characterization - UV-Vis and Photoluminescence Spectroscopy.

#### **UNIT-V: Application of Nanomaterials**

(14hrs)

Energy-fuel cells, hydrogen storage, nanophosphors for High Definition TV, Next-Generation Computer Chips, Quantum electronic devices - CNT based applications and Field Emission Display - Biochemical sensor, smart materials. Nanocatalysis. Biological applications – diagnostic and imaging, targeted drug delivery - Nano coatings and paintings. Cosmetic applications. Ferroelectric materials, molecular electronics and nanoelectronics, applications of polymer and its composites. Nanotoxicology and Green Nanochemistry.

#### **TEXTBOOKS:**

- 1. B.S. Murty, P. Shankar, Baldev Raj, B B Rath, James Murday; Textbook of Nanoscience and Nanotechnology, 2013.
- 2.T. Pradeep, A Textbook of Nanoscience and Nanotechnology, Springer publishing service, 2017.
- 3. P. I. Varghese, T. Pradeep, A Textbook of Nanoscience and Nanotechnology, Tata McGraw-Hill Education, 2003.
- 4. Dinesh C Agrawal, Introduction to Nanoscience and Nanomaterials, World Scientific Publisher, 2013.

- M. Wilson, K. Kannangara, G Smith, M. Simmons, B. Raguse, Nanotechnology: Basic science and Emerging technologies, Overseas Press India Pvt. Ltd, New Delhi, 1<sup>st</sup> edition, 2005.
- 2. C.N.R. Rao, A. Muller, A.K.Cheetham (Eds), The chemistry of nanomaterials: Synthesis, properties and applications, Wiley VCH, Weinheim, 2004.
- 3. Kenneth J. Klabunde (Eds), Nanoscale Materials Science, John Wiley & Sons, Inc., 2001.
- 4. C.S.S.R.Kumar, J.Hormes, C.Leuschner, Nanofabrication towards biomedical applications, Wiley –VCH Verlag GmbH & Co, Weinheim, 2004.
- 5. W. Rainer, Nano Electronics and information Technology, Wiley, 2003.
- 6. K.E. Drexler, Nano systems, Wiley, 1992.
- 7. G.Cao, Naostructures and Nanomaterials: Synthesis, properties and applications, Imperical College Press, 2004

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- 2. https://nptel.ac.in/
- 3. https://chem.libretexts.org/
- 4. http://www.ilpi.com/genchem/web.html#12
- 5. <a href="http://www.zyvex.com/nano/">http://www.zyvex.com/nano/</a>
- 6. https://www.instanano.com/
- 7. https://www.azonano.com/nanotechnology-equipment-index.aspx
- 8. http://www.e-booksdirectory.com/listing.php?category=238

# **Question Paper Pattern**

Section	Question Component	Numbers	Marks	Total
Section- A	MCQ:1-10, Fill in:11-15 T/F:16-20 Answer all questions	1 – 20	1	20
	Short Answer /Problems Answer any 5 out of 8 questions	21–28	7	35
Section- C	Essay Answer any 3 out 5 questions	29–33	15	45
TOTAL MARKS			100	

Castian	I Ini4	No. o	f Questions
Section	Unit	Theory	Problem
	Unit– 1	4	
	Unit– 2	4	
Section-A	Unit–3	4	
	Unit–4	4	
	Unit–5	4	
	Unit– 1	2	
	Unit-2	1	
Section-B	Unit-3	2	
	Unit–4	2	
	Unit–5	1	
	Unit– 1	1	
	Unit-2	1	
Section-C	Unit–3	1	
	Unit-4	1	
	Unit–5	1	

# CORE PRACTICAL—IV ELECTROANALYTICAL CHEMISTRY PRACTICAL

SUBJECT CODE:	PRACTICAL	MARKS: 100
SEMESTER: III & IV	CREDITS:4	TOTAL HOURS: 60

#### **COURSE FRAMEWORK:**

To help the students to understand and apply the concepts of electroanalytical chemistry.

#### **COURSE OUTCOME:**

On completion of the course the students will be able to

- 1. explain the principle of conductivity, potentiometry and colorimetry experiments.
- 2. determine the strength of unknown solutions by potentiometric and conductometric methods.
- 3. Determine the strength of unknown solutions by colorimetry.

# **UNIT-I: Conductometric Experiments**

- Determination of equivalent conductance of strong electrolytes and verification of Debye-Huckel-Onsager equation.
- 2. Determination of dissociation constant of weak electrolyte using Ostwald's dilution law.
- 3. Conductometric titration between simple and mixture of strong and weak acids and base and precipitation titration involving a single halide.

#### **UNIT-II:** Potentiometric Experiments

- 4. Determination of pH and calculation of pKa.
- 5. Determination of solubility product of sparingly soluble salt.
- 6. Potentiometric titrations between simple and mixture of strong and weak acids and base.
- 7. RedoxTitrations byEMFmeasurements
- 8. Precipitation titration of mixture of halides by EMF measurements.

#### **UNIT-III: Colorimetric Experiments**

- 9. Photoelectric method: Estimation of iron, nickel, manganese and copper.
- 10. \*Determination of  $Cr^{2+}$  and  $Mn^{2+}$  ions present in water sample by Colorimetry.(\*For CIA only)

- 1. B.Viswanathan and P.S.Raghavan, Practical Physical Chemistry, Viva books, 2012.
- 2. B.D.Khosla, V.C.Garg and A.Khosla, Senior Practical Physical chemistry, S.Chandand Co., New Delhi, 2011.
- 3. P.S.Sindu, Practical Physical Chemistry-A modern Approach, MacMillan India Ltd, 1<sup>st</sup> edition, 2006.
- 4. C.W.Garland, J.W.Nibler and D.P.Shoemaker, Experiments in Physical Chemistry, Tata McGraw-Hill, NewYork, 8<sup>th</sup> edition, 2003.
- 5. A.M.Halpern,G.C.McBane,Experiments in Physical Chemistry,W.H.Freeman and Co, New York, 3<sup>rd</sup> edition, 2003.

# CORE PRACTICAL- V ANALYTICAL CHEMISTRY PRACTICAL

SUBJECT CODE:	PRACTICAL	MARKS100
SEMESTER: III & IV	CREDITS:4	TOTALHOURS: 60

#### **COURSE FRAMEWORK:**

To impart the quantitative estimation of organic compounds, mixture of inorganic metal ions and spectral interpretations of organic compound and inorganic complexes.

#### **COURSE OUTCOME**

On completion of the course the students will be able to

- 1. imbibe the techniques of analysis of complex chemical materials
- 2. quantitative estimation of organic compounds and inorganic metal ions
- 3. interpret all specrto-analytical data for molecular identification

### **Unit-I: Estimations (Any Four)**

- 1. Estimation of aniline
- 2. Estimation of phenol
- 3. Estimation of glucose (Bertrand's Method)
- 4. Saponification of fat or oil.
- 5. Iodine value of an oil.

# Unit-II: Spectral Interpretation of Organic Compounds –UV, IR, PNMR and Mass Spectra

- 1. 1,3,5-Trimethylbenzene
- 2. Pinacolone
- 3. Benzylbromide
- 4. Phenylacetone
- 5. Isopropylalcohol
- 6. 2-N,N-Dimethylamino ethanol
- 7. 4-Picoline
- 8. Cinnamaldehyde

# **Unit-III: Spectral Interpretation of Inorganic Compounds**

- 1. <sup>31</sup>P NMR Spectra of methylphosphate
- 2. <sup>31</sup>P NMR Spectra of HPF<sub>2</sub>
- 3. <sup>19</sup>F NMR Spectra of CIF<sub>3</sub>
- 4. <sup>1</sup>H NMR Spectra of Tris (ethylthioacetoacetanato) cobalt (III)
- 5. Expanded high resolution NMR spectra of (N-propyl isonitroso acetylacetoneiminato) (acetylacetoneiminato)Nickel(II)
- 6. ESR Spectra of the aqueous  $ON(SO_3)_2^2$ -ion.
- 7. ESR Spectra of the H atoms in CaF<sub>2</sub>
- 8. ESR Spectra of the  $[Mn (H<sub>2</sub>O)<sub>6</sub>]^{2+}ion$
- 9. ESR Spectra of the bis(salicyladiminato)copper(II)
- 10. IR Spectra of the sulphato ligand
- 11. IR Spectra of the nitro and nitrito pentaminecobalt(III)chloride
- 12. IR Spectra of the dimethylglyoxime ligand and its Nickel(II)complex.
- 13. IR Spectra of carbonyls
- 14. Mossbauer spectra of FeSO<sub>4</sub>.7H<sub>2</sub>O
- 15. Mossbauer spectra of FeCl<sub>3</sub>
- 16. Mossbauer spectra  $[Fe(CN)_6]^{3-}$
- 17. Mossbauer spectra [Fe(CN)<sub>6</sub>]<sup>4</sup>-

## **Unit- IV: Quantitative Analysis of Complex Materials**

To impart the techniques of analysis of alloys; preparation and analysis in Organic complexes.

# (a) Analysis of Alloys

- 1. Analysis of copper and nickel from copper-nickel alloy.
- 2. Estimation of copper and zinc in brass.
- 3. Estimation of iron and nickel in stainless steel.
- 4. Estimation of iron and magnesium from the mixture.

# (b) Analysis of Inorganic Complex Compounds: (for internal assessment only)

- 1. Preparation of cis and trans potassiumbis (oxalato) diaquochromate and analysis of each of these for chromium.
- 2. Preparation of potassiumtris(oxalato)aluminate(III) and analysis for iron and oxalate.

- 1. J. Mendham, R.C.Denney, J. Basset and G.H.Jeffery, Vogel's Textbook of quantitative Inorganic Analysis, 4<sup>th</sup> edition ELBS, Longmann,1978.
- 2. A.I.Vogel, Text Book of Practical Organic Chemistry, ELBS, London, 5<sup>th</sup> edition, 1989.

#### EXTRA DISCIPLINARY ELECTIVE

# EDE – 1 NUTRITION AND DIETETICS

SUBJECT CODE:	THEORY	MARKS: 100
SEMESTER: II/III	CREDITS: 3	TOTAL HOURS: 45

#### **COURSE FRAMEWORK:**

- To introduce the students to the principle of Human Nutrition.
- To understand the relationship between Nutrition and human well being.
- To understand the modifications in nutrients and dietary requirements for various diseases.

#### **COURSE OUTCOME**

On completion of the course the students will be able to

- 1. acquire knowledge about importance of nutrition and diseases caused by malnutrition
- 2. get an awareness on role of vitamins in diet
- 3. get an awareness on role of minerals in diet
- 4. get an awareness on role of water in diet
- 5. gain knowledge on types of diets for various diseases.

Unit-I: Nutrition (9 hrs)

Food pyramid –Development of Nutrition as a Science-Definition of Nutrition.

Under nutrition, over nutrition and malnutrition. protein energy malnutrition - kwashiorkor, Marasmus and Mrasmic Kwashiorkor. Assimilation of food-digestion, absorption, transport, utilisation of nutrients in the body

Unit-II: Vitamins (9 hrs)

Fat soluble vitamins – vitamin A, D, E and K – function effects of deficiency, sources, requirements, units of measurement and hyper vitaminosis. Function, effects of deficiency. Water soluble vitamins- sources and requirements, ascorbic acid, thiamine, riboflavin and Niacin. Importance of folic acid, Vitamin B12 pyridoxine, Biotin and Pantothanic acid to the body.

Unit-III: Minerals (9 hrs)

Distribution in the body, functions, food sources, requirements and effects of deficiency of calcium, phosphorous, Iron and iodine. Trace elements in human nutrition - copper, iron, zinc-functions, food sources, requirements and effects of deficiency. Selenium and vitamin E relationship. Chromium and glucose tolerance factor.

Unit-IV: Water (9 hrs)

Distribution of water in the body, water in take and loss, exchange of water in the body, composition of body fluids.

Unit-V: Dietetics (9 hrs)

Role of Dietician, Basic concepts in Diet Therapy, Routine Hospital Diets. Regular diet, light diet, soft diet, full liquid diet and tube feeding. Modifications of Diet – Febrile conditions, infections and surgical conditions. Diets of gastro intestinal disorders, renal diseases, liver diseases, obesity, cardiovascular disorders and diabetes mellitus. Geriatrics-Role of diet.

### **TEXT BOOKS**

- 1. Mudambi S.R., M.V. Rajagopal, Fundamentals of Food and Nutrition, 5<sup>th</sup> Edition, Wiley Eastern Ltd., 2007.
- 2. Harbans Lal, Food and Nutrition, CBS Publishers & Distributors, 1st edition, 2021.
- 3. Antia, F.P. "Clinical Dietetics and Nutrition", 2<sup>nd</sup> Ed, Oxford University Press, Delhi, reprinted in 2009.

- 1. Dr. Susan A. Lanham, Thomas R. Hill, Alison M. Gallagher, Hester H. Vorster Introduction to Human Nutrition by, Wiley-Blackwell, 3rd Edition, 2019,
- 2. Martin Eastwood, Principles of Human Nutrition, Wiley-Blackwell, 2<sup>nd</sup> Edition, 2003.
- 3.H.-D. Belitz, Werner Grosch, Food Chemistry Springer Science & Business Media, 4<sup>th</sup> edition, 2009.

# **Question Paper Pattern**

Section	Question Component	Numbers	Marks	Total
Section- A	MCQ:1-10, Fill in:11-15 T/F:16-20 Answer all questions	1 – 20	1	20
Section-B	Short Answer /Problems Answer any 5 out of 8 questions	21–28	7	35
Section- C	Essay Answer any 3 out 5 questions	29–33	15	45
TOTAL MARKS			100	

Continu	Unit	No. o	f Questions
Section	Unit	Theory	Problem
	Unit– 1	4	
	Unit– 2	4	
Section-A	Unit–3	4	
	Unit–4	4	
	Unit–5	4	
	Unit– 1	2	
	Unit– 2	1	
Section-B	Unit–3	2	
	Unit–4	2	
	Unit–5	1	
	Unit– 1	1	
	Unit-2	1	
Section-C	Unit–3	1	
	Unit-4	1	
	Unit–5	1	

# EDE -2 APPLIED CHEMISTRY

SUBJECT CODE:	THEORY	MARKS: 100
SEMESTER: II/III	CREDITS: 3	<b>TOTAL HOURS: 45</b>

#### **COURSE FRAMEWORK:**

- To gain knowledge on fuels, fertilizers and water technology.
- To know about the food nutrients and adulterants in food, artificial sugar and beverages.
- To learn about the polymer chemistry and its application.
- To acquire knowledge on drugs like Anesthetics, Analgesics, Antibiotics, Antipyretics.
- To understand the basic fundamentals of Nanochemistry.

#### **COURSE OUTCOME**

On completion of the course the students will be able to

- 1. gain knowledge on fuels, fertilizers and water technology.
- 2. detect adulterants in food and get an awareness about artificial sugar and beverages.
- 3. differentiate various polymer materials
- 4. acquire knowledge on various diseases and drugs
- 5. understand the concepts of nanomaterials

#### **Unit-1: Chemical industries**

(9hrs)

Fuels: Fuels - types of fuels with examples - liquid fuels - gaseous fuels - nuclear fuels. Energy-sources of energy - renewable and non-renewable energies-non-conventional energies. Fertilizers: Definition, requirement of a fertilizer, Classification of fertilizers; Urea, ammonium sulphate, NPK fertilizer, superphosphate, triple superphosphate (uses only).

Water Technology: Sources of water, soft and hard water, methods of removal of hardness, Purification techniques - zeolite method, reverse osmosis and ion exchange.

Unit-2: Food science (9 hrs)

Food and Nutrition - Sources of food, types; Carbohydrates, Proteins, Fats, Minerals and vitamins (sources and their physiological importance) – Balanced diet -Food adulteration-contamination of Wheat, Rice, Milk, Butter, Ghee etc., with clay stones, water and toxic chemicals – Detection of adulterated foods by simple analytical techniques. Artificial sugar viz., saccharin, Aspartame and cyclamate. Beverages – soft drinks – soda -fruit juices –alcoholic beverages examples.

# **Unit–3: Polymer science**

(9 hrs)

Classification of polymers-biopolymers and biodegradable polymers. Plastics, polythene, PVC, Bakelite, polyesters, melamine - formaldehyde resins - Freon, Teflon-(uses only). Building materials - cement, ceramics, glass and refractories - definition, composition and application only.

# **Unit-4: Pharmaceutical products**

(9 hrs)

Definition and Uses of each: Anaesthetics – General and local (Chloroform, diethylether); Analgesics – Narcotic and synthetic; Antipyretics (aspirin, paracetamol and ibuprofen) and anti-inflammatory agents (diclofenac, celecoxib). Antibiotics: penicillin, streptomycin and chloramphenicol. (Structures not required) Cancer and Diabetes– Causes and treatment.

Unit-5: Nano ethics (9 hrs)

Definitions - Nano, nanoscience, and nano technology. Nano in nature – difference between bulk and nanomaterials-challenges in nanotechnology. Applications of Nanotechnology - Nanomedicine: diagnosis, biocompatible nanomedical materials. Industrial applications of nanomaterials: nano coatings and nanotextiles as antibacterial and anti - odour agents in deodorant/antiperspirant, shaving/depilatory products, foot powder, oral care.

- 1. M. Swaminathan, Food Science and Experimental Foods, Ganesh and Company, 1979.
- 2. Jayashree Ghosh, Fundamental Concepts of Applicated Chemistry, S. Chand & Co. Publishers,2<sup>nd</sup> edition, 2006.

- 3. S. Lakshmi, Pharmaceutical Chemistry, S.Chand & Sons, New Delhi, 3<sup>rd</sup> edition,1995.
- 4. V. R. Gowariker, N. V. Viswanathan and Jayader Sreedhar, Polymer Science, Wiley Eastern Ltd., New Delhi, 2012
- 5. V. Veeraiyan, Text book of Ancillary Chemistry, Highmount publishing house, Chennai, 1<sup>st</sup> edition, 2009.
- 6. S. Vaithyanathan, Text book of Ancillary Chemistry; Priya Publications, Karur, 2006.

# **Question Paper Pattern**

Section	Question Component	Numbers	Marks	Total
Section- A	MCQ:1-10, Fill in: 11-15 T/F:16-20 Answer all questions	1 – 20	1	20
Section-B	Short Answer /Problems Answer any 5 out of 8 questions	21–28	7	35
Section- C	Essay Answer any 3 out 5 questions	29–33	15	45
TOTAL MARKS			100	

Castion	IIn:4	No.of	f Questions	
Section	Unit	Theory	Problem	
	Unit-1	4		
	Unit-2	4		
Section A	Unit–3	4		
	Unit-4	4		
	Unit-5	4		
	Unit-1	2		
	Unit-2	1		
Section B	Unit–3	2		
	Unit-4	2		
	Unit-5	1		
Section C	Unit-1	1		
	Unit-2	1		
	Unit-3	1		
	Unit-4	1		
	Unit–5	1		

# EDE –3 ENVIRONMENTAL CHEMISTRY

SUBJECT CODE:	THEORY	MARKS: 100
SEMESTER: II / III	CREDITS: 3	TOTAL HOURS: 45

#### **COURSE FRAMEWORK:**

- To gain knowledge about types of environmental pollution and waste management.
- To acquire knowledge on current issues on disaster management and green chemistry

# **COURSE OUTCOME:**

On completion of the course the students will be able to

- 1. identify various pollutions and its hazards.
- 2. demonstrate the types of waste and their management.
- 3. understand the facts of toxicology and global warming.
- 4. apply the green chemical concepts in existing chemical reactions.
- 5. create an awareness on disaster management and emergency preparedness.

#### **UNIT-1: Environmental Pollution**

(9 hrs)

Air Pollution - sources — oxides of nitrogen, sulphur, ozone, hydrocarbons and particulate matter - effects and control measures - Air quality and emission standards. Water Pollution sources — organic, inorganic and heavy metals — Effects- Eutrophication — Transport of pollutants in the aquatic ecosystem - control measures of Ocean, Oil and Ground water pollution - Soil Pollution sources - Industrial, Domestic, Agricultural - Effects of soil pollutants on plants, animals and ground water - Radioactive pollution — sources- radioactive elements, Effects of radiation on surrounding environment and control measures.

## **UNIT-2:** Waste Management

(9 hrs)

Wastes – sources - Global scenario of wastes - Waste collection, Storage and segregation - Transportation and disposal methods of hazardous waste. Control measures and Impacts of biomedical and e-wastes in environment. Plastic wastes: Sources, Facts & figures of plastic waste scenarios in National & International - Effect of plastic wastes on environment. Different steps in the treatment of industrial waste- equalization, neutralization, sedimentation, oil separation, floatation, coagulation.

### **UNIT- 3: Environmental Toxicology and Current Issue**

(9hrs)

Environmental Toxicology and Pharmacokinetics -Toxic effects and dose response relationship - a brief idea of carcinogens and non-carcinogens, Biotransformation, Biomarker, Xenobiotics, Toxicity due to Hydrocarbons and pesticides. Global warming - Greenhouse effect, Ozone layer depletion and climate change—Facts and figures of current global warming scenarios in the world—Remedial measures.

# **UNIT-4: Energy and Green Technologies**

(9 hrs)

Energy—renewable, non-renewable energy sources, Geothermal, wind, Tidal, solar, nuclear and bio energy—Waste as renewable sources of energy—conversion of methane in to synthetic gas, factors effecting methane formation-Green Chemistry-Principles of green chemistry—inception and evolution—Importance of solvents—catalysts and their role—biological alternatives—Green Technologies in pharmaceutical, polymer, textile agrochemical industry.

## UNIT- 5: Environmental Quality and Disaster Management (9hrs)

Basic concepts of sustainable development - Guidelines for the preparation of environmental impact statement - Environmental quality standards International organization for standardization - ISO 14000, 19000 and 22000 standards and certification, Environmental safety – Risk management and emergency preparedness -Earthquakes, Tsunami, Landslides, Cyclones, Floods, and Forest fires predictions, Forecasting and mitigation measures of environmental hazards.

#### **TEXTBOOKS**

- 1. B.K. Sharma, Environmental Chemistry, Goel Publishing House, 12<sup>th</sup> edition, 2011.
- 2. Asim K.Das, Environmental Chemistry with Green Chemistry, Books and Allied (P) Ltd, Arun, 1<sup>st</sup> edition, 2010.
- 3. P.S. Sindhu, Environmental Chemistry, New Age International publishers,2<sup>nd</sup> Edition, 2010.

- Bhide and Sundaresan, Solid Waste Management in Developing Countries Indian National Scientific Documentation Center, New Delhi, 2000.
- 2. George Tehobanaglous- Milary Theiren and Samuel, Avigil Integrated Solid

- Waste Management, McGraw Hill Inc, 1993.
- 3. John Pitchel, Waste Management Practices, Municipal, Hazardous, and Industrial, Taylor & Francis Group, LLC, 2005.
- 4. Thomous S. Spiro and William M. Stiglicini, Chemistry of the Environment, Prentice Hall of India Pvt. Ltd., 2002.
- 5. Bregman JI Environmental Impact Statements, Lewis Publishers, London, 1999.
- 6. Canter LW, Environmental Impact Assessment, McGraw Hill, New York, 1996.
- 7. Khanal SK, Surampalli RY, ZhangTC, Lamsal BP, Tyagi RD, Kao CM, Bioenergy and Biofuel from Biowastes and Biomass, American Society of Civil Engineers, Virginia, USA, 2010.
- 8. Lee S and Shah YT, Biofuels and Bioenergy: Processes and Technologies, CRC Press, BocaRaton, FL, USA, 2013.

# **Question Paper Pattern**

Section	Question Component	Numbers	Marks	Total
Section- A	MCQ:1-10, Fill in:11-15 T/F:16-20 Answer all questions	1 – 20	1	20
Section-B	Short Answer /Problems Answer any 5 out of 8 questions	21–28	7	35
Section- C	Essay Answer any 3 out 5 questions	29–33	15	45
TOTAL MARKS			100	

Continu	T I 24	No.of Questions		
Section	Unit	Theory	Problem	
	Unit-1	4		
	Unit– 2	4		
Section-A	Unit–3	4		
	Unit–4	4		
	Unit–5	4		
	Unit– 1	2		
	Unit–2	1		
Section-B	Unit–3	2		
	Unit–4	2		
	Unit–5	1		
	Unit– 1	1		
Section-C	Unit-2	1		
	Unit–3	1		
	Unit–4	1		
	Unit–5	1		

# EDE -4 FORENSIC SCIENCE

SUBJECT CODE:	THEORY	<b>MARKS: 100</b>
SEMESTER: II/III	CREDITS: 3	<b>TOTAL HOURS: 45</b>

#### **COURSE FRAMEWORK:**

- To gain knowledge about types of poisons, explosives.
- To acquire knowledge about forgery, tracking and fire investigation.

#### **COURSE OUTCOME:**

On completion of the course the students will be able to

- 1. study of poisons, mode of action, detection and estimation of poisons, basics of pesticides and insecticides
- 2. acquiring knowledge about classification and characteristics of explosives, chemical synthesis of explosives like TNT, RDX, postblast residue collection and analysis.
- 3. investigation of crimes, forged signatures, checking original currency notes, detection of gold purity.
- 4. Investigation of tracks and traces, DNA finger printing for tissue identification, detecting steroid consumption in athletes and race horses.
- 5. study of chemistry of fire, types, fire scene patterns, collection of arson evidence, investigation of clue materials.

#### **UNIT-1: Poisons and Pesticides**

(9 hrs)

Definition of poisons, types of poisons – metal, synthetic chemical, biochemical, gaseous poisons. Mode of ingestion–oral ,inhalation, intravenous. Action and impact on human health. Detection of poisons - carbon monoxide, cyanide, ethanol and formaldehyde.Metallic poison–Reinch test –Marsch Berzelius and Gutzeit tests.

#### **UNIT-2:** Explosives

(9 hrs)

Classification of explosives—low explosives and high explosives, home made explosives, military explosives.Common explosives-TNT, PETN and RDX. Explosion process, post blast residue collection and analysis.

#### **UNIT-3: Forgery and Counterfeiting**

(9 hrs)

Forgery in documents, different types of forged signatures - simulated and traced forgeries, detection of forgery - uses of ultraviolet rays, comparison of type written letters,

checking silver line watermark in currency notes, alloy analysis using AAS to detect counterfeit coins - detection of gold purity in 22 carat ornaments – detecting gold plated jewels-authenticity of diamond

#### UNIT-4: Tracks and Traces

Foot prints - costing of foot prints - residue prints, walking pattern or tyre marks -miscellaneous traces and tracks, glass fracture, tool marks, paints, fibers. Analysis of biological substances - blood, semen, saliva, urine and hair - Cranial analysis (head and teeth) DNA Finger printing for tissue identification in dismembered bodies -detecting steroid consumption in athletes and race horses.

#### **UNIT-5:** Arson and fire investigation

(9 hrs)

(9 hrs)

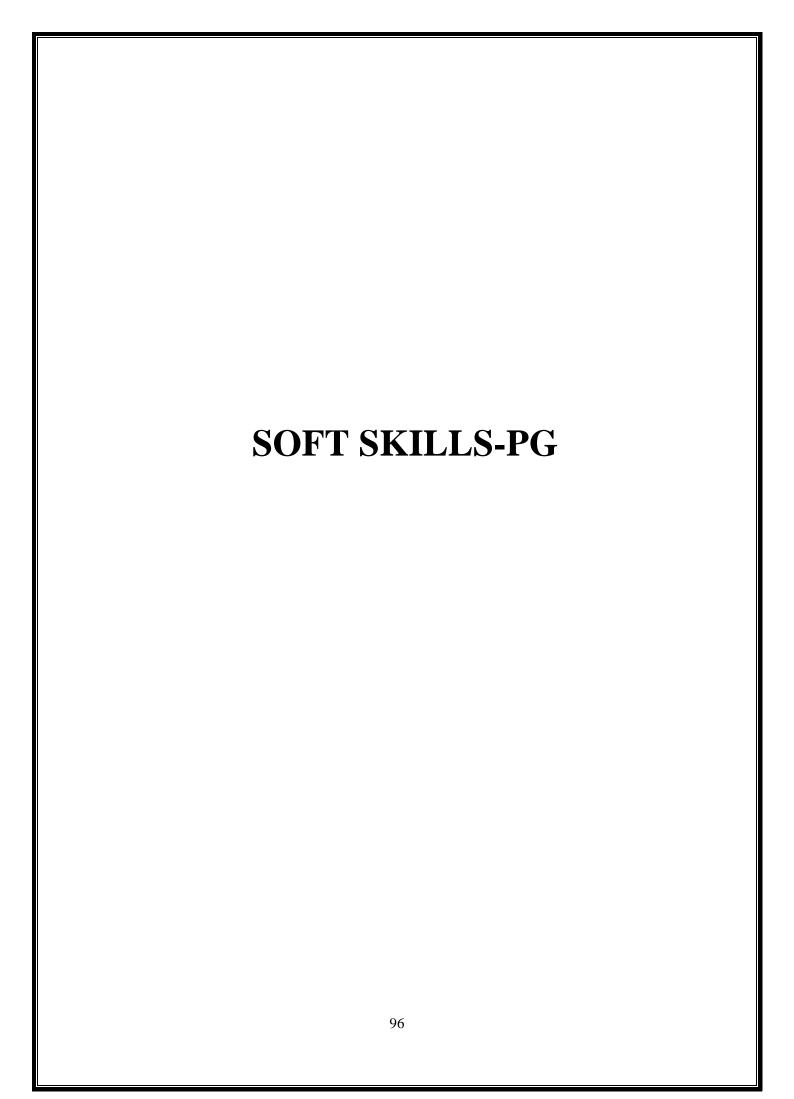
Chemistry of fire, conditions for fire and fire scene patterns. Location of point of ignition. Recognition of type of fire. Searching the fire scene. Collection and preservation of arson evidence. Analysis of fire debris. Analysis of ignitable liquid residue. Scientific investigation and evaluation of clue materials. Information from smoke staining.

- 1. T.H.James, Forensic Sciences, Stanley Thornes Ltd,1987.
- 2. Sopfestein, Richard Saferstin and Criminalistics-An Introduction to Forensic Science (College Version), Printicehall, 8<sup>th</sup> edition, 2003.
- 3. Almirall JR and Furton K G, Fire scene evidence, CRCPress, 2004.
- 4. Redsicker DR and Cannor JJ, Practical:Fire and arson investigation,Routledge, 2<sup>nd</sup> edition,1996.

# **Question Paper Pattern**

Section	Question Component	Numbers	Marks	Total
Section- A	MCQ:1-10, Fill in: 11-15 T/F:16-20 Answer all questions	1 – 20	1	20
Section-B	Short Answer /Problems Answer any 5 out of 8 questions	21–28	7	35
Section- C	Essay Answer any 3 out 5 questions	29–33	15	45
TOTAL MARKS			100	

C4:	T I 94	No. of Questions	
Section	Unit	Theory	Problem
	Unit-1	4	
	Unit–2	4	
Section-A	Unit–3	4	
	Unit-4	4	
	Unit–5	4	
	Unit-1	2	
	Unit–2	1	
Section-B	Unit–3	2	
	Unit-4	2	
	Unit–5	1	
	Unit-1	1	
Section=C	Unit-2	1	
	Unit–3	1	
	Unit-4	1	
	Unit–5	1	



# DEPARTMENT OF ENGLISH FIRST YEAR- FIRST SEMESTER 2022-23

# **Personality Enrichment**

#### **UNIT-I:- Self Disclosure**

- Characteristics of self-disclosure.
- Self-disclosure benefits and appropriateness.
- Self-disclosure and self-awareness.
- Self-disclosure and feedback.

# **UNIT-II: Anger, Stress and Managing Feelings**

- The nature of stress.
- Managing stress through social support systems.
- The nature of anger.
- Guidelines for managing anger constructively.
- Dealing with an angry person.

# **UNIT – III : Interpersonal Effectiveness**

- Managing anxiety and fear.
- Breathing—an antidote to stress.
- Progressive muscle relaxation.
- Understanding your shyness.
- Building one's self esteem.
- Avoiding self blame.
- Taking risks.
- Tolerating failure.
- Persisting and celebrating success.
- Self talk.

### **UNIT – IV: Study Skills**

- Importance of study environment.
- Using VCR3 to increase memory power: visualizing, concentrating, relating, repeating, reviewing.
- Memory hindrances.
- Memory helpers.
- Knowing vs memorizing.
- Memory and studying.
- The SQ3 R method; survey, write questions, read, recite, review.
- Mnemonic devices –rhymes–acronyms –pegging.
- Cooperative learning.

# **UNIT- V: Goal Setting and Managing Time**

- The basis of effective goals.
- Steps to be followed to obtain optimum results from goal setting.
- Identifying the reasons for procrastination.
- Guidelines to overcome procrastination.
- Priority management at home and college.

- 1. Johnson, D.W. Reachingout–Interpersonal Effectiveness and Self Actualization, 6<sup>th</sup> edition, Boston: Allyn and Bacon, 1997.
- 2. Sherfield, R.M., Montgomery, R.J. and Moody, P.G. Developing Soft Skills. 4<sup>th</sup> edition, NewDelhi:Pearson, 2010.
- 3. Robbins, S.P. and Hunsaker, Phillip, L. Training in Interpersonal skills, Tips for managing people at work, 5th edition, New Delhi: PHI Learning, 2009.

#### FIRST YEAR – SECOND SEMESTER

#### WORK PLACE COMMUNICATION SKILLS

# **UNIT-I:** Goal Setting

- SMART Goals.
- Blue print for success.
- Short Term, Long Term, Life Time Goals.

# **UNIT- II: Team Building and Working**

- Team Work necessity.
- Personal, Social and Educational.

#### **UNIT-III: Emotional Intelligence**

- Definition.
- Emotional.quotient.
- Importance of Emotional Intelligence.
- Emotion Scales.
- Managing Emotions.

#### **UNIT-IV:** Creativity

- Out of the box thinking.
- Lateral Thinking.
- Stimulating innovation and change.

# **UNIT-V: Decision Making and Empowerment**

- Importance and necessity of Decision Making.
- Process and practical way of Decision Making.
- Weighing Positives and Negatives.
- Power tactics.
- Coalition.
- Managerial empowerment.
- Entrepreneurship.

- 1. Covey Sean, Seven Habits of Highly Effective Teens, New York, Fireside Publishers, 1998.
- 2. Carnegie Dale, How to win Friends and Influence People, New York: Simon and Schuster, 1998.
- 3. Thomas A Harris, I amok, You areok, New York, Harper and Row, 1972.
- 4. Daniel Coleman, Emotional Intelligence, Bantam Book, 2006.

#### SECOND YEAR – THIRD SEMESTER

#### SELF AND TIME MANAGEMENT SKILLS

# **UNIT- I: Stress Management**

- Definition of Stress.
- Types of Stress.
- Symptoms.
- Stress coping ability.
- Stress inoculation training.
- Techniques to manage Stress.

# **UNIT-II: Crisis and Conflict Management Skills**

- Definition of Crisis.
- Ways to overcome Crisis.
- Critical Thinking and Innovation.
- Problem Solving.
- Types of conflict.
- Conflict stimulation.
- Conflict resolution–Approaches.

# **UNIT-III: Interpersonal Skills**

- Group decision making.
- Types of leadership.
- Emotional intelligence.
- Effective leadership.
- Negotiation skills.

# **UNIT – IV: Time Management**

- Concept.
- Limitations.

- Attendance, Self-Discipline and Punctuality.
- Adherence to Time.
- Maintaining Work/Life Balance.

#### **UNIT-V: Self-Actualization**

- SWOC Analysis.
- Self-Regulation.
- Self-Evaluation.
- Self-Management.
- Self-Monitoring.
- Self-Criticism.
- Self-Motivation.
- Self Esteem.
- Importance of Self Confidence.

- Wentz, Fredrick H. Soft skills Training A workbook to develop skills for employment by, Create Space Independent Publishing Platform; Large edition, May14, 2012.
- 2. Mitra, Barun K. Personality Development and Soft skills, Oxford University Press, 2011.
- 3. Mackenzie, Alec R. The TimeTrap: The Classic book on Time Management, NewYork: AMACOM Books, 2009.

#### SECOND YEAR –FOURTH SEMESTER

# SPOKEN AND PRESENTATION SKILLS

#### Unit- I

- Body Language.
- Kinesics, Proxemics, Paralinguistic, Chronemics.
- Nuances of Speech Delivery.
- Personality Development: Building self-esteem.

#### Unit-II

- Team work and participating in group discussions.
- Team building and Team work.
- Team briefing.
- Role of Team leader.
- Conflict resolution.
- Methodology of Group discussions.
- Role Functions in Group Discussion.
- Types of Non –functional Behavior.
- Improving group performance.
- Participating in Mock group discussions.

#### Unit- III

- Interviews.
- Types of Interviews.
- Preparing for interviews.
- Facing interviews.
- Reviewing performance.
- Participating in mock interviews.

#### **Unit-IV**

- Etiquettes for Public Speaking (extempore and lectures).
- Telephone Conversations and Business Meetings.

#### Unit-V

- Business Presentations.
- Preparing successful presentations.
- Thinking about audience.
- Making effective use of visual aid.
- Delivering presentation-using prompts, dealing with questions and interruptions.
- Mock presentations.

- 1. Peter, Francis, Soft Skills and Professional Communication, New Delhi: Tata McGraw Hill, 2012.
- 2. Singh, Prakash and Raman, Meenakshi, Business Communication, New Delhi: Oxford UP, 2006.
- 3. Bailey, Edward P., Writing and Speaking at Work: A Practical Guide for Business Communication, Pennsylvania: Prentice Hall, 2007.
- 4. Pease, Allan and Peas, Barbara, The Definitive Book of Body Language., New York: Random House, 2006.
- 5. DeBono, Edward., Serious Creativity, Reprint, Harper Business, 1993.