MANONMANIAM SUNDARANAR UNIVERSITY TIRUNELVELI
PG - COURSES – AFFILIATED COLLEGES
M.Sc. CHEMISTRY
(Choice Based Credit System)
(For those who joined from 2021- 2022 onwards)

VISION OF THE UNIVERSITY

To provide quality education to reach the un-reached.

MISSION OF THE UNIVERSITY

- To conduct research, teaching and outreach programmes to improve conditions of human living.
- To create an academic environment that honours women and men of all races, caste, creed, cultures and an atmosphere that values intellectual curiosity, pursuit of knowledge, academic freedom and integrity.
- To offer a wide variety of off-campus educational and training programs, including the use of information technology, to individuals and groups.
- To develop partnership with industries and government so as to improve the quality of the workplace and to serve as catalyst for economic and cultural development.
- To provide quality/inclusive education, especially for the rural and un-reached segments of economically downtrodden students including women, socially oppressed and differently abled.

PREAMBLE

All the changes in life in one-way or other involve chemistry. Chemistry is central to the current revolutions in science. No educated person today can understand the modern world without a basic knowledge of chemistry. The existence of a large number of chemical factories, mines and related industries necessitates chemistry education. An advanced course in chemistry will be a fascinating experience because it helps us understanding our surroundings. Hence, the Programme M.Sc. (Chemistry) is offered to meet current needs of aspiring youths and also create awareness about the in-depth scientific aspects to the society.

ELIGIBILITY

A Bachelor's degree in B. Sc Chemistry.

VISION OF THE PROGRAMME

Provide quality education and training in the field of chemistry to enable successful careers for the post graduate students in the field of education, research and industry applications of chemical science.

MISSION OF THE PROGRAMME

- To empower the youth through quality education and to provide professional leadership.
- To train and mentor students to become technically competent, responsible scientists, scientifically literate professionals and strong academicians who will constructively contribute to the overall growth of the society.
- To usher in construction of the thinking of students to scientifically tackle modern problems and global challenges.

PROGRAMME EDUCATIONAL OBJECTIVES (PEOs)

- PEO1: To impart knowledge in fundamental aspects of all branches of chemistry
- PEO2: To acquire deep knowledge in the study of spectroscopy, Disconnection approach, Synthetic chemistry, Coordination chemistry, Inorganic polymers, Group theory, Quantum chemistry, etc.
- PEO3: To acquire knowledge in the specialized areas of chemistry like Green chemistry, Nanoscience and Nanotechnology, Chemistry of Industrial products, Medicinal chemistry, Industrial processes, Catalysis, Forensic chemistry.
- PEO4: To impart the basic analytical and technical skills to work effectively in the various fields of chemistry.
- PEO5: To motivate critical thinking and analysis skills to solve complex chemical problems, e.g., analysis of data, synthetic logic, spectroscopy, structure and modeling, team-based problem solving, etc.
- PEO6: To enable the students to be competent, creative and highly valued professionals in industry, academia or government.

PROGRAMME OUTCOMES (POs):

On successful completion of the Programme, students will be able to

- PO1: Function as responsible individuals with ethical values, accountable to the community.
- PO2: Gain detailed knowledge of the major areas of chemistry including a wide range of factual information and experimentally observed phenomena.
- PO3: Apply chemical concepts in new situations and computational software in chemistry efficiently.
- PO4: Think critically and analyze chemical problems.
- PO5: Work effectively and safely in a laboratory environment.
- PO6: Present scientific and technical information resulting from laboratory experimentation by means of oral presentation, scientific poster or a written report.
- PO7: Pursue higher education / employable/ entrepreneur.
- PO8: Work in teams as well as independently in academia, industry or government.

PROGRAMME SPECIFIC OUTCOMES (PSOs)

Upon successful completion of M.Sc. Chemistry programme, graduates will be able to

- PSO1: Apply advanced concepts of organic, analytical, physical and inorganic chemistry to solve complex problems to improve human life.
- PSO2: Possess skill in spectral, analytical, qualitative and quantitative techniques which will be useful in industry.
- PSO3: Gain knowledge in recent and advanced developments in the area of Green Chemistry, Chemistry of Industrial products and formulation, Forensic Chemistry, Industrial Processes, Catalysis, Nanoscience and Nanotechnology, Medicinal Chemistry, Natural Products Chemistry, Bioinorganic Chemistry, Computational Chemistry, Contrasting agents in medical Diagnosis, Sensors etc.
- PSO4: Design a synthetic route for new compounds and transform innovative ideas into reality.
- PSO5: Be competent in problem solving, critical thinking and analytical reasoning as applied to scientific problems.
- PSO6: Acquire understanding of Plagiarism and Intellectual Property Rights.
- PSO7: Use Computational software in chemistry efficiently.

- PSO8: Carry out research / investigation independently to solve practical problems and write / present a substantial technical report/document.
- PSO9: Transform learned knowledge and skills to qualify in the NET and other competitive exams for higher studies and job.

COURSE STRUCTURE

Sem.	Sub. No.	Course Status	Course Title	Contact Hrs/ week	Credits
I	1	Core - 1	Aromaticity and Organic Reaction Mechanism	4	4
	2	Core - 2	Fundamentals of Inorganic Chemistry, Nuclear Chemistry and Inorganic Polymers	5	4
	3	Core - 3	Quantum Mechanics and Spectroscopy – I	5	4
	4	Elective – I (*Choose any One*)	1.1 Green Chemistry – Techniques and Applications	4	4
			1.2 Chemistry of Industrial Products and Formulation		
			1.3 Forensic Chemistry		
	5	Core - 4 Practical - 1	Organic Chemistry Practical – I	4	2
	6	Core – 5 Practical - 2	Inorganic Chemistry Practical – I	4	2
	7	Core - 6 Practical - 3	Physical Chemistry Practical – I	4	2
	Subtotal			**30**	**22**
II	8	Core - 7	Stereochemistry, Organic Reagents and Photochemistry	5	4
	9	Core - 8	Coordination Compounds and Solid State Chemistry	4	4
	10	Core - 9	Electrochemistry and Spectroscopy - II	5	4
	11	Elective – II (*Choose any One*)	2.1 Nanoscience And Nanotechnology	4	4
			2.2 Medicinal Chemistry		
			2.3 Industrial processes and Catalysis		
	12	Core - 10 Practical - 4	Organic Chemistry Practical – II	4	2
	13	Core - 11 Practical - 5	Inorganic Chemistry Practical – II	4	2
	14	Core – 12 Practical - 6	Physical Chemistry Practical – II	4	2
	Subtotal			**30**	**22**

Sem	Sub. No	Course Status	Course Title	Contact Hrs/ week	Credits
III	15	Core - 13	Organic Spectroscopy and Rearrangements	5	4
	16	Core - 14	Spectral Methods-I, Organo Metallic and Analytical Methods	5	4
	17	Core - 15	Group Theory and Chemical Thermodynamics	4	4
	18	Core - 16	Scientific Research Methodology	4	4
	19	Core - 17 Practical - 7	Organic Chemistry Practical – III	4	2
	20	Core - 18 Practical - 8	Inorganic Chemistry Practical – III	4	2
	21	Core - 19 Practical - 9	Physical Chemistry Practical – III	4	2
	Subtotal			**30**	**22**
IV	22	Core - 20	Synthetic Strategies in Organic Chemistry	5	4
	23	Core - 21	Bioinorganic, Spectral Methods-II and Photochemistry	5	4
	24	Core - 22	Chemical Kinetics, Photochemistry and Surface Chemistry	5	4
	25	Core - 23	Selected Topics in Chemistry	4	4
	26	Core – 24 Practical-10 (*Hands on Training*)	Computational Software in Chemistry - Laboratory Course	4	2
	27	Core - 25	Project	7 + 5*	6
	Subtotal			**30**	**24**
	Total			**120**	**90**

*****Extra hours for the project

For the project, flexible credits are b/w 5-8 & Hours per week are b/w 10-16.

Total number of credits ≥ 90 : 90

Total number of Core Courses : 25 (14T+10P+1Project)

Total number of Elective Courses : 02

Total number of Courses : 27

Total hours : 120

EVALUATION

The evaluation of each course comprises two components that are Internal and External.

THEORY

External : Internal = 75 : 25

PRACTICAL

External : Internal = 50 : 50

COMPUTATIONAL SOFTWARE IN CHEMISTRY - LABORATORY COURSE

External : Internal = 50 : 50

PROJECT

External : Internal = 50 : 50

INTERNAL

THEORY

Maximum marks: 25

There is no minimum pass mark for internal. But, if it is less than 50%, it should be compensated in the external.

Components	**Marks**
The average of the best two tests from three compulsory tests	15
Assignment	05
Seminar	05
Total	25

Note: Re internal assessment test for the student will not be allowed.

PRACTICAL

Maximum marks: 50

There is no minimum pass mark for internal. But, if it is less than 50%, it should be compensated in the external.

The break-up for the internal component will be as follows:

Components	**Marks**
Number of Experiments	30
Record	10
Mid-Term and Model Test Average	10
Total	50

COMPUTATIONAL SOFTWARE IN CHEMISTRY - LABORATORY COURSE

The students must do the exercises depending on the availability of time and suitable computational chemistry software and maintain the file with printed copy of results. This file should be submitted at the end of semester during the viva – voce examination.

Maximum marks: 50

There is no minimum pass mark for internal. But, if it is less than 50%, it should be compensated in the external.

The break-up for the internal component is as follows:

Components	**Marks**
Number of Exercises	30
Periodical submission of Reports	10
Model Test Average	10
Total	50

PROJECT

Maximum marks: 50

There is no minimum pass mark for internal. But, if it is less than 50%, it should be compensated in the external.

Students will do the experiments and project work on a title approved by the respective project supervisor. Students will maintain daily records and present oral reports while doing project preparation. All the above process will be duly assessed by the project supervisor to award the internal mark.

EXTERNAL

THEORY

Maximum marks: 75

Passing minimum marks: 38

The external evaluation will be based on the examinations to be conducted by the University at the end of each semester.

Question Pattern:

Section – A

Answer **ALL** the Questions (Multiple choice questions) 10 x 1 = 10

[Two Questions from One Unit]

Section – B

Answer **ALL** the Questions choosing either (a) or (b) 5 x 5 = 25

[One Question from each Unit]

Section – C

Answer **ALL** the Questions choosing either (a) or (b) 5 x 8 = 40

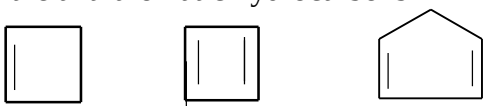
[One Question from each Unit]

Model Question Paper:

Code No. : **Subject Code : ZCHM11**

M.Sc. (CBCS) DEGREE EXAMINATION,
NOVEMBER 2021
First Semesterr
Chemistry
ORGANIC CHEMISTRY – I
(For those who joined in July 2021-22)

Time: Three hours Maximum: 75 marks

Q. No	PART A – (10 X 1 = 10 marks) Answer **ALL** the questions	CO	K - Level
	Choose the correct answer:		
1	Which one of the following compounds has dipolemoment? (a) Benzene (b) Azulene (c) Cyclobutane (d) Naphthalene	1	K4
2.	Choose the anti aromatic hydrocarbons  (i) (ii) (iii) (a) i (b) ii (c) iii (d) i, ii and iii	1	K4
3.	The crossover product is obtained in the ---------- reaction pathway (a) Intramolecular (b) Intermolecular (c) Inter – Intramolecular (d) Intra – Intermolecular	2	K2
4.	In aliphatic unimolecular nucleophilic substitution reaction, the geometry of first transition state resembles to that of ----------. (a) Reactant (b) Product (c) Intermediate (d)Second Transition state	2	K2
5.	The intermediate formed in Wolff rearrangement is ----------. (a) carbene (b) carbanion (c) aryne (d) nitrene	3	K2
6.	Nitrene is a ---------- species. (a) monovalent (b) divalent (c) trivalent (d) tetravalent	3	K2
7.	When 2-bromobutane undergoes elimination reaction (alk. KOH), 80% ----------- and 20% 1-butene are produced. (a) 2-butene (b) ethene (c) ethane (d) propene	4	K4
8.	Reaction intermediate of E_1CB reaction is ----------. (a) Benzene (b) Six membered cyclic transition state (c) Carbanion (d) Carbocation	4	K2
9.	Birch reduction reagent is ------. (a) Na/Hg (b) $NaBH_4$ (c) Na/liq. NH_3 (d) R-MgX	5	K2
10.	The intermediate formed in Wittig reaction is ------- (a) Carbonium ion (b) Carbanion (c) Aryne (d) Ylide	5	K2

PART B – (5 X 5 = 25 marks)
Answer **ALL** the questions choosing either (a) or (b)
Each answer should not exceed 250 words

11.	(a) Comment on the aromaticity of [10] and [14] annulenes.	1	K2
	Or		
	(b) Describe the structure and synthesis of adamantane.		K2
12.	(a) What do you mean by thermodynamic and kinetic controlled reactions? Explain with suitable example.	2	K2
	Or		
	(b) Write down the significance of the reaction constant (ρ) and substituent constant (σ) of Hammett equation.		K2
13.	(a) Explain the stability and structure of singlet and triplet carbenes.	3	K2
	Or		
	(b) Discuss the mechanism of Kolbe reaction.		K2
14.	(a) Discuss the aliphatic nucleophilic S_N2 mechanism with examples.	4	K2
	Or		
	(b) What are the conditions that favour E_1CB mechanism in an elimination reaction? Illustrate with two examples.		K2
15.	(a) Write a brief account on benzyne mechanism.	5	K2
	Or		
	(b) Give an account of the synthetic applications of Wittig reaction.		K2

PART C – (5 X 8 = 40)

Answer **ALL** the questions choosing either (a) or (b)

Each answer should not exceed 600 words.

16.	(a) Discuss the concept of antiaromaticity and homoaromaticity with examples.	1	K2 (30%) K4 (70%)
	Or		
	(b) Discuss the aromaticity of (i) Azulene and (ii) Sydnones		K2 (30%) K4 (70%)
17.	(a) How the following methods are useful in studying the reaction mechanism? (i) study of intermediates (ii) isotope labeling.	2	K2
	Or		
	(b) Discuss about the following: (i) Primary isotopic effect (ii) Hammond Postulate (4+ 4)		K2
18.	(a) Discuss the mechanism of (i) Hoffmann rearrangement (ii) Hofmann-Loffler reaction.	3	K2
	Or		
	(b) Narrate the generation, stability and reactions of free radicals.		K2
19.	(a) Explain how π and σ bonds behave as neighbouring groups to accelerate reactions. Show how they affect the stereochemistry.	4	K2
	Or		
	(b) Write short notes on (i) S_N1 mechanism (ii) Chugaev reaction (iii) Cope reaction.		K2
20.	(a) (i) Write an account of Smiles rearrangement. (ii) Write any four synthetic applications of $NaBH_4$.	5	K2
	Or		
	(b) Discuss the mechanism for (i) Mannich reaction (ii) Dieckmann condensation		K2

PRACTICAL

Maximum marks: 50

Passing minimum marks: 25

Practical examinations will be conducted at the end of each semester. The scheme of valuation is to be decided by the respective board of Question setters.

COMPUTATIONAL SOFTWARE IN CHEMISTRY - LABORATORY COURSE

Maximum marks: 50

Passing minimum marks: 25

The external examiner and internal examiner will conduct viva-voce regarding the computational chemistry software used by the students during the entire course to award external mark.

PROJECT AND VIVA-VOCE

Maximum marks: 50

Passing minimum marks: 25

Project report evaluation and Viva-Voce will be conducted by the external examiner and the Research Supervisor. The break-up for the project work is as follows:

Components	**Marks**
Project Report	30
Viva-Voce	20
Total	50

Note:

Scheme of evaluation of Project report includes choosing a universal problem, novelty of the title, purpose and importance of work for future development and methodology of writing the project report.

SEMESTER I

CORE 1	AROMATICITY AND ORGANIC REACTION MECHANISM	L	T	P	C
		4	0	0	4

Course Objectives:

- *To understand the concept of aromaticity, Novel ring systems and organic reaction mechanism determination.*
- *To study about reactive intermediates involved in organic reactions.*
- *To understand Aliphatic and Aromatic Nucleophilic substitution reaction, Elimination and Addition reaction mechanisms.*

UNIT I - AROMATICITY AND NOVEL RING SYSTEM (12 Hours)

Aromaticity: Benzenoid and non–benzenoid aromatic compounds – sextet theory – MO theory – Delocalisation and resonance - Huckel's rule – Aromatic – antiaromatic – homoaromatic and non–aromatic compounds - Musulin – Frost diagram - NMR and aromaticity - Annulenes and hetero annulenes – Azulene and sydnones - Fullerenes - Alternant and non – alternant Hydrocarbons.

Novel ring system: Nomenclature of bicyclic and tricyclic systems – structure and synthesis of Adamantane – Congressane.

UNIT II - DETERMINATION OF ORGANIC REACTION MECHANISM (12 Hours)

Reaction mechanism: Energy diagram of simple Organic reactions – Transition state and intermediate - Kinetic and Thermodynamic requirements of reactions – Hammond Postulate and microscopic reversibility.

Methods: Kinetic and Thermodynamic control of product formation. Kinetic methods of determination: Rate law – Primary and secondary isotope effect. Non-Kinetic methods of determination: Testing and Trapping of intermediates, Isotopic labeling, Cross–over experiment, Product analysis and stereo chemical evidence.

LFER: Hammett equation – Physical significance of σ and ρ – Applications and Limitations – Taft equation. Yukawa Tsuno equation, Swain-Lupton equation, Grunwald–Winstein equation.

UNIT III - REACTIVE INTERMEDIATES (12 Hours)

Carbenes: Generation, stability, structure and reactivity of carbenes – Simmons Smith cyclopropanation, Wolff rearrangement of acyl carbenes and their synthetic applications.

Nitrenes: Generation, stability, reaction of nitrenes - Mechanism of rearrangements through Nitrene intermediate: Schmidt, Hoffmann, Beckmann rearrangements.

Free radicals: Formation, structure, stability and reactivity - Fenton, Kolbe, Hofmann-Loffler, Barton – McCombie, Giese reactions and Barton-decarboxylation.

UNIT IV - ALIPHATIC NUCLEOPHILIC SUBSTITUTION AND ELIMINATION REACTIONS (12 Hours)

Aliphatic nucleophilic substitution: Mechanism of S_N1, S_N2, S_Ni, S_N1', S_N2' and S_Ni' reactions – Stereochemical aspects of these reactions - Effect of substrate, nucleophile, leaving group and solvent on the rate of substitution - Ambident nucleophile – NGP.

Elimination reaction: E_1, E_2 and E_1CB mechanisms - Stereochemical aspects of these reactions - Factors influencing elimination reactions - Hofmann and Satyzeff rules - Pyrolytic elimination - Chugaev and cope reactions - competition between substitution and elimination reactions.

UNIT V - AROMATIC NUCLEOPHILIC SUBSTITUTION REACTION AND ADDITION TO MULTIPLE BONDS (12 Hours)

Aromatic nucleophilic substitution reaction: Unimolecular, Bimolecular and Benzyne mechanisms - Reactivity, effect of substrate, leaving group and attacking nucleophile -typical reaction as oxygen and sulphur as nucleophile - Bucherer and Rosenmund reaction - Smiles rearrangement - Ortho-lithiation reaction and its application.

Catalytic hydrogenation - Birch reduction - Dieckmann condensation - Mannich reaction - Wittig reaction - Sharpless asymmetric epoxidation - Michael addition (1,2 and 1,4) - Addition of dialkyl groups to triple bonds. Addition of hydrides – $LiAlH_4$ and $NaBH_4$.

TEXT BOOKS

1. R.T. Morrison, and R.N. Boyd, *Organic Chemistry*, 7th edn, Pearson Education, 2010.
2. J. Mc Murry, *Fundamentals of Organic Chemistry*, 7th edn, Cengage Learning IndiaEdition, 2013.
3. P. Sykes, *A Guidebook to Mechanism in Organic Chemistry*, 6th edn, Pearson Education, 2003.
4. I.L. Finar, *Organic Chemistry*, Vol I, 6th edn, Pearson Education, 2002.
5. M.B. Smith, *March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure*,7th edn, Wiley, 2015.
6. S.M. Mukherjee and S.P. Singh, *Reaction Mechanism in Organic Chemistry*, Trinity Press, 2014.

7. John McMurry, *Fundamentals of Organic Chemistry*, Fifth edition, Thomson-Brooks/Cole, 2003.
8. Raj K. Bansal, *Organic Reaction mechanisms*, Tata Mc Graw Hill, Third Editon, 2007.

REFERENCE BOOKS

1. Jerry March, *Advanced Organic Chemistry: Reactions, Mechanisms and Structure*, Fourth edition, John Wiley & Sons (Asia) 2003.
2. S.H. Pine, *Organic Chemistry*, Fifth edition, Tata McGraw Hill Education, 2006.
3. T.W. Graham Solomons, C.B. Fryhle and S.A. Snyder, *Organic Chemistry*, 12th edn, Wiley, 2016.
4. J. Clayden, N. Greeves and S. Warren, *Organic Chemistry*, Second edition, Oxford University Press, 2014.
5. H. Togo, *Advanced Free Radical Reactions for Organic Synthesis*, Elsevier, 2004.
6. F.A. Carey and J. Sundberg, *Advanced Organic Chemistry, Part A: Structure and Mechanisms*, Fifth edition, Springer, 2007.
7. F.A. Carey and J. Sundberg, *Advanced Organic Chemistry, Part B: Reaction and Synthesis*, Fifth edition, Springer, 2007.

COURSE OUTCOMES (COs)

On completion of the course, the students will be able to

CO Nos	CO Statement	Cognitive Level
CO1	Analyze and predict the aromaticity of compounds and the nomenclature of bicyclic and tricyclic systems.	K4, K3, K2
CO2	Develop skills for identifying the kinetics of reactions.	K2, K5
CO3	Demonstrate the generation, stability, and reactivity of carbenes, nitrenes and free radicals.	K2
CO4	Explain and analyze the mechanism of substitution, elimination and addition reactions in aliphatic systems.	K2, K4
CO5	Infer the major types of nucleophilic substitution reactions on aromatics with their specific reactivity.	K2

K1 – Remember, K2 – Understand, K3 – Apply, K4 – Analyze, K5 – Evaluate, K6 - Create

MAPPING OF COURSE OUTCOMES WITH POs AND PSOs

CO	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PSO1	PSO2	PSO3	PSO4	PSO5	PSO6	PSO7	PSO8	PSO9
CO1	M	S	S	S	L	L	S	S	S	M	M	M	S	N	N	L	S
CO2	M	S	S	S	L	L	S	S	S	M	M	S	S	N	N	L	S
CO3	M	S	S	M	M	L	S	S	S	M	M	S	S	N	N	L	S
CO4	M	S	S	S	L	L	S	S	S	M	M	S	S	N	N	L	S
CO5	M	S	S	M	L	L	S	S	S	M	M	S	S	N	N	L	S

S – Strongly Correlated, M – Moderately Correlated, L – Weakly Correlated, N – No Correlation

CORE 2	FUNDAMENTALS OF INORGANIC CHEMISTRY, NUCLEAR CHEMISTRY AND INORGANIC POLYMERS	L	T	P	C
		5	0	0	4

Objectives:

- *To understand different type of bonds and to study different theories of bonding.*
- *To understand the acid-base concept, reactions in non-aqueous medium and to study applications of redox potential in inorganic systems.*
- *To introduce nuclear chemistry and to study the applications of radio isotopes.*
- *To understand structures and bonding in inorganic polymers and metal clusters.*

UNIT I - CHEMICAL PERIODICITY, CHEMICAL FORCES AND REDOX POTENTIAL (15 Hours)

Cause of Periodicity; Atomic radius: Covalent radius; Vander Waals' radii; Ionic radii; Ionization Potential; Electron affinity and electronegativity (Their variation in the periodic table and factors affecting them). Anomalous ionization potential and electron affinities; Applications of electronegativity, Group - electronegativity, Electronegativity equilization.

Slater Rules: Statement, applications and limitations.

Chemical Forces: Ion – dipole forces, dipole – dipole interactions, induced dipole interactions, instantaneous dipole – induced dipole interactions, Repulsive forces, H – bonding and its types – Effect of chemical forces on melting point, boiling point and solubility.

Redox potential: Factors affecting Redox potential - Applications of redox potentials: Latimer diagram.

UNIT II - CHEMICAL BONDING (15 Hours)

Valence Bond theory: Lewis structure – Concepts and VB theory of H_2 molecule - Stereochemistry of hybrid orbitals – Calculation of s and p characters of equivalence and nonequivalence of hybrid orbitals - VSEPR theory**.**

M.O. theory – Linear combination of Atomic orbitals (s – s, s – p, d – p, p – p and d –d overlapping) - s , p, d and quadruple bond. – M.O. diagrams of hetero nuclear diatomic molecules (CO, NO, HF) and triatomic molecules (BeH_2, H_2O, CO_2) – Walsh diagrams – Structure and hybridization - Bents rule and apicophilicity.

Ionic Bond: Lattice energy – Consequences- Born-Lande equation, Born Haber cycle and numerical problems involving it for the calculation of electron affinity or lattice energy – Kapustinskii equation.

UNIT III - ACID BASE CONCEPTS AND NON-AQUEOUS SOLVENTS (15 Hours)

Acid Base concepts: Lewis, Solvent systems, Lux Flood and Usanovich Acid – Base concepts. Group characteristics of Lewis acids – Reactions of Lewis acids Relative strength of Acids and Bases, Steric effect, Proton sponges, Solvation effects and Acid Base anomalies.

HSAB: Classification of Hard and Soft acids and bases – Pearson's concept – Acid – base strength and Hardness and Softness – Symbiosis – Theoretical basis of Hardness and Softness – Electronegativity and Hardness and Softness – Applications of HSAB.

Non-aqueous solvents: Classification of protic and aprotic solvents – General characteristics of solvents - Self ionization and leveling effect. Reactions in non-aqueous solvents - acid-base reactions, complex formation, solvolysis, solvation, Metatheses - Reactions in liquid NH_3, $SO2$, H_2SO_4 - Molten salts.

UNIT IV - NUCLEAR CHEMISTRY (15 Hours)

Atomic nuclei: Nuclear shell structure – nuclear reactions : types, Q-value, threshold energy, cross sections and excitation functions. Direct nuclear reactions – transmutation reactions: stripping and pick-up – high energy reactions : neutron evaporation and spallation – heavy ion reactions – photonuclear reactions. Nuclear fusion and stellar energy – nuclear fission : mass distribution of fission products – fission energy – fission neutrons – theory of nuclear fission – spontaneous fission. Waste disposal and atomic power project in India.

Radio isotopes: Preparation - Analytical applications: radio chromatography, neutron activation analysis, neutron absorptiometry and radiometric titrations.

UNIT V - INORGANIC POLYMERS AND METAL CLUSTERS (15 Hours)

Inorganic polymers: General characteristics, degree of polymerization, catenation and heterocatenation - property correlation - Polyacids - structures of isopoly and heteropoly anions - Polymeric sulphur nitride - Borazines - Phosphazenes - Phosphazene polymers - Boranes and carboranes - Structure and bonding in boranes - Wade'srule.

Structure and Bonding of Inorganic Metal clusters: Dinuclear Clusters: Cu(II) carboxylate, Chromium(II) acetate, $Mo_2Cl_8^{4-}$ and $Re_2Cl_8^{2}$- - Trinuclear Clusters: Re_3Cl_9 - Tetranuclear Clusters: $W_4(OR)_{12}$, $W_4(OR)_{16}$, $Mo_4Cl_{12}^{4-}$ - Hexanuclear Clusters: $[Nb_6Cl_{12}]^{2+}$, $[Os_6(CO)_{18}]^{2-}$ and $[Mo_6Cl_8]Cl_4$– Capping rule – poly atomic Zintl ions.

TEXT BOOKS

1. James E. Huheey, Ellen A. Keiter, Richard L. Keiter and O.K. Medhi, *Inorganic chemistry: principles of Structure and Reactivity*, 4th Edition, Pearson Education India, 2006.
2. J.D. Lee, *Concise Inorganic Chemistry*, Wiley, 5th Edition, 2014.
3. Wahid.U.Malik , G.D.Tuli and R.D.Madhan , *Selected Topics in Inorganic Chemistry* , S.Chand& Company, New Delhi, 2009.
4. P.Atkins , T.Overton , J.Rourke , M.Weller and F.Armstrong , *Inorganic Chemistry* , 5th edition , Oxford University press, 2010.
5. C.E.Housecraft and A.G.Sharpe , *Inorganic Chemistry* , 4th edition , Pearson, 2012.
6. Samuel Glasstone, *Source Book of Atomic Energy*, 3rd edition, East West, 1979.
7. H.J. Arnikar, *Essentials of Nuclear Chemistry*, Wiley Eastern, 4th Edition, 2000.

REFERENCE BOOKS

1. F. Albert Cotton, Geoffrey Wilkinson, Carlos A. Marilo and Manfred Bochman, *Advanced Inorganic Chemistry*, Wiley Interscience Publication, 6th Edition, 1999.
2. N.N. Greenwood and Earnshaw, *Chemistry of the Elements*, Pergamon Press, 2nd Edition, 1997.
3. B.E. Douglas, D.H. McDaniel and J.J. Alexander, *Concepts and Models of Inorganic Chemistry*, John Wiley and Sons. 3rd Edition, 2010.
4. K.F. Purcell and J.C. Kotz, *Advanced Inorganic Chemistry*, Cengage Learning, 2012.
5. W.l.Jolly ,*Modern Inorganic Chemistry* , 2nd Edition , McGraw-Hill ,1991.
6. J.E.Mark , R.West&H.R.Allcock , *Inorganic Polymers* , Academic Press ,1992.
7. G. Friedlander, J.W. Kennedy, E.S. Macies and Julian Malcolm, *Nuclear and Radiation Chemistry*, Wiley Interscience publication, 1981.
8. Gregory Choppin, Jan-OlovLiljenzin, Jan Rydberg and Christian Ekberg, *Radiochemistry and Nuclear Chemistry*, Academic Press, 4th Edition, 2013.

COURSE OUTCOMES (COs)

Upon completion of the course, the students will be able to

CO Nos	CO Statement	Cognitive Level
CO1	Recall the basic concepts of atomic structure, periodic table, periodic properties and chemical bonding of elements.	K1
CO2	Explain poly acids, cage compounds and Inorganic polymers.	K2
CO3	Apply the concept of hybridization to identify the structure of molecules by VBT, MOT and VSEPR theory.	K3
CO4	Distinguish hard and soft acids and bases and explain their relative strengths.	K4
CO5	Explain various nuclear reactions and the analytical applications of radio isotopes.	K2 , K3

MAPPING OF COURSE OUTCOMES WITH POs AND PSOs

CO	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PSO1	PSO2	PSO3	PSO4	PSO5	PSO6	PSO7	PSO8	PSO9
CO1	M	S	S	L	L	L	S	S	S	S	M	M	M	N	N	S	S
CO2	M	S	S	M	L	L	S	S	S	S	M	S	M	N	N	S	S
CO3	M	S	S	M	L	L	S	S	S	S	M	S	M	N	N	S	S
CO4	M	S	S	M	M	L	S	S	S	S	M	S	M	N	N	S	S
CO5	S	S	S	S	S	L	S	S	S	S	M	S	M	N	N	S	S

CORE 3	QUANTUM MECHANICS AND SPECTROSCOPY – I	L	T	P	C
		5	0	0	4

Objectives:

- *To have a good foundation in understanding the physical and mathematical aspects of quantum mechanics that leads to classical thermodynamics.*
- *To become familiar with the required mathematics for solving quantum mechanical problems.*
- *To understand and appreciate the quantum mechanical approach to the atomic and molecular electronic structure.*
- *To know quantization of energy and the interaction of electromagnetic radiation with matter.*
- *To learn the fundamentals of molecular spectroscopy.*
- *To know the application of spectroscopy to study the structure of molecules.*

UNIT I - MATHEMATICS FOR QUANTUM MECHANICS (QM) AND QM POSTULATES (15 hours)

Coordinate systems, Complex numbers - Functions (odd & even, orthogonality and normalization) - Operators: Linear, Differential, and Hermitian and Hamiltonian operators - Quantum mechanical treatment of angular momentum - simultaneous measurement of several properties. Statement of Heisenberg Uncertainty Principle by using the evaluation of commutator of $[x, p_x]$ and their significance. Eigen functions and eigen values - Failure of Classical Mechanics and the need for QM - Postulates of QM - The time-dependent and time - independent Schrodinger wave equations.

UNIT II - SOME QM MODELS AND THEIR APPLICATIONS (15 hours)

Particle in a box (1D & 3D), degeneracy and its application to linear conjugated molecular systems. Bohr's correspondence principle. QM tunneling, Rigid Rotor: wave equation and solution calculation of rotational constants and bond length - Harmonic Oscillator: wave equation and solution, anharmonicity force constant and its significance. The Hydrogen atom and H-like ions: Solution to H and H-like wave equation, radial and angular functions, quantum numbers n, l and m and their importance. Radial distribution functions and H-like orbitals and their representation.

UNIT III - APPLICATION OF QM TO MULTI-ELECTRON ATOMS (15 hours)

Approximation Methods: Need for approximation methods - The electron spin, Pauli exclusion principle and Slater determinant for He atom. The variation method - trial variation

function and variational integral (examples of variational calculations from particle in a box and Helium atom). Molecular QM and Chemical Bonding - Hydrogen molecule ion - the use oflinear variation function, the LCAO method - Hydrogen molecule: Molecular orbital theory and Heitler-London treatment. Electronic structure of conjugated systems: Huckel method applied to ethylene, allyl system, 1,3-butadiene and benzene.

UNIT IV - INTRODUCTION TO SPECTROSCOPY AND ROTATIONAL SPECTROSCOPY (15 hours)

Electromagnetic radiation: Quantization of energy, rotational, vibrational, and electronic energy levels and transitions in molecules; regions and representation of spectra. Resolution and intensity of spectral transition: signal-to-noise ratio, width of spectral lines - collision broadening, Doppler broadening, Heisenberg uncertainty principle; intensity of spectral lines-selection rules and transition probability, transit ion moment integral, Einstein absorption and emission coefficients, Boltzmann distribution.

Diatomic molecules as rigid rotors: Rotational energy levels, intensity of spectral lines, selection rules, effect of isotopic substitution. Diatomic molecules as non-rigid rotors: rotational transitions, centrifugal distortion constant; rotational spectra of linear and symmetric top polyatomic molecules.

UNIT V - VIBRATIONAL SPECTROSCOPY (15 hours)

Vibrating diatomic molecule: Energy of diatomic molecules as simple harmonic oscillator-energy levels, vibrational transitions, selection rules; anharmonic oscillator energy levels, selection rules, vibrational transitions. Diatomic vibrating rotator: Born-Oppenheimer approximation, vibration-rotation spectra, selection rules, P, Q, R branches. Vibrations of polyatomic molecules: symmetry and fundamental vibrations, normal modes of vibration, overtones, combination, difference bands; influence of rotations on the spectra of polyatomic molecules-parallel and perpendicular vibrations in linear and symmetric top molecules.

Raman Effect: Rayleigh and Raman scattering, Stokes' and anti-Stokes' radiation, molecular polarizability, Raman selection rules.Raman spectra: rotational Raman spectra- linear molecules, symmetric top and spherical top molecules; vibrational Raman spectra-symmetry and Raman active vibrations, rule of mutual exclusion; rotation-vibration Raman spectra of diatomic molecules. Applications of IR and Raman spectroscopy: skeletal and group vibrations, fingerprinting and absorption frequencies of functional groups for inorganic and organic compounds.

TEXT BOOKS

1. A. K. Chandra, *Introductory Quantum Chemistry*; 4th Edition, Tata McGraw Hill, 2001.
2. R.K. Prasad, *Quantum Chemistry through problems and Solutions*, New Age International Publishers, New Delhi., 1997.
3. R.P. Rastogi and V.K. Srivastava, *An Introduction to Quantum Mechanics of Chemical Systems*, Oxford & IBH Publishing Co., NewDelhi, 1986.
4. C. N. Banwell and E. M. McCash, *Fundamentals of Molecular Spectroscopy*; 4th Edition, McGraw Hill Education, 2016.
5. K.V. Raman, R. Gopalan and P.S. Raghavan, *Molecular Spectroscopy*, Thomson and Vijay Nicole, Singapore, 2004.

REFERENCE BOOKS

1. W. J. Moore, *Physical Chemistry*, 5th edition, Orient Longman, 1976.
2. P. Atkins, J.D. Paula and J. Keeler, *Physical Chemistry*, 11th Edition, Oxford University press, 2018.
3. D.A. McQuarrie and J.D. Simon, *Physical Chemistry*: *A Molecular Approach*, Viva Books Private Limited, New Delhi, 2020.
4. D.A. McQuarie, *Quantum Chemistry*, Viva Books, 2016.
5. R.L. Flurry, *Symmetry Groups: Theory and Chemical Applications*, Prentice Hall, 1980.
6. Ira N. Levine, *Quantum Chemistry*, 7th edition, Pearson, 2013.
7. Ira N. Levine, *Molecular Spectroscopy*, John Wiley & Sons, New York, 1975.
8. K. Nakamoto, *Infrared and Raman Spectra of Inorganic and coordination Compounds*, Part B: 5th ed., John Wiley & Sons Inc., New York, 1997.
9. G. M. Barrow, *Introduction to Molecular Spectroscopy*, McGraw Hill, 1962.

COURSE OUTCOMES (COs)

On completion of the course, the students will be able to

CO Nos	CO Statement	Cognitive Level
CO1	Explain the mathematical and physical aspects of quantum mechanics which illustrates the relationship between mathematics and fundamental of quantum mechanics.	K2
CO2	Solve quantum mechanical problems.	K3
CO3	Analyze the quantum mechanical aspects in various areas of applications in chemistry.	K4
CO4	Explain the basic idea of quantization of energy and spectroscopy and apply to the rotational spectra of diatomic molecules.	K2, K3
CO5	Explain the basic principles of vibrational spectra of diatomic molecules including both IR and Raman spectra.	K2

MAPPING OF COURSE OUTCOMES WITH POs AND PSOs

CO	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PSO1	PSO2	PSO3	PSO4	PSO5	PSO6	PSO7	PSO8	PSO9
CO1	M	S	M	M	L	L	S	S	S	M	M	N	S	N	S	M	S
CO2	M	S	S	S	L	L	S	S	S	M	M	N	S	N	S	M	S
CO3	M	S	S	S	L	L	S	S	S	S	S	N	S	N	S	M	S
CO4	M	S	S	M	L	L	S	S	S	S	S	N	S	N	S	M	S
CO5	M	S	S	S	L	L	S	S	S	S	S	N	S	N	S	M	S

ELECTIVE - I	1.1 GREEN CHEMISTRY – TECHNIQUES AND APPLICATIONS	L	T	P	C
		4	0	0	4

Objectives:

- *To understand the basic principles of Green chemistry and Green techniques.*
- *To study Green catalysis and Green solvents.*
- *To learn Renewable energy sources, their working principle and applications.*

UNIT I – BASIC PRINCIPLES OF GREEN CHEMISTRY (12 Hours)

Green chemistry principles – Waste minimization and atom economy – atom economic reactions and calculations – Reduction of non-renewable raw materials usage – considerations in protecting group and catalysts need – process intensification – Reduction of energy requirements – alternative energy sources and energy efficient improvements – Reduction of risk and hazards – Inherently safer design and alternative solvents. Green metrics – selected metrics used: Effective Mass Yield – *E* factor – Reaction Mass Efficiency – Mass Intensity and Mass Productivity.

UNIT II – GREEN CATALYSIS (12 Hours)

Introduction to green catalysis – heterogeneous catalysis – applications of zeolites, silica, alumina, clay, polymers, cyclodextrin and solid supported catalysts in green chemical reactions. Bio-catalysis - role of enzymes in catalytic oxidation, catalytic reduction, catalytic hydrolysis and catalytic carbon-carbon formation reactions. Green aspects – microbial production of ethanol. Phase-transfer catalysis and its advantage –applications of crown ethers in oxidation, substitution, elimination and esterification reactions.

UNIT III – GREEN SOLVENTS (12 Hours)

Role of solvents in synthesis – Application of green solvents –Super critical fluids – super critical carbon dioxide and super critical water. Aqueous phase reactions – Diels Alder reaction, Wurtz reaction, Claisen rearrangement, Aldol condensation, Knoevenagel reaction, Michel reaction. Ionic liquids - properties of ionic liquids -applications of ionic liquids as catalysts and solvents. An introduction to tunable and switchable solvent systems.

UNIT IV – GREEN TECHNIQUES AND ALTERNATIVE ENERGY SOURCES (12 Hours)

Photochemical reactions – photo reduction reactions, photochemical ring closure of dienes. Green techniques using microwaves – merits and demerits of microwave techniques – mechanism of microwave heating – effects of solvents in microwave assisted synthesis – microwave assisted reactions - Hoffman elimination, Heck reaction, Suzuki reaction, Microwave solvent free reactions – Deacetylation, saponification of esters. Sonochemistry –

basics of sonochemistry – ultrasound assisted reactions – Friedal-Crafts reaction, Simmons-Smith reaction, Cannizzaro reaction, Strecker synthesis and Reformatsky reaction.

UNIT V – RENEWABLE ENERGY RESOURCES (12 Hours)

Introduction to renewable energy sources - types of renewable energy sources - Solar cells: basic principles, types and their applications - Fuel cells - basic principles, types and their applications – working principle and applications of Biofuel cells - brief introduction about hydroelectric, biomass, wind power and geothermal power and their applications and limitations - energy from some other natural sources.

TEXT BOOKS

1. Mike Lancaster, *Green Chemistry: An Introductory Text*, RSC, 2002.
2. Editors -James Clark and Duncan MacQuarrie, *Handbook of green chemistry and technology*, Blackwell Science, 2002.
3. Edited by – Paul T. Anastas, *Green Processes Vol 7: Green Synthesis*, Wiley – VCH, 2012.
4. V.K Ahluwalia and M. Kidwai, *New Trends in Green Chemistry*, Anamaya Publishers, 2004.

REFERENCE BOOKS

1. Roger Arthur Sheldon, Isabel Arends and Ulf Hanefeld, *Green Chemistry and Catalysis*, Wiley – VCH, 2007.
2. John Twidell and Tony Weir, *Renewable Energy Resources*, Routledge Third Edition, 2015.
3. Francesca M. Kerton, *Alternative Solvents for Green Chemistry*, RSC Publishing, 2009.
4. Edited by Suresh C. Ameta and Rakshit Ameta, *Green Chemistry: Fundamentals and Applications*, Apple Academic Press, 2013.
5. Gadi Rothenberg, *Catalysis: Concepts and Green Applications*, Wiley-VCH, 2008.

COURSE OUTCOMES (COs)

Upon completion of the course, the students will be able to

CO Nos	CO Statement	Cognitive Level
CO1	Explain the basic principles of green chemistry, alternative energy sources and green metrics.	K2
CO2	Apply the green catalysis in chemical reactions.	K3
CO3	Identify the role of important green solvents in organic reactions.	K5
CO4	Illustrate name reactions and analyze the various green reactions using microwave techniques.	K2, K4
CO5	Explain the principles of renewable energy resources and generate its importance to the environment.	K2, K6

MAPPING OF COURSE OUTCOMES WITH POs AND PSOs

CO	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PSO1	PSO2	PSO3	PSO4	PSO5	PSO6	PSO7	PSO8	PSO9
CO1	S	S	S	S	S	L	S	S	S	S	S	S	S	N	L	S	S
CO2	S	S	S	S	S	L	S	S	S	S	S	S	S	N	L	S	S
CO3	S	S	S	S	M	L	S	S	S	S	S	S	S	N	L	S	S
CO4	S	S	S	S	S	L	S	S	S	S	S	S	S	N	L	S	S
CO5	S	S	S	S	M	L	S	S	S	S	S	S	S	N	L	S	S

ELECTIVE - I	1.2 CHEMISTRY OF INDUSTRIAL PRODUCTS AND FORMULATION	L	T	P	C
		4	0	0	4

Objectives:

- *To study paint formulations, various cosmetics and manufacture and refining of pulp.*
- *To learn milk processing, milk products and textile fibres.*

UNIT I - PAINTS AND PIGMENTS (12 Hours)

General characteristics of pigments - Types of pigments, methods of preparation and properties of white pigments - Paints, varnishes and Lacquers – function and classification - Function of vehicle, solvent, thinner, pigment, dyes, filler, resins, drier and additives in paint formulations - oil and alkyd paints - drying mechanism, epoxy coatings - Luminous paints.

UNIT II - COSMETICS (12 Hours)

Cosmetics – Definition, classification - Additives and its role in cosmetics – surfactants – Humectants – Antiseptics, Preservatives and Anti -oxidants. Perfumes – source, classifications, blending and fixations.

Formulation of the following cosmetics: Cleansing cream, all-purpose cream, shampoos, deodorants - Antiperspirants - face powder - Compact powder, sunscreen lotion, skin colorant – lipstick. Cosmetic soaps - moisturizing soap and medicated soap. Dentifrices - toothpaste and mouth washers.

UNIT III - PULP AND PAPER SCIENCE (12 Hours)

Raw materials for paper - Important fibre producing plants - Woody & non woody fibres used in paper industry - Pulp Manufacture: Mechanical pulping, Thermomechanical and Refiner mechanical pulping, semi-chemical & chemical pulping, Kraft pulping. Papermaking: Beating and Refining of pulp - Evaluation of Paper: Physical, optical, electrical properties and Chemical properties of paper.

UNIT IV - DAIRY CHEMISTRY (12 Hours)

Milk – definition of milk, composition - factors affecting the composition - physicochemical properties of milk, fat, proteins, enzymes, vitamins, minerals, milk processing - pasteurisation, sterilization, homogenisation, effect of heat on milk. Milk products - Definition and composition of butter, ghee, ice cream, milk powder, cheese. Special milk - definition and advantages of sterilized milk, flavoured milk, standardized milk, toned milk, double toned milk.

UNIT V - TEXTILE FIBRES **(12 Hours)**

Introduction and classification of textile fibres - characteristics of textile fibres - Manufacture of eco-friendly regenerated cellulosic fibre – viscose, cuprammonium rayon. Manufacture of Nylon-6 and Nylon 6,6. Brief study of physical & chemical properties of cotton, wool and silk. Enhancement of fibre properties by surface treatments - Plasma treatment, enzyme treatment, antimicrobial treatment - UV protection.

TEXT BOOKS

1. J. Bentley and G.P.A. Turner, *Introduction to Paint Chemistry and Principles of Paint Technology,* Fourth edition, Springer US, 1998.
2. Harry Ralph Gordon and Rosen Meyer R, *Harry's Cosmeticology*, Volume 2, Ninth edition, Chemical publishing company, 2015.
3. H. Butler, *Poucher's Perfumes, Cosmetics and Soaps*, 10th edition, springer, 2010.
4. Pratima Bajpai, *Environmentally Friendly Production of Pulp and Paper*, John wiley, 2010.
5. Jenness Robert and Patton Stuart, *Principles of Dairy Chemistry*, Scientific international, 2018.
6. De Sukumar, *Outlines of Dairy technology*, Oxford press, 1980.
7. H.V Sreenivasa Murthy, *Introduction to textile fibres*, Revised edition, Woodhead publishing India, 2015.
8. Seema Sekhri, *Textbook of Fabric Science - Fundamental to finishing,* PHI Learning, Delhi, Second Reprinting, 2013.

REFERENCES BOOKS

1. D. Stoye and W. Freitag, *Paints, Coatings and Solvents*, Second edition, Wiley-VCH, 1998.
2. Ernest Flick, *Cosmetic and Toiletry Formulations* Volume 8, Second Edition, 2007.
3. Pratima Bajpai, *Biermann's Handbook of Pulp and Paper: Raw Material and Pulp Making*, Third edition, Elsevier, 2018**.**
4. P. Walstra, T.J. Geurts, A. Noomen, A. Jellema and M.A.J.S. Van Boekel, *Dairy technology: Principles of Milk Properties and Processes. Part II: Processes*, Marcel decker Inc. 1999.
5. Robert R Mather and Roger H Wardman, *The chemistry of textile fibres*, second edition, Royal Society of Chemistry, 2015.

COURSE OUTCOMES (COs)

On completion of the course, the students will be able to

CO Nos	CO Statement	Cognitive Level
CO1	Acquire knowledge of paints and pigments and investigate its drying mechanism.	K2
CO2	Apply and formulate the role of cosmetics in industries.	K3, K6
CO3	Identify the fibre for paper making and evaluate its properties.	K5
CO4	Apply processing operations of milk and milk products in day to day life.	K3
CO5	Explain types of textile fibres and analyze its characters by various treatments	K2, K4

MAPPING OF COURSE OUTCOMES WITH POs AND PSOs

CO	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PSO1	PSO2	PSO3	PSO4	PSO5	PSO6	PSO7	PSO8	PSO9
CO1	S	S	S	S	M	L	S	S	S	S	S	M	L	N	N	M	S
CO2	S	S	S	S	M	L	S	S	S	S	S	M	L	N	N	M	S
CO3	S	S	S	S	M	L	S	S	S	S	S	M	L	N	N	M	S
CO4	S	S	S	S	M	L	S	S	S	S	S	M	L	N	N	M	S
CO5	S	S	S	S	M	L	S	S	S	S	S	M	L	N	N	M	S

ELECTIVE - I	1.3 FORENSIC CHEMISTRY	L	T	P	C
		4	0	0	4

Objectives:

- *To understand the importance of Forensic science, GPS, Finger printing and Forensic serology.*
- *To learn the role of chemistry in Forensic science, toxicology and DNA finger printing.*
- *To understand the concept of Cyber technology.*

UNIT I - ELEMENTARY FORENSIC SCIENCE (12 Hours)

Definition of Forensic science, The role of Forensic laboratory, Biometrics in Personal Identification- Introduction, Concepts of Biometric Authentication, Role in person Identification, Techniques and Technologies - Finger Print Technology, Face Recognition, IRIS, Retina Geometry, Hand Geometry, Speaker Recognition, Signature Verification. Geo-forensics - Global Positioning System, Basic principles and applications.

UNIT II - FINGER PRINTING AND FORENSIC SEROLOGY (12 Hours)

Fingerprinting - General principles of Finger Printing, Fingerprinting systems, Fingerprint Detection - Powder tests – dry powder method, detection using cellophane tape, small particle reagent analysis, vacuum metal deposition method, Chemical tests – silver nitrate test, iodine fuming, ninhydrin, superglue (cyanoacrylate), Physical Developer, and ruthenium oxide tests. Optical methods – Reflected Ultraviolet Imaging Systems, laser tests.

Forensic Serology – Blood types, Polymorphic Proteins and Isoenzymes, Characterization of Blood stains, Blood stains patterns. Testing of Saliva.

UNIT III - FORENSIC ANALYSIS (12 Hours)

Forensic Drug Analysis – How drugs work - analysis of selected drug classes –Gamma hydroxybutyric acid (GHB), Gamma butyro lactone (GBL), Marijuana, Anabolic steroids, Heroin, Cocaine, Amphetamines.

Forensic analysis of Inks and paints – Questioned documents – Physical analysis, chemical analysis of inks and paper – analytical methods – Optical microscopy, Fluorescent techniques, TLC, FT-IR.

UNIT IV- FORENSIC TOXICOLOGY AND DNA FINGER PRINTING (12 Hours)

Forensic Toxicology – Overview - Sample types – Blood and Plasma, Urine, Vitreous fluid, Hair. Types of Forensic Toxicology – Alcohol, Postmortem toxicology, Sport Toxicology. Analytical methods in Forensic Toxicology – Breath alcohol test (BrAC).

DNA Fingerprinting – An introduction to DNA, Forensic DNA typing - methods of DNA typing - RFLP and PCR methods – Procedures for DNA typing, Applications of DNA testing.

UNIT V - CYBER TECHNOLOGY AND FORENSIC SCIENCE (12 Hours)

Use of computers in Forensic science - Forensic Databases, Image Databases, DNA Databases, Paint Databases. Forensic Archiving of X-Ray Spectra, Video Image Processing and Animation Software, Use of Networks in Forensic Science.

Computer related crime - Definitions and types - Framework for Investigating Computer-Related Crime, Human Aspects of Computer-Related Crime.

TEXT BOOKS

1. Anil K. Jain, Arun A. Ross and Karthik Nandakumar, *Introduction to Biometrics*, Springer, 2011.
2. David E. Newton, *Forensic Chemistry*, Fact on File, Inc, 2007.
3. Suzanne Bell, *Forensic Chemistry*, Pearson International, Second Edition, 2014.
4. Edited by Stuart H. James and Jon J. Nordby, *Forensic Science - An Introduction to Scientific and Investigative Techniques,* CRC Press, 2003.

REFERENCE BOOKS

1. Editor – G.R. Sinha, *Advances in Biometrics - Modern Methods and Implementation Strategies*, Springer, 2019.
2. Editor – Jay A. Siegel, *Forensic Chemistry -Fundamentals and applications*, Wiley-Blackwell, First edition, 2016**.**
3. Max M. Houck**,** *Forensic Science-Modern methods of solving crime*, Praeger Publishers, 2007.
4. Kelly M. Elkins, *Introduction to Forensic chemistry***,** CRC Press, 2019.
5. Matthew Johll, *Investigating Chemistry: A Forensic Science Perspective*, W.H. Freeman & Co, Second Edition, 2008.

COURSE OUTCOMES (COs)

Upon completion of the course, the students will be able to

CO Nos	CO Statement	Cognitive Level
CO1	Acquire knowledge on forensic science and apply through biometric and finger printing technique.	K2, K3
CO2	Interpret the different methods of finger printing and characterization of blood stains.	K5
CO3	Analyze the selected drugs, inks and paints using different techniques.	K4
CO4	Identify the samples using forensic toxicology methods and DNA finger printing.	K3
CO5	Explain the proper applications of computer network in forensic science to investigate the crimes.	K2, K6

MAPPING OF COURSE OUTCOMES WITH POs AND PSOs

CO	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PSO1	PSO2	PSO3	PSO4	PSO5	PSO6	PSO7	PSO8	PSO9
CO1	S	S	S	S	M	M	S	S	S	S	S	N	S	N	L	S	S
CO2	S	S	S	S	M	M	S	S	S	S	S	N	S	N	L	S	S
CO3	S	S	S	S	M	M	S	S	S	S	S	N	S	N	M	S	S
CO4	S	S	S	S	M	M	S	S	S	S	S	N	S	N	S	S	S
CO5	S	S	S	S	M	M	S	S	S	S	S	N	S	N	S	S	S

CORE 4	ORGANIC CHEMISTRY PRACTICAL - I	L	T	P	C
		0	0	4	2

Objectives:

- *To introduce the students to have hands on experience to perform various reactions.*
- *The students can Separate and characterize the two component mixtures.*

1. Qualitative analysis of Organic mixture (atleast six two component mixtures)

- Separation of organic mixtures
- Elemental analysis
- Functional group(s) identification
- Preparation of derivatives
- Physical properties determination (melting point and boiling point) for both components and their derivatives.

Analysis may be performed in micro (or) macro scale depending upon the conditions of the laboratory.

2. For Class Work Only:

1. Separation of Caffeine from Tea / Coffee.
2. Separation of green, blue, red inks by TLC method.

TEXT BOOKS

1. A.I. Vogel, *Elementary Practical Organic Chemistry: Small Scale Preparations, Qualitative Organic Analysis, Quantitative Organic Analysis*, Pearson Education, 2011.
2. K. Bansal Raj, *Laboratory Manual of Organic Chemistry*, New Age International, 2009.
3. V. Venkateswaran, R. Veeraswamy and A. R. Kulandaivelu, *Basic Principles of Practical Chemistry*, Sultan Chand & Sons, 2004.

REFERENCES BOOKS

1. R.G. Engel, D.L. Pavia, G.M. Lampman and G.S. Kriz, *A Microscale approach to Organic Laboratory*, 5th edition, Paperback – International Edition, 2012.
2. P.B. Cranwell, L.M. Harwood, and C. J. Moody, *Experimental Organic Chemistry*, 3rd edn,Wiley-Blackwell**,** 2017.
3. J. Leonard, B. Lygo and G. Procter, *Advanced Practical Organic Chemistry*, 3rd edn, CRC Press, 2013.

COURSE OUTCOMES (COs)

On completion of the course, the students will be able to

CO Nos	CO Statement	Cognitive Level
CO1	Explain the basic separation procedures of organic mixtures.	K2
CO2	Select the separation methods to separate the organic mixtures.	K3
CO3	Classify the functional groups using systematic procedure.	K4
CO4	Determine the physical properties of organic compounds	K5
CO5	Develop skills to isolate natural products from plants.	K3

MAPPING OF COURSE OUTCOMES WITH POs AND PSOs

CO	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PSO1	PSO2	PSO3	PSO4	PSO5	PSO6	PSO7	PSO8	PSO9
CO1	M	S	S	S	S	S	S	M	S	S	M	L	S	N	N	S	S
CO2	M	S	S	S	S	S	S	S	S	S	M	L	S	N	N	S	S
CO3	M	S	S	S	S	S	S	S	S	S	M	L	S	N	N	S	S
CO4	M	S	M	S	S	S	S	S	S	S	M	L	M	N	N	S	S
CO5	S	S	S	S	S	S	S	S	S	S	M	L	S	N	N	S	S

CORE 5	INORGANIC CHEMISTRY PRACTICAL - I	L	T	P	C
		0	0	4	2

Objectives:

- *To learn the principles and methods of qualitative analysis of familiar and less familiar cations present in a mixture.*
- *To identify the methodology to analyze qualitatively a metal ion in the presence of another metal ion.*

Qualitative Analysis:

Qualitative analysis of mixture containing two familiar and two less familiar cations: Pb, Cu, Bi, Cd, Zn, Co, Ni, Mn, Ca, Ba, Sr, W, Se, Te, Mo, Ce, Zr, V, Ti, and Li.

Course work

Th & U (Course Work)

TEXT BOOKS

1. V.V. Ramanujan, *Inorganic Semi-micro Qualitative Analysis*, 3rd Edition, National Publishing Company, Chennai, 1990**.**

REFERENCE BOOKS

1. G. Svehla, *Vogel's Qualitative Inorganic Analysis*, 7th Edition, Pearson Education India, 2008.

COURSE OUTCOMES (COs)

Upon completion of the course, the students will be able to

CO Nos	CO Statement	Cognitive Level
CO1	Recall the procedure for the identification of more familiar metal ions.	K1
CO2	Explain the principles and techniques and have skills of qualitative analysis of familiar and less familiar cations in a mixture.	K2, K3
CO3	Analyze a metal ion in the presence of another metal ion.	K4

MAPPING OF COURSE OUTCOMES WITH POs AND PSOs

CO	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PSO1	PSO2	PSO3	PSO4	PSO5	PSO6	PSO7	PSO8	PSO9
CO1	M	S	S	M	M	S	S	M	S	S	M	L	S	N	N	S	S
CO2	M	S	S	S	S	S	S	S	S	S	M	L	S	N	N	S	S
CO3	M	S	S	S	S	S	S	S	S	S	M	L	S	N	N	S	S

CORE 6	PHYSICAL CHEMISTRY PRACTICAL - I	L	T	P	C
		0	0	4	2

Objectives:

- *To learn the Principles of Conductometric Titrations.*
- *To understand the Principles of Thermometry.*

I. Conductometric Titrations

(a). Standard: NH_4Cl Link: NaOH Estimation: HCl and CH_3COOH in a mixture

(b) Standard: NH_4Cl Link: NaOH Estimation: NH_4Cl and HCl in a mixture

(c) Acid-Base and PrecipitationTitration

(i) Standard: $Pb(NO_3)_2$ Link:Na_2CO_3 Estimation: $HNO_3 + Pb(NO_3)_2$

(ii) Standard: $CuSO_4$ Link: NaOH Estimation: $H_2SO_4 + CuSO_4$

(d) Determination of Solubility Product

Conductometry - Solubility product of sparingly soluble silver salts (AgCl, AgBr and AgI).

II. Thermometry

Determination of Solution enthalpy of

(i) Oxalic acid - water

(ii) Ammonium oxalate - water

(iii) Ammonium chloride - water

(iv) Naphthalene - toluene

TEXT BOOKS

1. J. B.Yadav, *Advanced Practical Physical chemistry*, 20th Edn., GOEL publishing House, Krishna Pakashan Media, 2001.
2. J.N. Gurtur and R.Kapoor, *Advanced Experimental chemistry*, Vol.I. Chand & Co., NewDelhi, 1987.
3. B.C. Kosla, *Senior Practical Physical Chemistry*, Simla Printers, New Delhi, 1987.
4. Saroj Kumar and Naba Kumar, *Physical Chemistry Practical*, New Central Book Agency, 2012.

REFERENCE BOOKS

1. Findlay's *Practical Physical Chemistry*, Revised and edited by B.P. Levitt 9th Edn., Longman, London, 1985**.**
2. W.J. Popiel, *Laboratory Manual of Physical Chemistry*, ELBS, London, 1970**.**
3. G.W. Garland, J.W. Nibler and D.P. Shoemaker, *Experiments in Physical Chemistry*, 8th Edn. McGraw Hill, 2009.

COURSE OUTCOMES (COs)

On completion of the course, the students will be able to

CO Nos	CO Statement	Cognitive Level
CO1	Explain the principles of conductometric titrations and estimate the strength of solutions.	K2, K5
CO2	Explain the basic principles of thermometry and determine the heat of solution as well as the amount of solute present in the solution.	K2, K5
CO3	Determine the solubility product of sparingly soluble salts using conductometric technique.	K5

MAPPING OF COURSE OUTCOMES WITH POs AND PSOs

CO	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PSO1	PSO2	PSO3	PSO4	PSO5	PSO6	PSO7	PSO8	PSO9
CO1	M	S	S	S	S	S	S	S	S	S	M	L	S	N	M	S	S
CO2	M	S	S	S	S	S	S	S	S	S	M	L	S	N	M	S	S
CO3	M	S	S	S	S	S	S	S	S	S	M	L	S	N	M	S	S

SEMESTER II

CORE 7	STEREOCHEMISTRY, ORGANIC REAGENTS AND PHOTOCHEMISTRY	L	T	P	C
		5	0	0	4

Objectives:

- *To understand the concept of Stereochemistry and conformation of organic molecules.*
- *To study synthetic utility of important organic reagents.*
- *To understand Photochemistry and Pericyclic reactions.*

UNIT I - STEREOCHEMISTRY **(15 Hours)**

Concept of chirality: – Stereogenicity – Topicity - Enantiotopic, diastereotopic hydrogens and prochiral centres – axial and planar chirality – stereochemistry of compounds containing two dissimilar asymmetric carbons, ansa compounds and para cyclophanes.

R/S notations of Spiranes, allenes and Biphenyl ortho derivatives - E/Z notation of compounds containing one and two double bonds.

Regiospecific, Regioselective and chemoselective reactions - Stereospecific and stereoselective synthesis – Methods of Asymmetric synthesis including enzymatic and catalytic process – SAMP/RAMP as chiral auxiliaries - Cram's rule and Prelog's rule – Cram chelation model and Felkin – Aln model.

UNIT II - CONFORMATIONAL ANALYSIS **(15 Hours)**

Conformation and configuration-conformational free energy-conformational analysis of mono substituted (alkyl, halogens) and 1,1-disubstituted (alkyl) and 1,2-1,3-and 1,4-dimethyl substituted cyclohexanes - compounds existing in boat form-conformation of cyclohexanone, decalin and perhydrophenanthrene-Curtin-Hammett principle- conformation and reactivity of acyclic and cyclic compounds (6membered).

UNIT III - REAGENTS IN ORGANIC SYNTHESIS **(15 Hours)**

Gilman's reagent – LDA – DCC – 1,3 – dithane (umpolung synthesis) – Selenium dioxide. Fetizon's reagent – Dimethyldioxirane (DMDO) – Pyridinum chloro chromate (PCC) – Luche reagent – IBX - Lemieux – Von Rudloff reagent – Lemieux–Johnson reagent – Woodward and prevost hydroxylation. Merrifield resin – Vaskas catalyst.

UNIT IV - ORGANIC PHOTOCHEMISTRY **(15 Hours)**

Introduction – Difference between Thermal and Photochemical reactions - Jablonskii diagrams - intersystem crossing - energy transfer process – Quantum efficiency -

Photosensitization – Geometry of excited states – Possible electron transitions in saturated ketones - Reactivity of electronically excited ketones - alpha cleavages or Norrish type-I and Norrish Type II cleavages - Paterno-Buchi reaction – Photo reduction – Photo addition – Photo oxidation - Barton reaction – Photo Fries rearrangement - cis-trans isomerisation – Photo chemistry of α, β unsaturated carbonyl compounds – Photochemistry of arenes – Photochemistry of vision - Di-π methane rearrangement.

UNIT V - PERICYCLIC REACTIONS (15 Hours)

Atomic and molecular orbitals - Woodward-Hoffmann rules, FMO and correlation diagram approaches:

Electrocyclic reaction: Concepts of con and dis rotatory motions for 4n and 4n+2system – Cyclisation of butadiene and 1,3,5-hexatrienes - Stereochemical course of electrocyclic reaction in terms of conservation of orbital symmetry.

Cycloaddiation: suprafacial and antarafacial, [2+2] and [4+2] cyclo addition reactions - Dimerisation of ethylene and Diels-Alder reaction.

Sigmatropic rearrangements: Sigmatropic migration of hydrogen and carbon - (1,3) and (1,5) shifts. (3,3) shift – Claisen, Cope and Aza-Cope rearrangements - Fluxional tautomerism.

TEXT BOOKS

1. I.L. Finar, *Organic Chemistry*, Vol I, 6th edn, Pearson Education, 2002**.**
2. P.S. Kalsi, *Stereochemistry: Conformation and Mechanism*, 9th edn, New Age International Private Limited, 2017**.**
3. D. Nasipuri, *Stereochemistry of Organic Compounds: Principles and Applications*, Fourth edition, New Academic Science Publisher, 2012.
4. G.L. David Krupadanam, Fundamentals of Asymmetric Synthesis, University Press (India) Private, 2013.
5. B.P.Mundy, M.G.Ellerd, F.G.Favaloro, *Name Reactions and Reagents in Organic Synthesis*, 2nd Ed., 2005.
6. Dr Jagdamba Singh & Dr. L.D.S Yadav, *Orgnic Synthesis: Design, Reagents, Reactions and Rearrngements*, A Pragati Second Revised Edition, 2007**.**
7. Raj K. Bansal, *Organic Reaction mechanisms*, Tata Mc Graw Hill, Third Editon, 2007**.**
8. Gurdeep R. Chatwal, *Reaction mechanism and Reagents in organic chemistry*, Himalaya publishing House, Bombay 1992**.**

9. Sanyal and Sanyal, *Reactions, Rearrangements and Reagents*, 4th edn, Bharati Bhawan Publishers and Distributors, 2003.
10. S.M. Mukherjee and S.P. Singh, *Reaction Mechanism in Organic Chemistry*, Trinity Press, 2014.
11. J. Singh, *Photochemistry and Pericyclic Reactions*, Third edition, New Age International Publishers, 2012.
12. S. Sankararaman, *Pericyclic Reactions - Applications and Theory*, Wiley – VCH, 2005.

REFERENCE BOOKS

1. E.L. Eliel, *Stereochemistry of Carbon Compounds*, Tata McGraw Hill education, 2013.
2. R. Noyori, *Asymmetric Catalysis in Organic Synthesis*, John Wiley & Sons 1994.
3. W. Carruthers and I. Coldham, *Modern Methods of Organic Synthesis*, Fourth edition, Cambridge University Press, 2015.
4. F.A. Carey and J. Sundberg, Advanced Organic Chemistry, Part B: Reaction and Synthesis, Fifth edition, Springer, 2007.
5. I. Fleming, *Pericyclic Reactions*, Second edition, Oxford University Press, Oxford, 2015.
6. N.J. Turro, J.C. Scaiano, and V. Ramamurthy, *Modern Molecular Photochemistry of Organic Molecules*, University Science Books, 2010.

COURSE OUTCOMES (COs)

Upon completion of the course, the students will be able to

CO Nos	CO Statement	Cognitive Level
CO1	Recognize three dimensional structures of any organic molecule with orientation of atoms or groups.	K3
CO2	Analyze the conformation and the reactivity of acyclic and six-membered cyclic compounds.	K4
CO3	Develop the skill to choose the appropriate reagents for organic reactions.	K3
CO4	Illustrate the fundamental concepts of photochemistry and its application in organic reactions	K2
CO5	Explain the core concepts of Pericyclic reactions and its mechanisms in organic substrates and to predict whether the chemical reaction is thermal or photochemical.	K2, K5

MAPPING OF COURSE OUTCOMES WITH POs AND PSOs

CO	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PSO1	PSO2	PSO3	PSO4	PSO5	PSO6	PSO7	PSO8	PSO9
CO1	M	S	M	M	L	L	S	S	S	M	M	S	M	N	M	S	S
CO2	M	S	M	S	L	L	S	S	S	M	M	S	M	N	M	S	S
CO3	M	S	S	S	L	L	S	S	S	M	M	S	S	N	L	S	S
CO4	M	S	M	M	L	L	S	S	S	S	M	S	M	N	M	S	S
CO5	M	S	S	S	L	L	S	S	S	S	M	S	S	N	M	S	S

CORE 8	COORDINATION COMPOUNDS AND SOLID STATE CHEMISTRY	L	T	P	C
		4	0	0	4

Objectives:

- *To know the nature of metal-ligand bond and to study various theories of bonding in coordination compounds.*
- *To study the stability, chemical reactions and magnetic properties of coordination compounds.*
- *To study the crystal structures, defects in solid crystals, band theory of solids and super conductors.*

UNIT I - CRYSTAL FIELD THEORY (12 Hours)

Basic concepts - Splitting of d - orbitals in Oh, Td, Tetragonal distortions and square planar symmetries – Crystal field stabilization energy [CFSE] in Oh and Td complexes – Factors affecting CFSE – Applications of CFSE - Jahn-Teller distortion - Static and dynamic Jahn Teller effect. – Limitations of CFT.

MOT: Ligand Field theory - sigma and pi bonding in Oh complexes – MO of Td and square planar complexes - Application of MOT to explain spectrochemical series.

UNIT II - STABILITY AND REACTIONS OF COORDINATION COMPOUNDS (12 Hours)

Stability of complexes - Thermodynamic and kinetic stabilities - stepwise and overall stability constants of the metal complexes - factors affecting stability - chelate and template effects – Template Synthesis. Determination of stability constants: Bjerrum's method, spectrophotometric method, continuous variation (Job's) method.

Reactions of complexes: Lability – inertness - Ligand substitution reactions of square planar complexes - Trans effect and trans influence - Theories of trans effect - use of trans effect in synthesis of complexes - Substitution reactions in octahedral complexes - acid hydrolysis, base hydrolysis and anation reactions – Racemization and isomerisation reactions - Electron transfer reactions - Inner sphere and outer sphere processes - complementary and non-complementary reactions-Electron transfer reactions in mixed valence complexes.

UNIT III - MAGNETIC PROPERTIES OF METAL COMPLEXES (12 Hours)

Magnetic Susceptibility – Types of Magnetic behaviours – Magnetically diluted and concentrated materials – Determination of magnetic susceptibility: Guoy Balance and Faraday methods – temperature dependence of magnetic susceptibility – Quenching of orbital contribution and effect of Spin –orbit coupling to magnetic moment – Spin – state cross over

–Magnetic properties of complexes with A, E and T terms; Magnetic properties of Lanthanides and Actinides – Comparison of magnetic properties of Oh, Td and square planar complexes of Fe(II), Co(II), Ni(II) and Cu(II).

UNIT IV - SOLID STATE – I **(12 Hours)**

Efficiency of Packing in crystals – Limiting radius ratio – Description of crystal structures - calcite, zinc blende, wurtzite, rutile, fluorite, antifluorite, CsCl, CdI_2, K_2NiF_4 - spinels and perovskite. Crystal defects in solids - line and plane defects - Point defects: Schottky and Frenkel defects - Non-stoichiometric defects - Colour centres. Determination of crystal structures – Powder method and Rotating Crystal method.

UNIT V - SOLID STATE – II **(12 Hours)**

Free electron and Band Theory – Types of Solids: Conductors and insulators – intrinsic and extrinsic semi conductors – p-n and n-p-n junctions. Optical and electrical properties of Semiconductors: Photo voltaic effect – Hall effect. Super conductivity - high temperature super conductors - BCS theory - Cooper electrons - Meissener effect and levitation.

TEXT BOOKS

1. James E. Huheey, Ellen A. Keiter and Richard L. Keiter, *Inorganic chemistry: principles Structure and Reactivity*, 4th Edition, Pearson education, 2006.
2. J.D. Lee, *Concise Inorganic Chemistry*, Wiley, 5th edition, 2014.
3. Wahid U. Malik, G.D. Tuli and R.D. Madhan, *Selected Topics in Inorganic Chemistry*, S. Chand & Company, New Delhi, 2009.
4. Anthony R. West, *Solid State Chemistry and its Application*, Wiley, 2nd Edition, 2014.
5. P.Atkins , T.Overton , J.Rourke , M.Weller and F.Armstrong , *Inorganic Chemistry* , 5th edition , Oxford University press, 2010.
6. L.V. Azaroff, *Introduction to Solids*, Tata McGraw Hill Publishing, India, 1992.
7. H.V. Keer, *Principles of the Solid State*, Wiley Eastern, 1993.
8. D.K. Chakrabarthy, *Solid State Chemistry*, New Age Publisheres, 1996.
9. D. Bannerjee, *Coordination Chemistry*, Tata McGraw Hill, 1993.

REFERENCE BOOKS

1. F. Albert Cotton, Geoffrey Wilkinson, Carlos A. Marilo and Manfred Bochman, *Advanced Inorganic Chemistry*, Wiley Interscience Publication, 6th Edition, 2008.
2. K.F. Purcell and J.C. Kotz , *Inorganic Chemistry* , Cengage Learning , 2012.
3. C.E. Housecraft and A.G.Sharpe, *Inorganic Chemistry*, 4th edition, Pearson, 2012.
4. M.C. Day Jr and J. Selbin , *Theoretical Inorganic Chemistry* , Literary Licensing, LLC, 2012.

5. S.F.A. Kettle, *Physical Inorganic Chemistry - A Coordination Chemistry Approach*, Springer-Verlag, 1996.
6. R.Gopalan and V.Ramalingam, *Concise Coordination Chemistry*, Vikas Publishing House (p), New Delhi, 2003.
7. G. Chatwal and M.S. Yadu, *Coordination Chemistry*, 1st edition, Himalaya publishing House, 1992.
8. C. Kittel, *Introduction to Solid State Physics*, Wiley Eastern, 5th Edition, 1993.
9. D.M. Adams, *Inorganic Solids: an Introduction to Concepts in Solid state structural Chemistry*, Wiley**,** 1974.

COURSE OUTCOMES (COs)

On completion of the course, the students will be able to

CO Nos	CO Statement	Cognitive Level
CO1	Recall the basic terms in coordination chemistry, Applications and limitations of CFT.	K1
CO2	Explain the stability and reactions of various coordination complexes.	K2
CO3	Compare the magnetic properties of Octahedral, Tetrahedral and Square planar coordination complexes.	K4
CO4	Classify the types of defects in solids and apply this knowledge to identify the type of defect present in compounds.	K2 , K3
CO5	Distinguish metals, semiconductors and insulators and explain the properties and applications of semiconductors.	K4 , K2

MAPPING OF COURSE OUTCOMES WITH POs AND PSOs

CO	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PSO1	PSO2	PSO3	PSO4	PSO5	PSO6	PSO7	PSO8	PSO9
CO1	M	S	M	L	L	L	S	S	S	M	M	L	L	N	L	M	S
CO2	M	S	M	M	L	L	S	S	S	M	M	L	S	N	S	S	S
CO3	M	S	S	S	L	L	S	S	S	S	M	L	S	N	S	S	S
CO4	M	S	S	S	L	L	S	S	S	S	M	L	S	N	S	S	S
CO5	M	S	S	S	L	L	S	S	S	S	M	L	S	N	S	S	S

CORE 9	ELECTROCHEMISTRY AND SPECTROSCOPY - II	L	T	P	C
		5	0	0	4

Objectives:

- *To understand the concepts of Electrochemistry.*
- *To analyze the applications of Electrochemistry.*
- *To know quantization of energy and the interaction of electromagnetic radiation with matter.*
- *To learn the fundamentals of molecular spectroscopy.*
- *To know the application of spectroscopy to study the structure of molecules.*

UNIT I - ELECTROCHEMISTRY - I (15 Hours)

The nature of electrolytes - ion-ion and ion-solvent interactions. Mean ion activity -The Debye-Huckel equation – Bjerrum equation - Conductivity - transport numbers - Nernst Einstein equation - Stork Einstein equation - Debye-Huckel Onsager equation - Conductivity at high frequency and at high field strength. Double layer-polarized and non-polarized electrodes - Lippmann equation - Models for doublelayer - Helmholtz, Guoy&Chapmann – Stern models - Zeta potential - Electro-kinetic phenomena – Electro-osmosis. Streaming potential - electrophoresis.

UNIT II - ELECTROCHEMISTRY - II (15 Hours)

Electrode potential - Types of potential generation - Nernst equation - Hydrogen scale - other reference electrodes - concentration cells - Liquid junction potential - membrane equilibria. Butler-Volmer equation - Tafel equation - electrolysis & overvoltage - Theories of hydrogen overvoltage - Application of EMF measurements & conductivity. Batteries - fuel cells - corrosion. Zero current potentiometry - constant current potentiometry. Polarography – pulse polarography - Differential pulse polarography - Stripping voltammetry. Cyclic voltammetry - electrogravimetry - Coulometric methods.

UNIT III - ELECTRONIC SPECTROSCOPY (15 Hours)

Electronic spectra of molecules: Born-Oppenheimer approximation, Franck-Condon Principle, selection rules, intensity of electronic transition, vibronic coupling, types of electronic transitions. Chemical analysis by electronic spectroscopy: assignment of electronic transitions, application to the study of organic compounds.

Emission spectroscopy: Fate of electronically excited molecules-dissociation, reemission, fluorescence, phosphorescence; emission spectra of molecules.

Lasers: Nature of stimulated emission - coherence and monochromaticity, population inversion, cavity and mode characteristics, Q-switching, mode locking; types of lasers - solid-state, gas, chemical, and dye lasers.

Photoelectron spectroscopy (PES): Principle and technique of PES, ultraviolet PES, X-ray PES and Auger electronic spectroscopy.

UNIT IV - MAGNETIC RESONANCE SPECTROSCOPY (NMR AND EPR) (15 Hours)

Theory of NMR spectroscopy: Nuclear spin and magnetic nuclei, nuclear magnetic moment, behavior of a bar magnet in a magnetic field, the NMR transition, the Bloch equations, relaxation mechanisms. Parameters of NMR: measuring the chemical shift, shielding and deshielding of magnetic nucleus, chemical shifts in aliphatic and aromatic compounds, factors affecting chemical shift - inductive effect, anisotropy of chemical bonds, hydrogen bond, temperature, solvent. Spin-spin splitting: effect of spin-spin splitting on the spectrum, mechanism of spin. Spin splitting, chemical exchange, coupling constants; application of spin-spin splitting to structure determination - germinal and vicinal long-range coupling; factors influencing geminal and vicinal coupling. FT NMR spectroscopy: principle of FT NMR-FIDs, Fourier transformation; ^{13}C, ^{19}F, ^{31}P NMR - range of chemical shift values,

Electron paramagnetic resonance (EPR) spectroscopy: Theory of EPR spectroscopy, presentation of the spectrum, nuclear hyperfine splitting in isotropic systems. EPR spectra of anisotropic systems: anisotropy in g-value, causes of anisotropy, anisotropy in hyperfine coupling, EPR spectra of triplet states and zero field splitting.

UNIT V - NQR AND MOSSBAUER SPECTROSCOPY AND MASS SPECTROMETRY

(15 hours)

Principle of NQR spectroscopy: Nuclear charge distribution and quadrupole moment, quadrupole nucleus and its interaction with electric field gradient, nuclear orientations, the asymmetry parameter , quadrupole transitions in spherical and axially symmetric fields, quadrupole energy levels, field gradient. NQR spectra: effect of magnetic field on the spectra, relationship between electric field gradient and molecular structure.

Principle of Mössbauer spectroscopy: Doppler shift, recoil energy, experimental technique-sources, absorber, calibration.Mössbauer spectra: isomer shift, quadrupole splitting, magnetic hyper fine interaction, chemical applications- isomer shift and quadrupole splitting in iron complexes.

Mass spectrometry: Ion production-electron impact and chemical ionization, field desorption, FAB, electrospray ionization, Determination of molecular formula: molecular ion and isotope peaks, fragmentation, rearrangements; mass spectra of different classes of organic compounds.

TEXT BOOKS

1. S. Glasstone, *An Introduction to Electrochemistry*, East-West Press, 2006.
2. J.O.M. Bockris and A.K.N. Reddy, "*Modern Electrochemistry*" *vol.1, 2A & 2B*, Plenum Press, Springer US, 2007.
3. D.R. Crow, *Principles and applications of electrochemistry*, 4th Edition, CRC Press, 1994.
4. K.V. Raman, R. Gopalan and P. S. Raghavan, *Molecular Spectroscopy*, Thomson and Vijay Nicole, Singapore, 2004.
5. C.N. Banwell and E. M. McCash, *Fundamentals of Molecular Spectroscopy*, 4th Edition, McGraw Hill Education, 2016.
6. D.H. Williams and I. Fleming, *Spectroscopic Methods in Organic Chemistry*, 6th Edition, Tata McGraw Hill, 2011.
7. R.M. Silverstein and F. X. Webster, *Spectroscopic Identification of Organic Compounds*, 7thEdition, John Wiley & Sons, 2005.

REFERENCE BOOKS

1. P. Atkins and J.D. Paula, *Atkins' Physical Chemistry*, 9th Edition, Oxford University Press, 2009.
2. I.N. Levine, *Molecular Spectroscopy*, John Wiley & Sons, New York, 1975.
3. A.U. Rahman, *Nuclear Magnetic Resonance-Basic Principles*, Springer-Verlag, New York, 1986.
4. D.L. Andrews, *Lasers in Chemistry*, 3rdEdition, Springer-Verlag, 1997.
5. R.S. Drago, *PhysicaI Methods in Chemistry*; Saunders: Philadelphia, 1977.
6. J.A. Weil, J. R. Bolton and J. E. Wertz, *Electron Paramagnetic Resonance; Elementary Theory and Practical Applications*, Wiley Interscience, 1994.
7. B.P. Straughan and S.Walker. *Spectroscopy, Volume-3*, Chapman & Hall, 1976.

COURSE OUTCOMES (COs)

Upon completion of the course, the students will be able to

CO Nos	CO Statement	Cognitive Level
CO1	Explain the concepts of electrochemistry and basic ideas of electrochemical processes.	K2
CO2	Analyze the applications of electrochemistry such as batteries and fuel cells.	K4, K3
CO3	Illustrate the electroanalytical techniques such as Polarography, Differential pulse polarography, Stripping voltammetry. Cyclic voltammetry, etc.	K2
CO4	Explain the basic principles of nuclear magnetic resonance (NMR) and Electron paramagnetic resonance (EPR) spectroscopy techniques.	K2
CO5	Illustrate the principles of Nuclear quadrupole resonance and Mössbauer spectroscopy techniques and Mass spectrometry.	K2

MAPPING OF COURSE OUTCOMES WITH POs AND PSOs

CO	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PSO1	PSO2	PSO3	PSO4	PSO5	PSO6	PSO7	PSO8	PSO9
CO1	M	S	M	M	L	L	S	S	S	M	M	L	M	N	L	S	S
CO2	M	S	S	S	L	L	S	S	S	M	M	L	S	N	L	S	S
CO3	M	S	M	M	L	L	S	S	S	S	M	L	S	N	M	S	S
CO4	M	S	M	M	L	L	S	S	S	S	M	L	M	N	L	S	S
CO5	M	S	M	M	L	L	S	S	S	S	M	L	M	N	L	S	S

ELECTIVE - II	2.1 NANOSCIENCE AND NANOTECHNOLOGY	L	T	P	C
		4	0	0	4

Objectives:

- *To study structure, properties and synthetic methods of nanomaterials.*
- *To understand nano composites and carbon nanostructures.*
- *To learn nano medicines, nano robots and dendrimers.*

UNIT I - NANOSTRUCTURE AND NANOMATERIALS (12 Hours)

Definition and terminology of Nano particles and Nano structural materials - crystalline and amorphous materials – surface energy – surface area to volume ratio – surface relaxation – Types of nanostructured materials - One dimensional (thin films, layers, coatings), Two dimensional (Nanotubes, Nanofibers, Nanowires) and Three dimensional nanostructured materials (Nano particles, Nano shells, Nano rings),-properties of nanomaterials - Mechanical properties, Optical properties, Magnetic properties, electrical conductivity – electronic properties – Engineered nanomaterials - Quantum dots, Buckyballs/nanotubes, Metal oxides, Nano capsules.

UNIT II - SYNTHETIC METHODS OF NANOMATERIALS (12 Hours)

Top-down and bottom-up approaches– nucleation and growth -homogeneous nucleation and heterogeneous nucleation-Synthesis of Nano particles by Physicalmethods-Mechanical milling, Physical vapor deposition, Laser ablation, Sputter deposition, Photo lithography– Chemical reductionmethod -Reduction of metal ions by Citrate and borohydride- capping agents-role of capping agents, Polyol synthesis - Biological methods - green synthesis – Viral nanotechnology.

UNIT III - NANO COMPOSITES (12 Hours)

Nanocomposites - Polymer-based Nanocomposites - Polyamide/clay Nano composites – Synthesis, characterization and properties of Nylon 6 - clay hybrid - Polystyrene/clay Nanocomposites – syndiotactic polystyrene/clay Nano composites, properties. Poly(butylenes terephthalate) (PBT) based nano composites. Bio-Nanocomposites - properties and applications.

UNIT IV - CARBON NANOSTRUCTURES AND FUNCTIONALIZATION (12 Hours)

Carbon nanotube (CNT) and its Applications: Carbon nanotube (CNT), structure of CNT, synthesis and functionalization of CNT, electronic, vibrational, mechanical and optical properties of CNT, applications of CNT and Fullerenes.

Graphene: Graphene, structure of Graphene, synthesis and functionalization of Graphene, electronic application of Graphene, Electrochemical deposition, Graphene Oxide and its application.

UNIT V - BIOMEDICAL NANOTECHNOLOGY (12 Hours)

Nanomedicines - Diagnosis of diseases, treating and preventing of diseases – targeted drug delivery systems – Tissue Engineering - scaffolds for tissue fabrications – materials for scaffolds – materials for hydrogel scaffolds - Medical Devices - Imaging, implantable sensors, cell specific gene therapy – nano robots and their bio-medical applications. Dendrimers - structural description and its biomedical applications.

TEXT BOOKS

1. C.N.R. Rao, A. Muller and A.K. Cheetham, *The Chemistry of Nanomaterials – Synthesis, properties and Application,* Wiley – VCH – verlog GMOH & Co., Wilhelm, 2004.
2. C.P.Poole Jr., and F.J. Owens, *Introduction to Nanotechnology*, John Wiley &Sons, 2006.
3. Rajendra Kumar Goyal, *Nanomaterials and Nanocomposites: Synthesis, Properties, Characterization Techniques, and Applications***,** First edition, CRC Press, 2018.
4. Joseph Koo, *Polymer Nanocomposites*, First Edition, McGraw-Hill, 2006.
5. Ahmet Gürses, *Introduction to Polymer–Clay Nanocomposites*, CRC Press, 2016.
6. Edited by Vinod Labhasetwar and Diandra L.Leslie-Pelecky, *Biomedical Applications of Nanotechnology*, John Wiley & Sons, 2007.
7. Editor - Stergios Logothetidis, *Nanomedicine and Nanobiotechnology*, Springer, 2012.

REFERENCE BOOKS

1. G.L. Hornyak, J. Dutta, H.F. Tibbals and A.K. Rao, *Introduction to Nanoscience*, CRC Press, Taylor & Francis Group, 2008.
2. Guozhong, *Nanostructures and Nanomaterials: Synthesis, Properties and Applications*, Imperial College Press, 2004.

3. Edited by Vikas Mittal, *Synthesis Techniques for Polymer Nanocomposites*, Wiley-VCH, 2015.
4. Sati N. Bhattacharya, Musa R. Kamal and Rahul K. Gupta, *Polymeric Nanocomposites - Theory and Practice* Hanser Gardner Publications, 2008.
5. Yury Gogotsi, *Carbon Nanomaterials*, CRC Press, First Edition, 2006.
6. Daniel Alfonso Melendrez Armada, John Edward Proctor and Aravind Vijayaraghavan, *An Introduction to graphene and carbon nanotubes*, CRC Press, 2016.
7. K. Tanaka and S. Iijima, *Carbon Nanotubes and Graphene*, Elsevier, Second Edition, 2014.
8. Editor - M. Reza Mozafari, *Nanomaterials and Nanosystems for Biomedical Application*, Springer, 2007.
9. Editor - Ajay Kumar Mishra, *Nanomedicine for Drug Delivery and Therapeutics*, John Wiley & Sons, 2013.

COURSE OUTCOMES (COs)

Upon completion of the course, the students will be able to

CO Nos	CO Statement	Cognitive Level
CO1	Explain the unique properties and structure of nanomaterials.	K2
CO2	Trace the different methods of synthesis of nanomaterials.	K2
CO3	Acquire knowledge about polymer based nanocomposites and applications of bio- nanocomposites.	K2, K3
CO4	Evaluate the synthesis and potential applications of carbon nanotubes and grapheme.	K5
CO5	Apply nanotechnology in bio-medical field.	K3

MAPPING OF COURSE OUTCOMES WITH POs AND PSOs

CO	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PSO1	PSO2	PSO3	PSO4	PSO5	PSO6	PSO7	PSO8	PSO9
CO1	M	S	M	M	L	L	S	S	S	M	S	M	L	N	L	S	S
CO2	S	S	S	S	L	L	S	S	S	S	S	S	M	N	M	S	S
CO3	S	S	S	M	L	L	S	S	S	S	S	M	M	N	M	S	S
CO4	M	S	S	S	L	L	S	S	S	S	S	S	M	N	M	S	S
CO5	S	S	S	S	L	L	S	S	S	S	S	M	M	N	M	S	S

ELECTIVE - II	2.2 MEDICINAL CHEMISTRY	L	T	P	C
		4	0	0	4

Objectives:

- *To introduce the mechanism of drug action, drug delivery systems and molecular docking.*
- *To learn drug design and drug synthesis.*
- *To learn various types of drugs and their mode of action.*

UNIT I - GENERAL ASPECTS OF MEDICINAL CHEMISTRY (12 Hours)

Medicinal chemistry - Definition and major processes involved in drug action – pharmacokinetics - Definition and elementary aspects of ADME – Pharmacodynamics – Definition - receptors and their structures - agonist and antagonist - concept of bioisosterism - prodrugs and soft drugs. Drug delivery systems - Definition and types - Carrier based drug delivery system, Transdermal drug delivery system, Mucoadhesive drug delivery system. Molecular docking - Definition and types - Rigid docking (Lock and Key), Flexible docking (Induced fit).

UNIT II: DRUG DESIGN (12 Hours)

Development of new drugs - Lead identification and optimization - Structure and Ligand based drug design - Structure Activity Relationship (SAR) of morphine and Penicillin - Physico – chemical parameters, Lipophilicity, partition coefficient, electronic ionization constants - Quantitative Structure Activity Relationship. Free – Wilson analysis, Hansch analysis, relationships between Free– Wilson and Hansch analysis – case study. Elementary treatment of Drug receptor interactions.

UNIT III - ANTISEPTICS, ANTIBIOTICS AND CELL MEMBRANE (12 Hours)

Structure and function of bacterial cell wall, Gram-positive and Gram-negative bacteria, comparison of bacterial and fungal cell wall - Microbe killers: Antiseptics and Disinfectants - Definition and mode of action. Antibiotics - Definition, classification and uses - Structure and mode of action of Bacitracin, Fosfomycin, Isoniazid, Ethambutol, β-Lactam antibiotics - Synthesis of penicillin G, ampicillin, amoxicillin, Cephalosporin. Mutations and origins of drug-resistance.

UNIT IV - DRUG SYNTHESIS (12 Hours)

Definition, synthesis and mode of action of following classes (i) Anxiolytics – Benzodiazepines (ii) Neuroleptics – Phenothiazines (iii) Hypnotics and Sedatives – Piperidinediones (iv) Local anesthetics – Aminobenzoic acid and its derivatives (v) Anti – coagulants – 1,3 – Indandione derivatives (vi) Hypoglycemic agents – Sulfonyl ureas (vii). Antihistaminic agents – Ethylenediamine derivatives (viii) Antimalarials – Aminoquinolines (ix) Analgesics and Antipyretics – Paracetamol, Phenylbutazone. (x) Anti – inflammatory – Diclofenac.

UNIT V - ANTINEOPLASTIC AGENTS AND CARDIOVASCULAR DRUGS (12 Hours)

Antineoplastic Agents: Introduction, cancer chemotherapy, special problems, role of alkylating agents and antimetabolites in treatment of cancer - Introduction of carcinolytic antibiotics and mitotic inhibitors - Synthesis of mechlorethamine, cyclophosphamide, melphalan, and uracil - Recent development in cancer chemotherapy.

Cardiovascular Drugs: Introduction and classification, cardiovascular diseases - Synthesis of amyl nitrate, sorbitrate, diltiazem, quinidine, verapamil, methyldopa, atenolol.

TEXT BOOKS

1. Ashutosh Kar, *Medicinal Chemistry*, New Age International, fourth edition, 2007.
2. Graham L. Patrick, *An Introduction to Medicinal Chemistry*, Oxford University Press, fifth edition, 2013.
3. Gareth Thomas, *Fundamentals of Medicinal chemistry*, Wiley-Blackwell, First Edition, 2003.
4. D. Sriram and P. Yogeeswari, *Medicinal Chemistry*, Pearson India, second edition, 2010.
5. N. Weaver, *Medicinal Chemistry*, Oxford, 2006.
6. G.R. Chatwal, *Medicinal Chemistry*, Himalaya, New Delhi, 2002.
7. P. Graham, *Instant Notes Medicinal Chemistry*, Viva, New Delhi, 2002.

REFERENCE BOOKS

1. Thomas Lemke and David A. Williams, *Foye's Principles of Medicinal Chemistry*, 7th edition, Lippincott Williams & Wilkins Pulications, 2012.
2. John M. Beale and John H. Block, *Wilson and Gisvold's Textbook of Organic Medicinal and Pharmaceutical Chemistry,* 12th Edition, Lippincott Williams & Wilkins Publications, 2010.

3. Ruben Vardanyan and Victor Hruby, *Synthesis of Essential Drugs*, 1st edition Elsevier Science, 2006.
4. Richard B. Silverman, *The Organic Chemistry of Drug Design and Drug Action*, 2nd edition, Elsevier Academic Press, 2004.
5. Camille Georges Wermuth, David Aldous, Pierre Raboisson, and Didier Rognan, *The Practice of Medicinal Chemistry*, 4th edition, Elsevier Academic Press, 2015.
6. T. J. Franklin and G. A. Snow, *Biochemistry and Molecular Biology of Antibacterial Drug Action*, 5th edition, Springer Science, 1998.

COURSE OUTCOMES (COs)

Upon completion of the course, the students will be able to

CO Nos	CO Statement	Cognitive Level
CO1	Categorize the drug delivery system and gain knowledge on molecular docking.	K4, K2
CO2	Acquire knowledge about structure activity relationship of drugs.	K2
CO3	Explain the structure and functions of antiseptics, antibiotics and differentiate bacterial and fungal cell walls.	K2, K4
CO4	Illustrate the synthesis and mode of actions of some important drugs.	K2
CO5	Create certain developments in cancer chemotherapy and cardiovascular drugs.	K6

MAPPING OF COURSE OUTCOMES WITH POs AND PSOs

CO	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PSO1	PSO2	PSO3	PSO4	PSO5	PSO6	PSO7	PSO8	PSO9
CO1	S	S	S	S	L	L	S	S	S	S	S	M	S	N	S	S	S
CO2	S	S	M	M	L	L	S	S	S	S	S	S	S	N	S	S	S
CO3	S	S	M	M	L	L	S	S	S	M	S	M	M	N	L	S	S
CO4	S	S	M	S	L	L	S	S	S	M	S	S	S	N	L	S	S
CO5	S	S	S	S	L	L	S	S	S	S	S	M	S	N	M	S	S

ELECTIVE - II	2.3 INDUSTRIAL PROCESSES AND CATALYSIS	L	T	P	C
		4	0	0	4

Objectives:

- *To learn unit operations and reverse osmosis in industrial plants.*
- *To study catalyst and homogeneous and heterogeneous catalysis in industries.*
- *To understand the environmental impact of chemical industries.*

UNIT I – UNIT OPERATIONS (12 Hours)

Concepts of unit operation and unit process. Basic Unit operation – batch and continuous, Distillation – azeotropic, steam and extractive distillation, Evaporation – single effect and multiple effect, Extraction – liquid-liquid and solid – liquid extractions, Crystallization – evaporative, cooling, precipitation and fractional crystallization. Size reduction and size separation – definition and objectives, factors affecting size reduction, Law governing Energy & Power requirements in comminution - size reduction equipment – ball mill, hammer mill and fluid energy mill.

UNIT II – REVERSE OSMOSIS (12 Hours)

Principle of Reverse Osmosis, dead - end filtration, cross – flow filtration, Industrial applications of reverse osmosis. Basic terms and definitions – recovery, rejection, flux, concentration polarization, beta, fouling, scaling, silt density index, modified fouling index, langelier saturation index. Membrane types and function – cellulose acetate membranes, polyamide and composite membranes. Membrane modules – plate and frame modules, tubular modules, spiral wound modules. Pretreatment of water – mechanical and chemical pretreatments.

UNIT III – CATALYST AND CATALYSIS (12 Hours)

Catalyst – general features and industrial applications, Catalysis – homogeneous catalysis and its limitations, heterogeneous catalysis – general kinetic behavior - chemisorption and active sites - physical form and preparation of bulk and supported catalysts – catalytic deactivation and reusability – advantages and operational modes of heterogeneous catalysis in industry.

UNIT IV – CATALYSIS IN PETROCHEMICAL INDUSTRY (12 Hours)

Overview of Petrochemical Industry and Refinery processes – importance of catalysis. Catalytic selectivity – mesoporous materials and shape selectivity – zeolites and zeotypes – zeolites in petrochemistry and refining – shape selective catalysis by zeolites – shape selectivity in conversion of methanol to hydrocarbon – shape selectivity in hydrocracking – shape selectivity in carbonylation.

UNIT V – ENVIRONMENTAL IMPACT OF CHEMICAL INDUSTRIES (12 Hours)

Environment and human interactions, Sources of Pollution – Atmospheric pollution, Aquatic pollution, land pollution, Control and treatment of pollution and wastes from industry – Control of atmospheric discharges, control of aquatic discharges, disposal of solid wastes from industrial sites. Hazards of the chemical industry – chemical exposure and toxicity – control techniques used in chemical plants.

TEXT BOOKS

1. Alan Heaton, *An Introduction to Industrial Chemistry*, Springer, Third Edition, 1996.
2. M. Gopala Rao and Marshall Sittig, *Dryden's Outlines of Chemical Technology*, East – West Press, Third Edition, 1997.
3. Jane Kucera, *Reverse Osmosis: Design, processes and applications*, Scrivener Publishing LLC and Wiley, Second Edition, 2015**.**
4. B.K Sharma, *Industrial Chemistry*, Goel Publishing House, Fifteenth Edition, 2006**.**

REFERENCE BOOKS

1. Editor – James A. Kent, *Handbook of Industrial Chemistry and Biotechnology*, Vol 1 &2, Springer, Twelfth Edition, 2012.
2. Editors - Lawrence K. Wang, Yung-Tse Hung, Howard H. Lo and Constantine Yapijakis, *Waste Treatment in the Process Industries*, CRC Press, First Edition, 2006.
3. Editors - Adriano Zecchina, Silvia Bordiga and Elena Groppo, *Selective Nanocatalysts and Nanoscience*, Wiley – VCH, 2011.
4. Editor – John Regalbuto, *Catalyst Preparation: Science and Engineering*, CRC Press, 2007.

COURSE OUTCOMES (COs)

On completion of the course, the students will be able to

CO Nos	CO Statement	Cognitive Level
CO1	Acquire knowledge on unit operations and unit process in industry.	K2
CO2	Explain reverse osmosis and how to apply it in the pretreatment of water.	K2, K3
CO3	Distinguish homogeneous and heterogeneous catalysis and analyze the advantages of heterogeneous catalysis in industry.	K4
CO4	Evaluate the role of catalysis in petrochemical industry.	K5
CO5	Save the environment from hazardous industrial chemical waste.	K6

MAPPING OF COURSE OUTCOMES WITH POs AND PSOs

CO	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PSO1	PSO2	PSO3	PSO4	PSO5	PSO6	PSO7	PSO8	PSO9
CO1	S	S	M	M	S	L	S	S	S	S	S	L	S	N	N	S	S
CO2	S	S	S	S	S	L	S	S	S	S	S	L	S	N	N	S	S
CO3	M	S	M	S	S	L	S	S	S	S	S	S	M	N	N	S	S
CO4	S	S	S	S	M	L	S	S	S	S	S	S	M	N	N	S	S
CO5	S	S	S	S	S	L	S	S	S	M	S	S	M	N	N	S	S

CORE 10	ORGANIC CHEMISTRY PRACTICAL - II	L	T	P	C
		0	0	4	2

Objectives:

- *To enable the students to develop analytical skill in organic quantitative analysis.*
- *To understand the techniques involved in the preparation of standard solutions, standardization and calculations in the estimations of compounds.*
- *To develop preparative skills in organic preparations.*

Estimation, Single stage preparations and chromatographic techniques have been included as the practical components.

Microscale preparations are recommended for the simple reasons, as they are both economic-friendly and eco-friendly.

A. Estimation

1. Estimation of Ethyl Methyl ketone
2. Estimation of phenol
3. Estimation of aniline
4. Estimation of ascorbic acid in tablets

B. List of single stage preparations:

1. Preparation of 1,2,3,4 –tetrahydro carbazole from cyclohexanone.
2. Preparation of Resacetophenone from Resorcinol.
3. Preparation of p-benzoquinone from hydroquinone.
4. Preparation of Dibenzylidene acetone.
5. Preparation of anthraquinone from anthracene
6. Preparation of benzophenone oxime from benzophenone
7. Preparation of Benzilic acid from Benzil
8. Preparation of Bis-2- naphthol from 2-naphthol.
9. Prepartion of m-dinitrobenzene from Nitrobenzene.

Note: Each student is expected to submit both Crude and recrystallized samples of the preparation during their regular practical for evaluation at the time of practical examinations.

For Class work Only:

1. Isolation of carotene from carrot.
2. Isolation of casein from milk
3. Isolation of Citric acid from Citric fruits.

TEXT BOOKS

1. A.I. Vogel, *Elementary Practical Organic Chemistry: Small Scale Preparations, Qualitative Organic Analysis, Quantitative Organic Analysis*, Pearson Education, 2011.
2. F.G. Mann and B.C. Saunders, *Practical Organic Chemistry*, 4th edn, Pearson Education India, 2009.
3. K. Bansal Raj, *Laboratory Manual of Organic Chemistry*, New Age International, 2009.
4. V. Venkateswaran, R. Veeraswamy and A. R. Kulandaivelu, *Basic Principles of Practical Chemistry*, Sultan Chand & Sons, 2004.
5. V.K. Ahluwalia, and R. Aggarwal, *Comprehensive Practical Organic Chemistry*, UniversitiesPress, 2004**.**

REFERENCE BOOKS

1. R.G. Engel, D.L. Pavia, G.M. Lampman and G.S. Kriz, *A Microscale approach to Organic Laboratory*, 5th edition, Paperback – International Edition, 2012.
2. P.B. Cranwell, L.M. Harwood and C.J. Moody, *Experimental Organic Chemistry*, 3rd edn, Wiley-Blackwell**,** 2017.
3. J. Leonard, B. Lygo and G. Procter, *Advanced Practical Organic Chemistry*, 3rd edn, CRC Press, 2013.
4. Moore, Dalrympk and Rodig, *Experimental methods in organic chemistry*, 3rd edition, Saunders College publishing, The Oxford Press, 1982.

COURSE OUTCOMES (COs)

On completion of the course, the students will be able to

CO Nos	CO Statement	Cognitive Level
CO1	Develop the skills to estimate organic compounds	K3
CO2	Estimate the amount of organic compound using quantitative organic estimation methods	K5
CO3	Illustrate various organic reactions and their utility in organic preparations.	K2, K3
CO4	Acquire the skills to isolate useful compounds from natural sources	K3
CO5	Determine the physical properties of organic compounds	K5

MAPPING OF COURSE OUTCOMES WITH POs AND PSOs

CO	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PSO1	PSO2	PSO3	PSO4	PSO5	PSO6	PSO7	PSO8	PSO9
CO1	M	S	S	S	S	S	S	S	S	S	M	L	S	N	N	S	S
CO2	M	S	S	S	S	S	S	S	S	S	M	L	S	N	N	S	S
CO3	M	S	M	S	S	S	S	S	S	S	M	L	S	N	N	S	S
CO4	S	S	S	S	S	S	S	S	S	S	M	M	S	N	N	S	S
CO5	M	S	M	M	S	S	S	S	S	S	M	M	M	N	N	S	S

CORE 11	INORGANIC CHEMISTRY PRACTICAL - II	L	T	P	C
		0	0	4	2

Objectives:

- *To understand the principles and various analytical methods of quantitative analysis of cations present in a mixture.*
- *To improve the skill in quantitative estimation of metal ions by complexometric titration.*
- *To understand the preparation and analysis of coordination complexes.*

A. Quantitative Analysis of Cations by Complexometric Method.

1. Estimation of Cu (II) in a solution containing Pb (II) or Ba (II) (Separation of Pb (II) or Ba(II) by Precipitation).
2. Estimation of Zn(II) in a solution containing Pb(II) or Ba(II) (Separation of Pb(II) or Ba(II) by precipitation).
3. Estimation of Mg(II) in a solution containing Pb(II) or Ba(II) (Separation of Pb(II) or Ba(II) by precipitation).
4. Estimation of Ca(II) in diet supplement pill.
5. Estimation of Pb and Sn in Solder alloy [Demasking by F^-].

B. Preparation and Analysis of Inorganic Complexes by Volumetric Method

1. Preparation and analysis of potassium tris(oxalato)ferrate(III) trihydrate $K_3[Fe(C_2O_4)_3].3H_2O$
2. Preparation and analysis of tris(thiourea)copper(I) sulphate dihydrate, $[Cu(tu)_3]_2SO_4.2H_2O$
3. Preparation, and analysis of potassium tris(oxalato)chromate(III) trihydrate $K_3[Cr(C_2O_4)_3].3H_2O$

C. Photo colorimetric analysis of Fe and Ni (Course work)

TEXT BOOKS

1. G.H. Jeffery, J. Bassett, J. Mendham and R.C. Denney, *Vogel's Textbook of Quantitative Chemical Analysis*, Revised 5th edition, ELBS, 1989.
2. Douglas A. Skoog, Donald M. West, F. James Holler and Stanley R. Crouch, *Fundamentals of Analytical Chemistry*, 8th Edition, Brooks/Cole-Thomson Learning, USA, 2004.

REFERENCE BOOKS

1. I.M. Kolthoff and V.A. Stenger, *Volumetric Analysis*, 2nd Edition, Interscience Publishers, New York, 1947.
2. Mounir A. Malati, *Experimental Inorganic/Physical Chemistry - An Investigative, Integrated Approach to Practical Project Work*, Woodhead Publishing Limited, Reprint, 2010**.**
3. W. G. Palmer, *Experimental Inorganic Chemistry*, Cambridge University Press, Reprint, 1970**.**
4. George Brauer, *Handbook of Preparative Inorganic Chemistry*, 2nd Edition, Academic Press, 1963**.**
5. Geoffrey Pass and Haydn Sutcliffe, *Practical Inorganic Chemistry - Preparations, reactions and instrumental methods*, Springer, 1974.

COURSE OUTCOMES (COs)

Upon completion of the course, the students will be able to

CO Nos	CO Statement	Cognitive Level
CO1	Describe the principles, techniques and skills related to quantitative determination of ions in a mixture by complexometric titration.	K_2
CO2	Estimate one metal ion in presence of another metal ion by complexometric method.	K5
CO3	Estimate the amounts of components present in Solder alloy.	K4, K5
CO4	Prepare and analyze the Inorganic complexes and estimate them by volumetric methods.	K6,K4, K5
CO5	Describe the basic principle of calorimetry and apply it for the estimation of ions present in solution.	K_2,K_3, K_5

MAPPING OF COURSE OUTCOMES WITH POs AND PSOs

CO	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PSO1	PSO2	PSO3	PSO4	PSO5	PSO6	PSO7	PSO8	PSO9
CO1	M	S	S	S	S	S	S	S	S	S	M	L	M	N	N	S	S
CO2	M	S	S	S	S	S	S	S	S	S	M	L	M	N	N	S	S
CO3	S	S	S	S	S	S	S	S	S	S	M	M	M	N	N	S	S
CO4	M	S	S	S	S	S	S	S	S	S	M	M	M	N	N	S	S
CO5	M	S	S	S	S	S	S	S	S	S	M	M	M	N	N	S	S

CORE 12	PHYSICAL CHEMISTRY PRACTICAL - II	L	T	P	C
		0	0	4	2

Objectives:

- *To motivate the students to understand the principles of conductometric titrations and Distribution law.*
- *To understand the Principles and applications of Thermometry.*

I. Conductometric experiments

(a) Estimation of K_2SO_4 using $BaCl_2$

(b) Estimation of CH_3COOH and $CH_3COOONa$ in a Buffer solution.

(c) Neutralization and Displacement reactions

Standard: CH_3COONa, Link: HCl Estimation: NaOH + CH_3COONa

(d) Determination of Dissociation constant of a weak acid.

II. Distribution law

(a) Distribution of Iodine between two immiscible solvents & Study of the equilibrium constant of the reaction $KI + I_2 \rightarrow KI_3$

(b) Distribution of benzoic acid between two immiscible solvents.

III. Thermometry Determination of Solution enthalpy of

(i) Benzoic acid - water

(ii) Potassium dichromate - water

(iii) Potassium nitrate - water

TEXT BOOKS

1. J. B.Yadav, *Advanced Practical Physical chemistry*, 20th Edn., GOEL publishing House, Krishna Pakashan Media, 2001.
2. B.C. Kosla, *Senior Practical Physical Chemistry*, Simla Printers, New Delhi, 1987.
3. Saroj Kumar and Naba Kumar, *Physical Chemistry Practical*, New Central Book Agency, 2012.

REFERENCE BOOKS

1. Findlay's *Practical Physical Chemistry*, Revised and edited by B.P. Levitt 9th Edn., Longman, London, 1985.
2. W.J. Popiel, *Laboratory Manual of Physical Chemistry*, ELBS, London, 1970.
3. G.W. Garland, J.W. Nibler and D.P. Shoemaker, *Experiments in Physical Chemistry*, 8th Edn. McGraw Hill, 2009.

COURSE OUTCOMES (COs)

On completion of the course, the students will be able to

CO Nos	CO Statement	Cognitive Level
CO1	Explain the basic principles of conductometric titrations and determine the Dissociation constant of weak acids.	K2, K5
CO2	Illustrate the principles of distribution law and estimate the distribution of solute in two immiscible solvents.	K2, K5
CO3	Outline the basic principles of thermometry and determine the solution enthalpy of solute in solvent.	K2, K5

MAPPING OF COURSE OUTCOMES WITH POs AND PSOs

CO	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PSO1	PSO2	PSO3	PSO4	PSO5	PSO6	PSO7	PSO8	PSO9
CO1	M	S	S	S	S	S	S	S	S	S	M	L	S	N	M	S	S
CO2	M	S	S	S	S	S	S	S	S	S	M	L	S	N	M	S	S
CO3	M	S	S	S	S	S	S	S	S	S	M	L	S	N	S	S	S

SEMESTER III

CORE 13	ORGANIC SPECTROSCOPY AND REARRANGEMENTS	L	T	P	C
		5	0	0	4

Objectives:

- *To study the concept of UV, IR, NMR spectroscopy, Mass spectrometry and their applications in organic systems.*
- *To interpret the spectral data of organic molecules.*
- *To understand the mechanism of Rearrangement reactions.*

UNIT I - ULTRAVIOLET, INFRA – RED SPECTROSCOPY, ORD AND CD (15 Hours)

UV-Visible: The absorption laws – Types of electronic transitions – effect of solvents and Hydrogen bonding on λ_{max} values. – Woodward – Fieser rules to calculate λ_{max} values of conjugated dienes and α,β - unsaturated ketones.

IR: Molecular Vibrations – Vibrational frequencies - Characteristic IR absorptions of different functional groups – Fermi resonance and Finger print region - factors influencing absorption of carbonyl and hydroxyl groups – electronic effect and effect of hydrogen bonding.

ORD and CD: Optical rotatory dispersion (ORD): Cotton effect - Octant rule and axial - halo ketone rule – Conformation and Configuration determination of simple systems - Circular Dichroism.

UNIT II - NMR SPECTROSCOPY (15 Hours)

Nuclear spin – magnetic moment of a nucleus – nuclear energy levels in the presence of magnetic field – relative populations of energy levels – macroscopic magnetization - Basic Principle of NMR experiments – CW and FT NMR.

^{1}H NMR: Chemical shift - number of signals - Factors influencing proton chemical shift (Electronegativity, Anisotropic effects and Vander walls' deshielding) and vicinal proton - Spin–spin coupling – proton coupling constants - Geminal, Vicinal and long range coupling constants - 1H NMR spectrum of simple organic molecules such as CH_3CH_2Cl, CH_3CHO etc. - Classification of spin systems – First order and Second order spectra - analysis of AX, AMX and ABX systems – spin decoupling – Nuclear Overhauser Effect – Chemical exchange.

^{13}C NMR: Principle of proton decoupled and OFF- resonance ^{13}C NMR spectra - comparison with ^{1}H NMR – factors affecting ^{13}C chemical shifts – ^{13}C NMR spectra of simple organic molecules (aliphatic, olefinic, alkynic, aromatic and carbonyl compounds).

UNIT III - MASS SPECTROMETRY (15 Hours)

Basic Principles– Base peak – molecular ion – nitrogen rule – metastable ions – isotopic peak - daughter ions – Mc–Lafferty rearrangement – RDA – General rules for fragmentation pattern – Fragmentation pattern of simple compounds of hydrocarbons, alcohols, amines, aldehyde, ketone, ether, acids, phenols ,nitro compounds, alicyclic compounds .

Alternative electron impact ionization technique – CI, FAB, ESI – MS, MALDI –MS, MALDI-TOF, ICP- MS.

UNIT IV - 2D NMR AND INTERPRETATION OF SPECTRUM (15 Hours)

2D NMR spectroscopy: H^1–H^1COSY, H^1–C^{13} COSY, NOESY, DEPT and INADEQUATE spectra.

Applications of combined spectroscopic techniques in elucidating the structure of organic molecules – One conjunction problem based on UV, IR, H^1 NMR, ^{13}C NMR and Mass spectroscopic techniques is compulsory under section – C. Problems shall be based on the reference books.

UNIT V - REARRANGEMENT REACTIONS (15 Hours)

Types of rearrangements: Nucleophilic, electrophilic and free radical and protrophic reactions.

Mechanism: Nature of migration – migrating aptitude and memory effects, ring enlargement and ring contraction rearrangements.

Reactions: Carbon to carbon migration: Pinacol – Pinacolone, Benzil – Benzilic acid, Arndt – Eistert synthesis, Demjanov and dienone-phenol rearrangements.

Carbon to oxygen migration – Brook, Cumene Hydro-peroxide and Dakin rearrangements.

Carbon to Nitrogen migration – Lossen, Neber and curtius rearrangements.

Miscellaneous: Von – Richter and Sommelet-Hauser rearrangements.

TEXT BOOKS

1. William Kemp, *Organic Spectroscopy*, Third Edition, MacMillan, Indian edition, 2019.
2. R.M. Silverstein, F.X. Webster and K.J. Kiemle, *Spectrometric identification of organic compounds*,John Wiley and Sons, Inc., 2005.
3. L.D. S. Yadav, , *Organic Spectroscopy*, Springer, 2005.
4. L.D. Field, S. Sternhell and J.R. Kalman, *Organic Structures from Spectra*, 4th edition, John Wiley and Sons, 2007**.**
5. Karen-Feinstein, *Guide to Spectroscopic Identification of Organic compounds*, 1st edition, CRC Press, 1994.
6. B.P.Mundy, M.G.Ellerd and F.G.Favaloro, *Name Reactions and Reagents in OrganicSynthesis*, 2nd Ed., 2005.
7. Dr Jagdamba Singh & Dr. L.D.S Yadav, Orgnic Synthesis: Design, Reagents, Reactions and Rearrngements, A Pragati Second Revised Edition, 2007**.**
8. Raj K. Bansal, Organic Reaction mechanisms, Tata Mc Graw Hill, Third Editon, 2007.
9. A. Hassner & I. Namboothiri. Organic Syntheses Based Name Reactions, Elsevier, 2012.
10. Sanyal & Sanyal, Reactions, Rearrangements and Reagents, 4th edition, Bharati Bhawan Publishers and Distributors, 2003.

REFERENCE BOOKS

1. R.M. Silverstein, F.X. Webster, K.J. Kiemle and D.L. Bryce, *Spectrometric identification of organic compounds*, 8th edition Wiley Publications, 2014.
2. Ian Fleming and Dudley Williams, *Spectroscopic methods in organic chemistry*, 7th edition, Springer Publications, 2019.
3. William Kemp, *Organic Spectroscopy*, Third Edition, MacMillan, 1994.
4. E. Pretsch, P. Buhlmann and M. Badertscher, *Structure Determination of Organic Compounds: Tables of Spectral Data*, 4th revised and enlarged edition, Springer Publications, 2009.
5. F. A. Carey and R.J. Sundberg, *Advanced Organic Chemistry, Part B: Reaction and Synthesis*, 5th edition, Springer, 2007**.**
6. W. Carruthers, and I. Coldham, *Modern Methods of Organic Synthesis*, 4th edn, CambridgeUniversity Press, 2015.

7. L. Kurti and B. Czako, *Strategic Applications of Named Reactions in Organic Synthesis*, Elsevier 2005.

COURSE OUTCOMES (COs)

Upon completion of the course, the students will be able to

CO Nos	CO Statement	Cognitive Level
CO1	Describe the basic principles of UV, IR, ORD and CD, and the applications of UV-Visible spectroscopy, IR spectroscopy, ORD and CD in structural elucidation of organic compounds.	K2, K3, K4
CO2	Interpret the 1H NMR and 13C NMR spectral data to elucidate the structure of organic compounds.	K2, K3, K4
CO3	Explain the fragmentation pattern in Mass spectrometry and use them in structural elucidation.	K3, K2
CO4	Interpret the 2D NMR spectrum and solve structure related problems	K2, K3
CO5	Illustrate the types and mechanisms of the prescribed rearrangement reactions and their applications in Organic synthesis.	K2, K3

MAPPING OF COURSE OUTCOMES WITH POs AND PSOs

CO	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PSO1	PSO2	PSO3	PSO4	PSO5	PSO6	PSO7	PSO8	PSO9
CO1	M	S	S	S	L	L	S	S	S	S	M	L	S	N	M	S	S
CO2	M	S	S	S	L	L	S	S	S	S	M	L	S	N	M	S	S
CO3	M	S	S	M	L	L	S	S	S	S	M	L	S	N	M	S	S
CO4	M	S	S	S	L	L	S	S	S	S	M	L	S	N	M	S	S
CO5	M	S	S	M	L	L	S	S	S	S	M	S	S	N	L	S	S

CORE 14	SPECTRAL METHODS-I, ORGANO METALLIC AND ANALYTICAL METHODS	L	T	P	C
		5	0	0	4

Objectives:

- *To study the applications of electronic and photo electronic spectroscopic techniques in coordination compounds.*
- *To study the applications of ORD and CD to determine absolute configuration of chelate complexes.*
- *To introduce organometallic compounds and to study their catalytic applications in homogeneous and heterogeneous systems.*
- *To understand the basic principles and applications of thermo and spectro analytical techniques.*

UNIT I - ELECTRONIC SPECTROSCOPY, ORD AND CD (15 Hours)

Electronic spectroscopy: Selection rules for electronic transitions - Hole formalism - LS Coupling and determination of term symbols – Hund's Rules - Splitting of terms – Orgel and Tanabe Sugano diagrams – Electronic spectra of I^{st}row transition metal complexes - Evaluation of 10 Dq, β and B' for octahedral d^2 and d^8 systems. Charge transfer spectra – types – Effect of solvent polarity on CT spectra - Effect of tetragonal distortion and spin - orbit coupling on spectra – Electronic spectra of lanthanide and actinide complexes.

ORD and CD - Optical isomerism in octahedral complexes – absolute configuration of chelate complexes from ORD and CD.

UNIT II - PHOTO ELECTRON SPECTROSCOPY (15 Hours)

Theory – types of PES – origin of fine structures – adiabatic and vertical transitions – PE spectra of homonuclear diatomic molecules (N_2, O_2) – hetero nuclear diatomic molecule (CO) – polyatomic molecules (H_2O, NH_3) - Koopman's theorem – application and limitation of the theorem. XPS (ESCA): structure of N_3^- ion, N (1s) spectrum of $[Co(en)_2(NO)_2]NO_3$, C(1s) spectrum of $C_2H_5COOCF_3$. Shake-up and shake-off processes – Structural and bonding information in metal carbonyls – Auger electron spectroscopy.

UNIT III - ORGANOMETALLIC CHEMISTRY–I (15 Hours)

The 18 e^- and 16 e^- rules and its correlation to stability – Synthesis, structures and bonding of metal carbonyls, metal nitrosyls and dinitrogen complexes – Identifications of bridging and

terminal CO groups by IR – Structure of Mononuclear, dinuclear [$Mn_2(CO)_{10}$, $Co_2(CO)_8$, $Fe_2(CO)_9$], Trinuclear [$M_3(CO)_{12}$ (M = Fe, Ru, Os)] and Tetranuclear [$M_4(CO)_{12}$ (M = Co, Rh, Ir)] Carbonyls. Synthesis, properties and structural features of metal complexes with alkene, alkyne and allyl systems. Metallocenes – synthesis, properties, structure and bonding with particular reference to ferrocene and berryllocene – covalent versus ionic bonding in beryllocene.

UNIT IV - ORGANOMETALLIC CHEMISTRY–II (15 Hours)

Organometallic compounds as catalysts and the requirements: Agostic interaction – Oxidative addition and reductive elimination - insertion and elimination reactions – nucleophilic and electrophilic attack of coordinating ligands.

Homogeneous catalysis: Wilkinson's catalyst and hydrogenation reactions, Tolman catalytic loop; hydroformylation (oxo) reaction, Wacker and Monsanto acetic acid processes.

Heterogeneous catalysis: synthesis gas and water gas shift reactions; Fischer Tropsch process and synthetic gasoline, Ziegler-Natta polymerization and mechanism of stereoregular polymer synthesis.

Hybrid Catalysis: Cluster compounds in catalysis, polymer-supported and phase-transfer catalysis-biphasic-systems.

UNIT V - THERMOANALYTICAL AND SPECTROANALYTICAL METHODS (15Hours)

Theory and principles of thermogravimetric analysis, differential thermal analysis and differential scanning colorimetry – characteristic features of TGA and DTA curves – factors affecting TGA and DTA curves – complementary nature of TGA and DTA – applications of thermal methods in analytical chemistry – thermometric titrations – the study of minerals and metal compounds. Principle and applications of spectrophotometry, spectrofluorimetry, atomic absorption spectroscopy and atomic emission spectroscopy based on plasma sources.

TEXT BOOKS

1. James E. Huheey, Ellen A. Keiter and Richard L. Keiter, *Inorganic chemistry: principles Structure and Reactivity*, 4th Edition, Pearson Education, 2006.
2. D.F. Shriver, P.W. Atkins and C.H. Langford, *Inorganic Chemistry*, ELBS, Oxford University Press, 1994.
3. B.K.Sharma, *Instrumental Methods of Chemical Analysis*, Meerut Krishna Prakashan, 2012.
4. P. Powell, *Principles of Organometallic Chemistry*, 2nd edition, Springer, 1998.
5. D.N. Satyanarayana, *Electronic Absorption Spectroscopy*, University Press, 2000.

6. P. Atkins, T. Overton, J. Rourke, M. Weller and F.Armstrong, *Inorganic Chemistry*, 5th edition, Oxford University press, 2010.
7. Russell S. Drago, *Physical Methods in Inorganic Chemistry*, Chapman and Hall, London, 1965.
8. Russell S. Drago, *Physical Methods for Chemists*, Surfside Scientific Publishers, 2nd Edition, 1977.
9. E.A.V. Ebsworth, David W.H. Rankin and Stephen Credock, *Structural Methods in Inorganic Chemistry*, ELBS, 1988.
10. B.P. Lever, *Inorganic Electronic Spectroscopy*, 2nd Sub Edition, Elseveir Science, 1986.

REFERENCE BOOKS

1. C. Elschenbroich and A. Salzer, *Organometallics – A Concise Introduction,* 2nd Edition, VCH Publication, 1992.
2. R. C. Mehrotra and A. Singh, *Organometallic Chemistry: A Unified Approach,* 2nd Edition, New Age International Publishers, 2005.
3. B.D.Gupta and A.J. Elias, *Basic Organometallic Chemistry: Concepts, Synthesis and Applications of Transition Metals* , 1st edition , University Press, CRC Press, 2010.
4. R.H.Crabtree, *Organometallic Chemistry of the Tranistion Metals*, Wiley, Newyork, 1988.
5. D.A. Skoog, F.J. Holler and T.A. Nieman, *Principles of Instrumental Analysis*, Saunders**,** 1992.
6. D.A. Skoog, D. M. West, F.J. Holler and S.R. Grouch, *Fundamentals of Analytical Chemistry*, Thomson Asia, 8th Edition, Third Reprint**,** 2005.
7. H.H. Willard, L.L. Merritt and J.A. Dean, *Instrumental Methods of Analysis*, CBS Publishers, 6th Edition, 1986.
8. F. Albert Cotton, Geoffrey Wilkinson, Carlos A. Marilo and Manfred Bochman, *Advanced Inorganic Chemistry*, Wiley Interscience Publication, 6th Edition, Reprint, 2012.

COURSE OUTCOMES (COs)

On completion of the course, the students will be able to

CO Nos	CO Statement	Cognitive Level
CO1	Describe the principles and applications of electronic and photo electronic spectroscopic techniques in coordination compounds.	K2, K3
CO2	Determine absolute configuration of chelate complexes by applying ORD and CD.	K3, K4, K5
CO3	Recall the EAN rule and explain the 18 & 16 electron rules to determine the stability of complexes.	K1, K2, K4
CO4	Classify terminal and bridging carbonyl groups in metal carbonyls using IR spectra.	K4
CO5	Categorize the different types of organometallic catalysts and explain their applications.	K4, K2, K3
CO6	Describe the principles and applications of thermo analytical techniques and determine the stability of complexes.	K2, K3, K4, K5

MAPPING OF COURSE OUTCOMES WITH POs AND PSOs

CO	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PSO1	PSO2	PSO3	PSO4	PSO5	PSO6	PSO7	PSO8	PSO9
CO1	M	S	S	M	L	L	S	S	S	S	M	L	M	N	L	S	S
CO2	M	S	S	M	L	L	S	S	S	S	M	L	M	N	L	S	S
CO3	L	S	M	L	L	L	S	S	S	S	M	L	M	N	M	S	S
CO4	M	S	M	M	L	L	S	S	S	M	M	M	M	N	M	S	S
CO5	M	S	S	M	L	L	S	S	S	S	M	S	M	N	L	S	S
CO6	M	S	S	S	L	L	S	S	S	S	M	M	M	N	M	S	S

CORE 15	GROUP THEORY AND CHEMICAL THERMODYNAMICS	L	T	P	C
		4	0	0	4

Objectives:

- *To understand the basic concepts of group theory.*
- *To understand the inter linking of quantum chemistry and group theory.*
- *To explain various concepts of thermodynamics.*
- *To apply the concepts of statistical thermodynamics for the study of equilibrium reactions and reaction rates.*
- *To understand the inter linking of quantum chemistry and statistical thermodynamics.*

UNIT I - GROUP THEORY-I (12 hours)

Symmetry elements and operations - Group Postulates and types of groups. Identification of Point groups of molecules and Schoenflies symbols. Construction of multiplication table for C_{2v}, C_{3v} and C_{2h}. Sub-groups and classes of symmetry operations. Rule of similarity transformations. Matrix representations of symmetry operations. Use of atomic wave functions as bases for point group representations. Reducible and irreducible representations. The Great Orthogonality theorem. Properties of Reducible and irreducible representations. Construction of character tables for C_{2v}, C_{3v}, C_{4v}, C_{2h} and D_2 point groups by using the Great Orthogonality theorem.

UNIT II - GROUP THEORY-II (12 hours)

Standard Reduction Formula -Vibrational modes as bases for group representations-Normal mode analysis for non linear molecules H_2O, $POCl_3$, trans-N_2F_2 and $PtCl_4$. Symmetry selection rules for infrared and Raman spectra. Mutual exclusion principle. Determination of Hybridisation of atomic orbitals in non-linear molecules (CH_4, XeF_4, and PF_5). Electronic spectra of ethylene and formaldehyde molecules. Construction of Projection operators and Molecular orbitals by Symmetry Adapted Linear Combinations. Simplification of HMO calculations using group theory. Calculation of delocalization energy for ethylene, *trans*-1,3-butadiene and benzene systems.

UNIT III - CHEMICAL THERMODYNAMICS (12 hours)

A general review of enthalpy, entropy and free energy concepts. Maxwell relations. Genesis of third law and its limitations - Thermodynamics of systems of variable compositions - partial molar quantities and their determination - chemical potential - Gibbs-Duhem equation - Duhem-Margules equation - Fugacity and its determinations - choice of state - Activity and

activity coefficients - electrolytes and non-electrolytes. Determination of activity and activity coefficients for electrolytes and non-electrolytes. Excess Thermodynamic functions.

UNIT IV - STATISTICAL THERMODYNAMICS (12 hours)

Thermodynamic probability and most probable distribution - Ensemble averaging, postulates of ensemble averaging, Canonical, Grand canonical and microcanonical ensembles. Maxwell-Boltzmann statistics – Partition functions – thermodynamic properties from partition function - translational, rotational, vibrational and electronic partition functions. Partition function and equilibrium constant. Quantum statistics - Fermi-Dirac and Bose-Einstein statistics - photon gas and electron gas. Heat capacities of diatomic gases. Einstein and Debye's theory of heat capacity of solids - population inversion - negative Kelvin temperature.

UNIT V - IRREVERSIBLE THERMODYNAMIC PROCESSES (12 hours)

Affinities and fluxes, reversible and irreversible processes, entropy production for some important irreversible processes, entropy flow due to exchange of matter and energy, entropy changes due to chemical reaction, affinity and coupling of chemical reaction, the phenomenological laws and equations and their applications in chemistry - Onsager reciprocal relations- validity and verification. Thermoelectric phenomena - Electro kinetic and thermo mechanical effects. Application of irreversible thermodynamics to biological and non-linear systems.

TEXT BOOKS

1. F.A. Cotton, *Chemical Applications of Group Theory*, 3rd Edn., Wiley, 2008.
2. G. Davidson, *Introductory Group Theory for Chemists*, Elsevier, 1971.
3. K.V. Raman, *Group Theory and its applications to Chemistry*, 3rd Edn., Tata Mc Graw- Hill Publishing Company, 1990.
4. M. S. Gopinathan and V. Ramakrishnan, *Group Theory in chemistry*, 2nd Edn., Vishal Publication, 2013.
5. K.V. Reddy, *Symmetry and Spectroscopy of molecules*, New Age International, 2007.
6. P.K. Bhattacharya, *Group Theory and its Chemical Applications*, Himalaya Publishing House, 2010.
7. K. Rajaram and J.C. Kuriacose, *Thermodynamics For Students of Chemistry*, 2nd Edition, S.L.N. Chand and Co, Jalandhar, 1986.
8. M.C. Gupta, *Statistical Thermodynamics*, New Age International, New Delhi, 1995.

REFERENCE BOOKS

1. R.L. Carter, *Molecular Symmetry and Group Theory*, Wiley, 1997.
2. R.L. Flurry, *Symmetry Groups: Theory and Chemical Applications*, Prentice Hall, 1980.
3. I.M.Klotz and R.M. Rosenberg, *Chemical thermodynamics*, 6th edition, W.A.Benjamin Publishers, California, 1972.
4. Lee, Sears and Turcotte, *Statistical Thermodynamics*, 2nd edition, Addison Wesley, 1973.
5. P.A.Rock, *Chemical Thermodynamics*, Oxford University press, 1983.
6. W.J. Morre, *Physical Chemistry*, 5th edition, Orient Longman, 1976.
7. G.W. Castellan, *Physical Chemistry*, 3rd edition, Addison Wesley, 1983.

COURSE OUTCOMES (COs)

Upon completion of the course, the students will be able to

CO Nos	CO Statement	Cognitive Level
CO1	Explain the basic concepts of group theory and construct character tables for various point groups.	K2, K3
CO2	Analyze the symmetry of molecules and apply the group theory into spectroscopy and hybridizations.	K4, K3
CO3	Illustrate the relationship between group theory and quantum mechanics.	K2
CO4	Summarize the concepts of statistical thermodynamics and the interlinking between the quantum mechanics and thermodynamics.	K2
CO5	Explain the irreversible thermodynamic processes and apply to biological and non-linear systems.	K2, K3

MAPPING OF COURSE OUTCOMES WITH POs AND PSOs

CO	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PSO1	PSO2	PSO3	PSO4	PSO5	PSO6	PSO7	PSO8	PSO9
CO1	M	S	M	S	L	L	S	S	S	M	M	L	S	N	M	S	S
CO2	M	S	S	S	L	L	S	S	S	M	M	L	S	N	S	S	S
CO3	M	S	M	M	L	L	S	S	S	M	M	L	M	N	S	S	S
CO4	M	S	S	M	L	L	S	S	S	M	M	L	M	N	M	S	S
CO5	M	S	S	S	L	L	S	S	S	M	M	L	S	N	S	S	S

CORE 16	SCIENTIFIC RESEARCH METHODOLOGY	L	T	P	C
		4	0	0	4

Objectives:

- *To introduce scientific research and to learn the survey for literature, chemical abstract, choosing a research problem, scientific writing of research articles, presentations and research proposal and funding agencies.*
- *To learn Plagiarism and Intellectual Property Rights.*
- *To introduce the basic principles, working and applications of Instrumental techniques like Surface Probe Microscopy.*

UNIT I - INTRODUCTION TO SCIENTIFIC RESEARCH (12 Hours)

Objectives of research – Types of research – Significance of research. Research methods versus methodology – Research and scientific method – Criteria of good research – Problems encountered by researchers in India.

Problem selection – Selection of research problem, sources of research problems, criteria/characteristics of a good research problem, errors in selecting a research problem - project proposal – funding agencies.

UNIT II - LITERATURE SURVEY (12 Hours)

Sources of information, Primary, Secondary, Tertiary sources, Journals, Journal abbreviations, Abstracts – Beilstein - Compendia and tables of information – Reviews – Current titles – Textbooks – Current contents - General treatises – Monographs and treatises on specific areas - Literature search – Information about a specific compound – Science citation index – Box to locate journals.

Introduction to Chemical Abstracts. Online searching, Database, *Scifinder*, *Scopus*, Citation Index, Impact Factor.

UNIT III - WRITING OF RESEARCH REPORT (12 Hours)

Format of the research report - style of writing the report - references and bibliography.

Research paper writing: Types of research papers – Structure of research papers – Research paper formats - Different formats for referencing – ways of communicating research paper – organizing a poster display, giving an oral presentation in seminars/conferences - Making effective presentations using Power Point and Beamer.

Research Proposal: Format of research proposal, individual research proposal and institutional proposal.

UNIT IV - PLAGIARISM AND INTELLECTUAL PROPERTY RIGHTS (12 Hours)

Plagiarism - Introduction, Reason for plagiarism, Types of plagiarism - Plagiarism of words, Patchwork plagiarism, Self-plagiarism, Cyber and Digital plagiarism, Accidental plagiarism, Plagiarism of Authorship, Plagiarism of Ideas. Plagiarism policies - IEEE, Springer, Elsevier. Software used for identifying plagiarism. Techniques to avoid plagiarism - Referencing, Paraphrasing, Creative Common License.

Intellectual Property Rights - Introduction. Difference between Industrial Property and Intellectual Property, Significance of Intellectual Property Rights. Forms of IPR - Patents, Copyright, Trademarks, Collective marks, Industrial Design, Integrated Circuit, Geographical Indication. Valuation of IPR, IPR and licensing.

UNIT V - ADVANCED INSTRUMENTAL TECHNIQUES (12 Hours)

Principles, techniques and applications:

Surface probe microscopy: Atomic force microscopy, Scanning tunnelling microscopy, Scanning electron microscopy, Transmission electron microscopy, HRTEM, Energy Dispersive X-ray analysis (EDX), X-ray photo electron spectroscopy. X-ray diffraction techniques - Powder and single crystal XRD, principle, techniques and applications.

TEXT BOOKS

1. Dr.C.R. Kothari, *Research Methodology: Methods and Techniques*, New Age International Publishers, 2nd Edition, New Delhi. 2014.
2. Ranjit kumar, *Research Methodology: A Step by Step Guide for Beginners*, Pearson Education; 2nd Edition, 2005.
3. Tanmoy Chakraborty and Lalita Ledwani, *Research Methodology in Chemical Sciences: Experimental and Theoretical Approach*, Apple Academic Press; 1st Edition, 2016.
4. Dr. N. Arumugam, *Research Methodology*, Saras Publication, First Edition, 2016.
5. Vinayak Bairagi and Mousami V. Munot, *Research Methodology - A Practical and Scientific approach*, CRC Press, 2019.
6. R. Gopalan, P. S. Subramanian and K. Rengarajan, *Elements of Analytical Chemistry*, Sultan Chand and Sons, New Delhi, 2005.
7. S. M. Khopkar, *Basic concepts of analytical chemistry*, New age international, third edition 2008.
8. Douglas A. Skoog, Donald M. West, F. James Holler and Stanley R. Crouch, *Fundamentals of Analytical Chemistry*, ninth edition, 2013.

9. Gary D. Christian, Purnendu K. Dasgupta and Kevin A. Schug, *Analytical Chemistry*, John Wiley & Sons, seventh edition, 2013.
10. G.R. Chatwal and S.K. Anand, *Instrumental Method of Chemical Analysis*, Himalaya Publishing house, fifth Reprint, 2016.

REFERENCE BOOKS

1. M.D. Barbara Gastel and Robert A. Day, *How to Write and Publish a Scientific Paper*, Greenwood Publishing Group Inc, 8th Edition, 2016.
2. R. Gopalan, *Thesis writing*, Vijay Nicole Imprints, 2005.
3. D.G Peters, J.M. Hayes and G.M. Hefige, *A brief introduction to Modern chemical analysis*, Saunders, 1976.
4. R.A Day and A.L. Underwood, *Quantitative analysis*, Prentice Hall, 1999.
5. D.A. Skoog, F.J. Holler and T.A. Nieman, *Principles of Instrumental Analysis*, 5th Edition, Bangalore, 2005.
6. Anthony R. West, *Solid state chemistry and its applications*, second edition, student edition, Wiley and sons, 2014.

COURSE OUTCOMES (COs)

On completion of the course, the students will be able to

CO Nos	CO Statement	Cognitive Level
CO1	Select research problem and various funding agencies.	K2
CO2	Write the research report and make effective presentations.	K3
CO3	Apply software for identifying plagiarism.	K3
CO4	Describe the forms of IPR and its significance.	K2, K3
CO5	Describe the surface probe microscopic techniques to analyze the sample surfaces.	K2, K4

MAPPING OF COURSE OUTCOMES WITH POs AND PSOs

CO	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PSO1	PSO2	PSO3	PSO4	PSO5	PSO6	PSO7	PSO8	PSO9
CO1	S	S	S	S	L	S	S	S	M	S	S	L	S	L	S	S	S
CO2	M	S	M	M	L	S	S	S	M	S	S	L	S	L	S	S	S
CO3	M	S	M	S	L	S	S	S	M	S	S	L	S	S	S	S	S
CO4	S	S	M	M	L	M	S	S	L	S	S	L	M	S	M	S	S
CO5	M	S	S	S	L	L	S	S	S	S	S	L	S	L	M	S	S

CORE 17	ORGANIC CHEMISTRY PRACTICAL - III	L	T	P	C
		0	0	4	2

Objectives:

- *To enable the student to develop analytical skill in organic quantitative analysis.*
- *To enable the students to understand the mechanism involved in two stage organic preparations.*

Estimations and two stage preparations comprising oxidation, bromination, nitration, hydrolysis, dehydration, diazotisation, coupling and photochemical reactions have been included as the practical components.

Microscale preparations are recommended for the simple reason, as they are both economic-friendly and eco-friendly.

A. List of Estimations

1. Glucose - Lane - Eynon and method
2. Glucose - Bertrand's method
3. Purity of Glucose
4. Determination of Percentage purity in an unsaturated acid.

B. List of Two stage preparations

1. Benzaldehyde → Benzoic acid → m-nitrobenzoic acid
2. Acetanilide → p-bromoacetanilide → p-bromoaniline
3. Acetanilide → p-nitroacetanilide → p-nitroaniline
4. Methyl Benzoate → m-nitro methylbenzoate → m-nitrobenzoic acid
5. Benzophenone → Benzpinacol → Benzpinacolone
6. Benzophenone → Benzophenone oxime → Benzanilide
7. Phthalic acid → Phthalic anhydride → Phthalimide
8. Aniline → Tribromoaniline → sym-tribromobenzene
9. Aniline → Diazoaminobenzene → p-aminoazobenzene

Students are expected to submit the recrystallised samples of the final products, at the time of practical examination, for evaluation by the examiners.

TEXT BOOKS

1. A.I. Vogel, *Elementary Practical Organic Chemistry: Small Scale Preparations, Qualitative Organic Analysis, Quantitative Organic Analysis*, Pearson Education, 2011.
2. F.G. Mann and B.C. Saunders, *Practical Organic Chemistry*, 4th edn, Pearson Education India, 2009.
3. V.K. Ahluwalia, and R. Aggarwal, *Comprehensive Practical Organic Chemistry*, Universities Press, 2004.
4. Raj K. Bansal, *Laboratory Manual of Organic Chemistry,* Second Edition, Wiley Eastern, 1990.

REFERENCE BOOKS

1. R.G. Engel, D.L. Pavia, G.M. Lampman and G.S. Kriz, *A Microscale approach to Organic Laboratory*, 5th edition, Paperback – International Edition, 2012.
2. P.B. Cranwell, L.M. Harwood and C.J. Moody, *Experimental Organic Chemistry*, 3rd edn, Wiley-Blackwell**,** 2017.
3. J. Leonard, B. Lygo and G. Procter, *Advanced Practical Organic Chemistry*, 3rd edn, CRC Press, 2013.
4. Moore, Dalrympk and Rodig, *Experimental methods in organic chemistry*, 3rd edition, Saunders College publishing, The Oxford Press, 1982.

COURSE OUTCOMES (COs)

On completion of the course, the students will be able to

CO Nos	**CO Statement**	**Cognitive Level**
CO1	Estimate the amount of organic compounds using quantitative organic estimation methods	K5
CO2	Develop the skills to handle corrosive and toxic chemicals in organic preparations.	K3
CO3	Categorize organic reactions and their mechanisms relevant to organic preparations.	K4
CO4	Carry out microscale organic preparations	K3, K6
CO5	Determine the physical properties of organic compounds	K5

MAPPING OF COURSE OUTCOMES WITH POs AND PSOs

CO	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PSO1	PSO2	PSO3	PSO4	PSO5	PSO6	PSO7	PSO8	PSO9
CO1	M	S	S	S	S	S	S	S	S	S	M	L	M	N	N	S	S
CO2	M	S	M	S	S	S	S	S	S	S	M	S	M	N	N	S	S
CO3	M	S	M	S	S	S	S	S	S	S	M	S	M	N	N	S	S
CO4	M	S	S	M	S	S	S	S	S	S	M	M	M	N	N	S	S
CO5	M	S	M	L	S	S	S	S	S	S	M	M	M	N	N	S	S

CORE 18	INORGANIC CHEMISTRY PRACTICAL - III	L	T	P	C
		0	0	4	2

Objectives:

- *To identify the methodology to separate and estimate mixture of metal ions quantitatively.*
- *To understand the principles for volumetric and gravimetric methods of estimation of cations present in a mixture.*

I. Quantitative estimation of a mixture containing two or three metal ions (Volumetric and Gravimetric Estimations)

1. Estimation of mixture of Cu^{2+}(V) and Ni^{2+}(G)ions.
2. Estimation of mixture of Fe^{2+}(V)and Cu^{2+}(G)ions.
3. Estimation of mixture of Fe^{2+}(V) and Ni^{2+}(G)ions.
4. Estimation of Cu^{2+} (V), Ba^{2+} (G) and Ca^{2+} (G) ions in a mixture.
5. Estimation of Cu^{2+} (V), Ba^{2+} (G) and Zn^{2+} (G) ions in a mixture.
6. Estimation of Fe^{2+} (V), Cu^{2+} (G) and Ni^{2+} (G) ions in a mixture.

II. Analysis of ores and alloys (coursework)

TEXT BOOKS

1. Mounir A. Malati, *Experimental Inorganic/Physical Chemistry - An Investigative, Integrated Approach to Practical Project Work*, Woodhead Publishing Limited, Reprint, 2010.
2. G.H. Jeffery, J. Bassett, J. Mendham and R.C. Denney*, Vogel's Textbook of Quantitative Chemical Analysis,* Revised 5th edition, ELBS, 1989.
3. Douglas A. Skoog, Donald M. West, F. James Holler and Stanley R. Crouch, *Fundamentals of Analytical Chemistry*, 8th Edition, Brooks/Cole-Thomson Learning, USA, 2004.

REFERENCE BOOKS

1. I.M. Kolthoff and V.A. Stenger, *Volumetric Analysis*, 2nd Edition, Interscience Publishers, New York, 1947.
2. W. G. Palmer, *Experimental Inorganic Chemistry*, Cambridge University Press, Reprint, 1970.

COURSE OUTCOMES (COs)

Upon completion of the course, the students will be able to

CO Nos	CO Statement	Cognitive Level
CO1	Describe the concept of volumetric and Gravimetric analysis.	K2
CO2	Explain the principles for volumetric and gravimetric methods of estimation of cations present in a mixture.	K2, K3
CO3	Separate and estimate mixture of metalions quantitatively.	K4, K5
CO4	Analyze and estimate the contents of Ores and Alloys.	K4, K5

MAPPING OF COURSE OUTCOMES WITH POs AND PSOs

CO	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PSO1	PSO2	PSO3	PSO4	PSO5	PSO6	PSO7	PSO8	PSO9
CO1	L	S	M	M	S	M	S	S	S	M	M	L	S	N	N	S	S
CO2	M	S	S	M	S	M	S	S	S	M	M	L	M	N	N	S	S
CO3	M	S	S	S	S	S	S	S	S	S	M	M	S	N	N	S	S
CO4	S	S	S	S	S	S	S	S	S	S	M	M	S	N	N	S	S

CORE 19	PHYSICAL CHEMISTRY PRACTICAL - III	L	T	P	C
		0	0	4	2

Objectives:

- *To learn and apply the Principles of Potentiometric Titrations.*
- *To understand the Principles and applications of Kinetics and Adsorption*.

I. Potentiometric Titrations

(a) Acid alkali titrations.

(b) Determination of dissociation constant of weak acids

(c) Determination of pH of buffer Potentiometrically

(d) Redox Titrations

(i) Fe^{2+} *vs* Ce^{4+}

(ii) Fe^{2+} *vs* $Cr_2O_7^{2-}$

(iii) Fe^{2+} vs $KMnO_4$

(iv) I^- *vs* $KMnO_4$

(e) Precipitation Titrations

(i) Mixture of Cl^- & I^- vs Ag^+

(f) Solubility Product**:** Determination of solubility product of sparingly soluble silver salts.

II. Kinetics: Study of Kinetics of KI - $K_2S_2O_8$ system

III. Adsorption:

(a) Freundlich Adsorption isotherm:

(i) Adsorption of oxalic acid on charcoal.

(ii) Adsorption of acetic acid on charcoal.

(b) Langmuir Adsorption isotherm:

(i) Adsorption of oxalic acid on charcoal.

(ii) Adsorption of acetic acid on charcoal.

TEXT BOOKS

1. J. B.Yadav, *Advanced Practical Physical chemistry*, 20th Edn., GOEL publishing House, Krishna Pakashan Media, 2001.
2. B.C. Kosla, *Senior Practical Physical Chemistry*, Simla Printers, New Delhi, 1987.
3. R.C. Das and B. Behra, *Experimental Physical Chemistry*, Tata McGraw Hill, New Delhi, 1983.
4. Saroj Kumar and Naba Kumar, *Physical Chemistry Practical*, New Central Book Agency, 2012.

REFERENCE BOOKS

1. Findlay's *Practical Physical Chemistry*, Revised and edited by B.P. Levitt 9th Edn., Longman, London, 1985.
2. W.J. Popiel, *Laboratory Manual of Physical Chemistry*, ELBS, London, 1970.
3. G.W. Garland, J.W. Nibler and D.P. Shoemaker, *Experiments in Physical Chemistry*, 8th Edn. McGraw Hill, 2009.

COURSE OUTCOMES (COs)

On completion of the course, the students will be able to

CO Nos	CO Statement	Cognitive Level
CO1	Explain the principles of potentiometric titrations and apply for various reactions such as neutralization, redox and precipitation reactions.	K2, K3, K5
CO2	Determine the Dissociation constant of weak acids, pH of buffer and solubility product of sparingly soluble salts potentiometrically.	K5
CO3	Describe the principles of chemical kinetics and study the kinetics of a system**.**	K2, K3, K4
CO4	Illustrate the principles of adsorption process and carry out experiments to find out whether a particular adsorption process is Freundlich or Langmuir Adsorption isotherm.	K2, K3, K4

MAPPING OF COURSE OUTCOMES WITH POs AND PSOs

CO	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PSO1	PSO2	PSO3	PSO4	PSO5	PSO6	PSO7	PSO8	PSO9
CO1	M	S	S	M	S	S	S	S	S	S	M	L	M	N	L	S	S
CO2	M	S	M	S	S	S	S	S	S	S	M	L	M	N	L	S	S
CO3	L	S	M	M	S	S	S	S	S	S	M	L	M	N	L	S	S
CO4	M	S	M	S	S	S	S	S	S	S	M	L	S	N	S	S	S

SEMESTER IV

CORE 20	SYNTHETIC STRATEGIES IN ORGANIC CHEMISTRY	L	T	P	C
		5	0	0	4

Objectives:

- *To study selected name reactions and synthetic utility of important organic reagents.*
- *To understand the concept of retrosynthesis and the terms involved, about one group and two group disconnections and protection and deprotection of important functional groups.*
- *To study about Steroids, Vitamins and Terpenoids.*

UNIT I - NAME REACTIONS IN ORGANIC SYNTHESIS (15 Hours)

Acyloin condensation, Shapiro reaction, Julia olefination, Bamford – Stevens reaction, Bouveault-Blanc Reduction, Oxymercuration, Mc Murray coupling, Mukaiyama aldol reaction, Hofmann-Loffler-Freytag reaction, Peterson olefination, Wittig reaction, Tischenko reaction, Ugi reaction, Nef reaction.

UNIT II - RETEROSYNTHETIC ANALYSIS (15 Hours)

Disconnection approach - Synthon-synthetic equivalent, target molecule - Functional group interconversions – Chemoselectivity - one group C-C and C-X disconnection (disconnection of alcohols, alkenes, and carbonyl compounds) -Two group C-C & C-X disconnections: 1,3 and 1,5 difunctionalised compounds, α,β- unsaturated carbonyl compounds, synthesis of 3,4,5 and 6 membered rings in organic synthesis. Diels- Alder reaction, Robinson annulation reaction.

Use of protecting groups for alcohols, amines, acids, carbonyl compounds- use of activating and blocking groups – Reversal of polarity (Umpolung) - Reterosynthetic analysis of the following compounds: cis - Jasmone, Trihexyl phenydyl, Isonootkatone, cascarillic acid, and 2,4-dimethyl-2-hydroxy pentanoic acid.

UNIT III - REAGENTS IN ORGANIC SYNTHESIS (15 Hours)

Uses of the following reagents in organic synthesis and functional group transformation:

2,3-Dichloro-5,6-dicyano-1,4-benzoquinone (DDQ), DMSO, Super hydrides - Dess-martin-periodinane.

Modern Reagents: Introductory treatment of the application of silicon (Tri alkyl silyl halides, organo silanes), Boron (9–BBN, borane, and alkyl borane), phosphorus (phosphoranes), Tin – allyl stannane, palladium (Stille coupling, Suzuki Coupling, Heck and Negishi reactions)

samarium (SmI_2), ruthenium (RuO_4, Ru-BINAP Complex), platinum (Adam's Catalyst) reagents.

UNIT IV - STEROIDS **(15 Hours)**

Classification- structural elucidation of cholesterol, irradiated products of ergosterol. Conversion of cholesterol to androsterone, progesterone, testosterone, 5α- and 5 β-cholanic acid. Conversion of Oestrone to Oestriol, Oestrodiol and vice-versa. Conformational structure of cholestane and Coprostane. General study of Bile acids and Prostoglandins.

UNIT V - VITAMINS AND TERPENOIDS **(15 Hours)**

Vitamins: Structural elucidation, synthesis of vitamins – A_1, B_1 and C - synthesis of vitamins B_2, B_6, D and E.

Terpenoids: Structural elucidation, synthesis of α-Pinene, Camphor, α-Cadinene, Zingiberene and squalene - synthesis of α-Santonin and Gibberelic acid.

TEXT BOOKS

1. B. P. Mundy, M. G. Ellerd, & F. G. Favaloro. *Name Reactions and Reagents in Organic Synthesis,* Wiley-Interscience, 2005.
2. A. Hassner and I. Namboothiri, Organic Syntheses Based Name Reactions, Elsevier, 2012.
3. W. Carruthers, and I. Coldham, *Modern Methods of Organic Synthesis*, Fourth edition, CambridgeUniversity Press, 2015.
4. Dr Jagdamba Singh and Dr. L.D.S Yadav, *Orgnic Synthesis: Design, Reagents, Reactions and Rearrngements,* A Pragati Second Revised Edition, 2007.
5. E. J. Corey & X. M. Cheng, *The Logic of Chemical Synthesis*, Wiley-India, 2011.
6. S. Warren & P. Wyatt, *Organic Synthesis: The Disconnection Approach*, John Wiley & Sons, 2008.
7. Sanyal and Sanyal, *Reactions, Rearrangements and Reagents,* Fourth edition, Bharati Bhawan Publishers and Distributors, 2003.
8. N.R. Krishnaswamy, *Chemistry of Natural Products; A Unified Approach*, CRC Press; 2nd edition, 2010.
9. I.L. Finar, *Organic Chemistry*, Vol II, 5th edition, Pearson Education India, 2002.

REFERENCE BOOKS

1. L. Kurti & B. Czako, *Strategic Applications of Named Reactions in Organic Synthesis*, Elsevier 2005.
2. Jie Jack Li, *Name Reactions*, Fifth edition (Springer), 2014.

3. Thomas Laue and Andreas Plagens, *Named Organic Reactions*, John Wiley & Sons, 1999.
4. F. A. Carey and R.J. Sundberg, *Advanced Organic Chemistry, Part B: Reaction and Synthesis*, 5th edition, Springer, 2007.
5. R. O.C. Norman and J. M. Coxon, *Principles of Organic Synthesis,* 3rd edition, 1993.
6. P. Wyatt & S. Warren, *Organic Synthesis: Strategy and Contro*l, Wiley-Blackwell, 2007.
7. S. Warren, *Designing Organic Synthesis*, John Wiley & Sons, 1994.
8. D. Goldsmith, M. C. Pirrung and A. T. Morehead, *Total Synthesis of Natural Products,*John Wiley & Sons, 2007.
9. R. Xu, Y. Ye and W. Zhao, *Introduction to Natural Products Chemistry*, CRC Press, 2011.
10. D. Barton, K. Nakanishi and O. Meth-Cohn, *Comprehensive Natural Products Chemistry*, Elsevier 1999.
11. D. L. Nelson and M. M. Cox, Lehninger's *Principles of Biochemistry*, Seventh edition, WH Freeman, 2017.
12. J.M. Berg, J.L. Tymoczko and L. Stryer, *Biochemistry*, Fifth edition, W.H.Freeman and Co, 2002.

COURSE OUTCOMES (COs)

Upon completion of the course, the students will be able to

CO Nos	CO Statement	Cognitive Level
CO1	Illustrate the prescribed organic name reactions with their mechanisms and apply in organic synthesis.	K2, K3
CO2	Design organic synthetic steps employing disconnection approach in the synthesis of drugs, natural products etc.	K3, K6
CO3	Identify suitable reagent for important organic reactions and building appropriate bonds.	K3
CO4	Explain the structural elucidation of cholesterol and various synthetic approaches of steroids in Natural Products synthesis.	K2
CO5	Infer the structural elucidation and the synthesis of vitamins and terpenoids	K2

MAPPING OF COURSE OUTCOMES WITH POs AND PSOs

CO	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PSO1	PSO2	PSO3	PSO4	PSO5	PSO6	PSO7	PSO8	PSO9
CO1	M	S	S	M	L	L	S	S	S	S	M	S	S	N	M	S	S
CO2	S	S	S	S	L	L	S	S	S	S	S	S	S	N	S	S	S
CO3	M	S	S	S	L	L	S	S	S	S	M	S	S	N	M	S	S
CO4	M	S	M	M	L	L	S	S	S	M	L	M	M	N	L	M	S
CO5	M	S	M	M	L	L	S	S	S	M	L	M	M	N	L	M	S

CORE 21	BIOINORGANIC, SPECTRAL METHODS-II AND PHOTOCHEMISTRY	L	T	P	C
		5	0	0	4

Objectives:

- *To introduce bioinorganic chemistry and to study role of metalloporphrins and metalloenzymes in various biological processes.*
- *To study the applications of Mossbauer and nuclear quadrupole resonance spectroscopic techniques in inorganic systems.*
- *To study the applications of NMR and EPR techniques in inorganic systems.*
- *To introduce inorganic photochemistry and to study applications in various systems.*

UNIT I - BIOINORGANIC CHEMISTRY– I (15 Hours)

Biological function, toxicity and deficiency of trace elements (N, O, F, Na, Mg, P, S, K, Ca, Cr, Mn, Fe, Co, Cu, Zn, As, Mo, Cd, Hg, I, Pb); classification of metallo-biomolecules. Metalloporphyrins – chlorophyll and photosynthesis; cytochromes, hemoglobin, myoglobin and dioxygen binding, vitamin B_{12} and co-enzyme – *in vivo* and *in vitro* nitrogen fixation. Iron storage and transport: ferritin, transferrins and siderophores, iron proteins: hemerythrin, cytochrome P450 enzyme, ferredoxin and rubredoxin.

UNIT II - BIOINORGANIC CHEMISTRY– II (15Hours)

Copper proteins and Enzymes:peroxidases,catalases,oxygenases, plastocyanin, azurin, hemocyanin and ascorbic oxidase – different types of Cu present in proteins and enzymes. Zinc enzymes: carboxypeptidase A, carbonic anhydrase and superoxide dismutase. Inhibition and poisoning of enzymes illustrated by xanthine oxidase and aldehyde oxidase. Chelate therapy – metal complexes as drugs, anticancer and antiarthritic agents. Metal complexes as probes of nucleic acids.

UNIT III - MOSSBAUER SPECTROSCOPY (15 Hours)

Splitting of resonance lines: quadrupole splitting and magnetic hyperfine splitting. Applications: MB spectra of iron compounds/complexes – structural elucidation, π- bonding effect, determination of high spin and low spin, spin state crossover and cis–trans isomers – nature of the complexes – mixed valence complexes. Tin compounds: MB spectra of Sn(II) and Sn(IV) compounds, oxidation states of Sn in its different compounds. Applications in bioinorganic chemistry: oxy and deoxy- hemerythrin - catalase, peroxidases, Fe-S protein systems.

UNIT IV - NMR AND ESR SPECTROSCOPY (15 Hours)

NMR Spectroscopy: ^{1}H, ^{19}F and ^{31}P – NMR – applications in structural problems based on number of signals, multiplicity, anisotropy (like H_3PO_3, H_3PO_2, $[HNi(PPh_3)_4]^+$, SF_4, TiF_4, PF_5, HPF_2, H_2PF_3, $PF_3(NH_2)_2$, P_4S_3, $P_4N_4Cl_6(NHC_6H_5)_2$, $P_3N_3(CH_3)_2Cl_4$, NF_3, NH_3 – mer- and fac-$Rh(PPh_3)_3Cl_3$. B^{11} NMR of $B_3H_8^-$ and $B_{10}H_{14}$. Fluxional molecules (including organometallic compounds) and study of fluxionality by NMR technique - NMR of paramagnetic molecules - contact shifts. Evaluation of Rate constants - monitoring the course of reaction using NMR.

EPR spectroscopy: Hyperfine splitting - Factors affecting magnitude of g-values - Zero field splitting and Kramers' degeneracy - Application of EPR in the study of transition metal complexes based on number of signals, multiplicity, anisotropy (bis(salicylaldimine)copper(II), $[Cu(bpy)_3]^{2+}$, $[Cu(Phen)Cl_2]$, $[(NH_3)_5Co\text{-}O_2\text{-}Co(NH_3)_5]^{5+}$ $Co_3(CO)_9Se$, $Co_3(CO)_9Rh$, $[CoF_6]^{4-}$, $[CrF_6]^{3-}$, $VO(acac)_2$, $[VO(H_2O)_6]^{2+}$, $[Fe(CN)_5NO]^{2-}$. Applications in predicting the covalent character of M-L bond and Jahn-Teller distortion in Cu(II) complexes. EPR spectroscopy of metallobiomolecules: copper and iron proteins.

UNIT V - PHOTOCHEMISTRY OF METAL COMPLEXES (15 Hours)

Properties of excited states of metal complexes – types of excited states, Frank Condon and thermally equilibrated excited (THEXI) states – photophysical processes: bimolecular deactivation and energy transfer, photochemical processes: electron transfer reactions, isomerisation and substitutional processes – Photochemistry of Cr(III) and Co(III) complexes - Photophysical and photochemical properties of $[Ru(bpy)_3]^{2+}$ and $[Cr(bpy)_3]^{3+}$. Applications of inorganic photochemistry: photochemical conversion and storage of solar energy – photochemical conversion of N_2 to NH_3 – TiO_2 as a green photocatalyst in removing air and water pollutants.

TEXT BOOKS

1. James E. Huheey, Ellen A. Keiter and Richard L. Keiter, *Inorganic chemistry: principles Structure and Reactivity*, 4th Edition, Pearson Education, 2006.
2. P. Atkins, T. Overton, J. Rourke, M. Weller and F.Armstrong, *Inorganic Chemistry*, 5th edition, Oxford University press, 2010.
3. Russell S. Drago, *Physical Methods in Inorganic Chemistry*, Chapman and Hall, London, 1965.
4. Russell S. Drago, *Physical Methods for Chemists*, Surfside Scientific Publishers, 2nd Edition, 1977.

5. E.A.V. Ebsworth, David W.H. Rankin and Stephen Credock, *Structural Methods in Inorganic Chemistry*, ELBS, 1988.
6. I.Bertini, H.B.Gray, S.J.Lippard and J.S.Valantine, *Bioinorganic Chemistry*, Viva Books, 1998.
7. S.J. Lippard and J.M. Berg, *Principles of Bioinorganic Chemistry*, Panima Company, New Delhi, 1997.
8. K.K. Rohatgi – Mukherjee, *Fundamentals of Photochemistry*, Wiley, New York, 3rd Edition, 2002.
9. D.E. Fenton, *Bio-coordination Chemistry*, Oxford Science Publications, 1995.

REFERENCE BOOKS

1. F. Albert Cotton, Geoffrey Wilkinson, Carlos A. Marilo and Manfred Bochman, *Advanced Inorganic Chemistry*, Wiley Interscience Publication, 6th Edition, 2008.
2. David W. H. Rankin, Norbert W. Mitzel and Carole A. Morrison, *Structural Methods in Molecular Inorganic Chemist*ry, John Wiley & Sons, 1st Edition, 2013.
3. John A. Weil and James R. Bolton, *Electron Paramagnetic Resonance Elementary Theory and Practical Applications*, 2nd Edition, John Wiley & Sons, 2007.
4. E.I. Solomon and A.B.P. Lever, *Inorganic Electronic Structure and Spectroscopy*, Vol. 2 , Applications and case studies , Wiley – Interscience, 2006.
5. R.V. Parish, *NMR, NQR, EPR and MOSSBAUER Spectroscopy in Inorganic Chemistry*, Ellis Horwood Limited, 1990.
6. A.W. Adamson and P.D. Fleischauer, *Concepts of Inorganic Photochemistry*, John wiley and sons, New York, 1975.
7. K. Kalyanasundaram, *Photochemistry of polypyridine and phorphyrin complexes*, Academic Press, London, 1992.

COURSE OUTCOMES (COs)

On completion of the course, the students will be able to

CO Nos	CO Statement	Cognitive Level
CO1	Describe the role of metalloporphrins and metalloenzymes in various biological processes.	K2
CO2	Apply metal complexes as drugs and probes of nucleic acids	K3
CO3	Explain the applications of Mossbauer, NMR and EPR Spectroscopy in inorganic compounds and interpret the data.	K2, K3, K4
CO4	Explain the photophysical and photochemical properties of metal complexes	K2
CO5	Develop photochemical conversion, storage of solar energy and green photocatalyst.	K6

MAPPING OF COURSE OUTCOMES WITH POs AND PSOs

CO	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PSO1	PSO2	PSO3	PSO4	PSO5	PSO6	PSO7	PSO8	PSO9
CO1	M	S	M	M	L	L	S	S	S	M	S	M	L	N	L	M	S
CO2	S	S	S	S	L	L	S	S	S	S	S	M	M	N	M	S	S
CO3	M	S	S	S	L	L	S	S	S	S	M	M	M	N	S	S	S
CO4	M	S	M	M	L	L	S	S	S	M	M	L	L	N	L	S	S
CO5	S	S	S	M	L	L	S	S	S	S	S	M	S	N	L	S	S

CORE 22	CHEMICAL KINETICS, PHOTOCHEMISTRY AND SURFACE CHEMISTRY	L	T	P	C
		5	0	0	4

Objectives:

- *To educate the kinetic theory of gases.*
- *To explain various concepts of Phase rule.*
- *To elucidate the use of chemical kinetics in understanding reaction mechanisms and to apply the theories and concepts of it for homogenous and heterogeneous catalyzed reactions.*
- *To understand the photochemical organic reactions and radiation chemistry reactions.*
- *To understand the surface phenomena.*

UNIT I - KINETIC THEORY OF GASES AND PHASE RULE (15 Hours)

Equations of state - molecular speeds - distribution of molecular velocities - one, two and three dimensions (Maxwell distribution of molecular velocity) - Maxwell distribution as energy distribution - Maxwell Boltzmann distribution law - Principle of equipartition energy and quantization - calculation of vibrational heat capacity - transport properties - thermal conductivity in a gas - the molecular collisions and mean free path in a gas - viscosity - diffusion of gases - nonsteady state - Poiseuille formula.

Phase rule and Lever rule - Derivation of phase rule from the concept of chemical potential. Plots for a mixture of three liquids consisting of one, two and three pairs of partially miscible liquids. Salting out phenomenon - systems composed of two solids and a liquid.

UNIT II - CHEMICAL KINETICS –I (15 Hours)

Simple collision theory, absolute reaction rate theory, thermodynamics treatment, potential energy surfaces, application of ARRT to simple bimolecular processes - steady state approximation, principle of microscopic reversibility & detailed balancing - chain reactions - general characteristics, study of kinetics of chain reactions like decomposition of acetaldehyde and N_2O_4; study of H_2-O_2 explosive reactions. Reactions in solutions - Factors determining reaction rates in solution; primary and secondary salt effects - influence of ionic strength and dielectric constant on reactions involving (i) ions (ii) dipoles (iii) ion and dipole. Electrostriction; influence of hydrostatic pressure; volume of activation. Linear free energy relationship, Hammett and Taft equations.

UNIT III - CHEMICAL KINETICS – II **(15 Hours)**

Theory of unimolecular reactions - Lindemann, Hinshelwood, RRK, RRKM and Slater treatments. General catalytic mechanisms. Equilibrium and steady state treatments. Enzyme catalysis, Michalis-Menten kinetics, activation energies of enzyme-catalyzed reaction. Acid - base catalysis - protolytic and prototropic mechanisms. Acidity functions - Kinetic methods of analysis. Fast reaction techniques - Relaxation theory and relaxation techniques - Temperature, Pressure, electric field and magnetic field jump methods; Flash photolysis and pulse radiolysis, ultrasonic absorption techniques, reaction in a flow system, continuous and stopped flow, shock wave tube method.

UNIT IV - PHOTOCHEMISTRY AND RADIATION CHEMISTRY **(15 Hours)**

Physical properties of the electronically excited molecules - excited state dipole moments, excited state pKa, excited state redox potential. Fluorescence, phosphorescence and other deactivation process - Stern-Volmer equation and its applications. Photosensitisation and chemiluminescence. Experimental techniques in photochemistry - flash photolysis technique. Radiation chemistry - source of high energy - interaction of high energy radiation with matter, radiolysis of water - definition of G value. Primary and secondary process, linear energy transfer - the hydrated electron and its reactions.

UNIT V - SURFACE CHEMISTRY AND CATALYSIS **(15 Hours)**

Micelles - surface active agents, classification of surface active agents, micellization, hydrophobic interaction, critical micellar concentration (CMC), factors affecting the CMC of surfactants, counter ion binding to micelles, thermodynamics of micellization - reverse micelles. Chemisorption and Physisorption; Langmuir's adsorption isotherm; competitive adsorption - Mechanisms of reactions on surfaces (Langmuir, Rideal and Langmuir-Hinshelwood mechanisms) Activation energies - Non-ideal adsorption; multiplayer adsorption; capillary condensation; measurement of surface area, BET equation , Gibbs adsorption isotherm - electrokinetic phenomena - zeta potential - Catalysis and types of catalysis - Heterogeneous catalysis - reactions and their kinetics.

TEXT BOOKS

1. J. Rajaram and J.C. Kuriokose, *Kinetics and Mechanisms of chemical transformation*, 1st Edn., Macmillan India, Delhi, 1993.
2. C. Kalidas, *Chemical Kinetics methods*, New-Age International, 1996.
3. K.J. Laidler, C*hemicalKinetics*, 3rd edn., Harper and Row Publishers, New York, 1987.
4. A.A. Frost and R.G. Pearson, *Kinetics and Mechanism*, 2nd edn., John Wiley and sons

INC., 1963.

5. D.K. Chakrabarty and B. Viswanathan, *Heterogeneous Catalysis*, New Age Science, 2008.

REFERENCE BOOKS

1. Walter J. Moore, *Physical Chemistry*, 5th edition, Orient Longman, 1976.
2. G.W. Castellan, *Physical Chemistry*, 3rd edition, Addision-Weslay, 1986.
3. P. Atkins, *Physical Chemistry*, 7th edition, Oxford University Press, 2000.
4. K.B. Ytsiimiriski, *Kinetic Methods of Analysis*, Pergamom press, 1993.
5. W. Adamson and A.P. Gast, *Physical chemistry of surfaces*, 6th Edn.,Wiley, 1997.
6. J.J. Bikerman, *Surface Chemistry: Theory and Applications*, 2nd Edition, Academic Press, 2013.

COURSE OUTCOMES (COs)

Upon completion of the course, the students will be able to

CO Nos	CO Statement	Cognitive Level
CO1	Explain kinetic theory of gases and phase rule and its applications.	K2, K3
CO2	Describe the concepts of chemical kinetics and make use of it in understanding reaction mechanisms.	K2,K3, K4
CO3	Illustrate various photochemical processes and experimental techniques in photochemistry.	K2, K4
CO4	Explain the basic ideas of radiation chemistry and its applications.	K2, K3
CO5	Describe the concepts of Adsorption processes and catalysis.	K2

MAPPING OF COURSE OUTCOMES WITH POs AND PSOs

CO	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PSO1	PSO2	PSO3	PSO4	PSO5	PSO6	PSO7	PSO8	PSO9
CO1	M	S	M	M	L	L	S	S	S	M	L	L	M	N	M	S	S
CO2	M	S	M	M	L	L	S	S	S	M	L	L	M	N	M	S	S
CO3	M	S	M	M	L	L	S	S	S	M	M	L	M	N	L	S	S
CO4	M	S	M	M	L	L	S	S	S	M	M	L	M	N	L	M	S
CO5	M	S	M	M	L	L	S	S	S	S	M	M	S	N	M	S	S

CORE 23	SELECTED TOPICS IN CHEMISTRY	L	T	P	C
		4	0	0	4

Objectives:

- *To understand the concept of Computational chemistry.*
- *To learn principle of corrosion, corrosion inhibition and separation techniques.*
- *To study Chemical sensors, Biosensors and Contrasting agents in medical diagnosis.*

UNIT I - COMPUTATIONAL CHEMISTRY (12 Hours)

Introduction to computational chemistry - quantum mechanics - schrodinger equation. Types of calculations – single point energy, geometry optimization, frequency prediction - Brief introduction of computational methods - Ab initio method, semi-empirical method, Density Functional Theory method, Molecular mechanics. Basis Sets - minimal basis sets, split valence basis sets, polarized basis sets, Diffuse functions, High angular momentum basis sets.

UNIT II - CORROSION SCIENCE (12 Hours)

Principles of Corrosion – Definition – Types of Corrosion - Electro chemical principles of Corrosion – Corrosion monitoring methods - Coupon (weight loss) – electrical resistance – gasometric – Potentiodynamic polarisation – impedance – hydrogen permeation – Corrosion inhibition – definition – Classification of inhibitors based on electrode process – mechanism of inhibitor action in acidic medium

UNIT III - SEPARATION TECHNIQUES (12 Hours)

Solvent extraction - Methods of extraction and applications of solvent extraction, solid-phase extraction, micro extraction (SPME), solid-phase nano extraction (SPNE).

Chromatography - thin layer chromatography, ion exchange chromatography and size exclusion chromatography – HPLC-outline study of instrument modules. Gas chromatography – basic instrumental set up-carriers, columns and detectors.

UNIT IV - SENSORS (12 Hours)

Definitions for sensors and biosensors - Technical definitions: calibration, selectivity, sensitivity, reproducibility, detection limits, response time; Introduction to Transducers - primary and secondary types, Active and passive, Analog and Digital transducers.

Sensors based on sensing layer - Chemical sensor - semi-conductor gas sensors, solid electrolyte gas sensors, ion-selective electrode sensors, humidity sensors and field effect transistor sensors. Bio-sensors - Enzymes based, Affinity-based biosensors, Inhibition-based biosensors; Cell-based biosensors (Membrane receptors and transporters).

UNIT V - CONTRASTING AGENTS IN MEDICAL DIAGNOSIS (12 Hours)

MRI imaging: Principles of MRI - development of MRI contrasting agents - types of contrasting agents – Gadolinium based contrasting agents, Manganese based contrast agents - Advantages and disadvantages - Fe(III) and Fe(II) based contrast agents - merits and demerits. Routes of administration - Targeted and organ specific contrast agents.

Radio isotopic Imaging agents: principle, functions and requirements of radio isotopic imaging agents - types of nuclear imaging - PET, SPEC and CAT imaging - nuclear imaging agents – ^{18}F, ^{99m}Tc.

TEXT BOOKS

1. Frank Jensen, *Introduction to Computational Chemistry*, Third Edition, John Wiley & Sons, 2017.
2. Andrew R. Leach, *Molecular modelling: principles and applications*, Second Edition, Prentice-Hall, 2001.
3. Edward Mc Cafferty, *Introduction to Corrosion Science*, First Edition, Springer, 2010.
4. D. Kealey and P.J. Haines, *Instant Notes Analytical chemistry*, First Edition, BIOS, 2002.
5. R. Gopalan, P. S. Subramanian and K. Rengarajan, *Elements of Analytical Chemistry*, Sultan Chand and Sons, New Delhi, 2005.
6. S. M. Khopkar, *Basic concepts of analytical chemistry*, Third edition, New age international, 2008.
7. G.R. Chatwal and S.K. Anand, *Instrumental Method of Chemical Analysis*, Himalaya Publishing house, fifth (Reprint), 2016.
8. Jiri Janata, *Principle of Chemical Sensors*, First edition, Springer Science, 1989.
9. Editor-Maartin Braddock, *Biomedical Imaging: The Chemistry of Labels, Probes and Contrast Agents*, Royal Society of Chemistry, 2012.

REFERENCE BOOKS

1. Christopher J. Cramer, *Essentials of Computational Chemistry: Theories and Models*, Second Edition, John Wiley & Sons, 2004.
2. James B. Foresman, *Exploring Chemistry with Electronic Structure Methods*, Second Edition, Gaussian Inc, 1996.
3. R Winston Revie and Herbert Henry Uhlig, *Corrosion and its Control*, Fourth Edition, John Wiley & Sons, 2018.

4. Douglas A. Skoog, Donald M. West, F. James Holler, Stanley R. Crouch, *Fundamentals of Analytical Chemistry*, Ninth edition, Brooks/Cole, 2013.
5. Brian R. Eggins, *Chemical Sensors and Biosensors*, First Edition, John Wiley & Sons, 2002.
6. Peter Grundler, *Chemical Sensors*, Springer, 2007.
7. Florinel-Gabriel Banica, *Chemical Sensors and Biosensors-Fundamentals and applications*, First Edition, John-Wiley &Sons, 2012.
8. Ursula E. Spichiger-Keller, *Chemical Sensors and Biosensors for Medical and Biological Applications*, Wiley-VCH, 1998.
9. Richard C. Dorf, *Sensors, Nanoscience, Biomedical Engineering, and Instruments: Sensors Nanoscience Biomedical Engineering*, CRC Press, 2006.
10. M.J. Usher and D.A. Keating, *Sensors and Transducers*, Second Edition, Macmillan Press, 1996.
11. Editors-Andre Merbach, Lother Helm and Eva Toth, *The chemistry of Contrasting Agents in Medical Magnetic Resonance Imaging,* Second Edition, John Wiley and Sons, 2013.
12. Editors-Valerie C. Pierre and Matthew J. Allen, *Contrast Agents for MRI*, Royal Society of Chemistry, 2018.

COURSE OUTCOMES (COs)

Upon completion of the course, the students will be able to

CO Nos	**CO Statement**	**Cognitive Level**
CO1	Describe the importance and applications of Computational Chemistry methods.	K2, K3
CO2	Be competent in separation and purification techniques.	K3, K4
CO3	Explain the corrosion monitoring methods and application of corrosion inhibitors.	K2, K3
CO4	Develop various types of sensors.	K3, K6
CO5	Choose contrasting agents in medical diagnosis.	K3, K6

MAPPING OF COURSE OUTCOMES WITH POs AND PSOs

CO	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PSO1	PSO2	PSO3	PSO4	PSO5	PSO6	PSO7	PSO8	PSO9
CO1	M	S	S	S	S	L	S	S	S	S	S	M	S	N	S	S	S
CO2	M	S	S	S	S	L	S	S	S	S	S	M	S	N	L	S	S
CO3	M	S	S	S	S	L	S	S	S	S	S	S	S	N	L	S	S
CO4	S	S	S	S	S	L	S	S	S	S	S	S	S	N	S	S	S
CO5	S	S	S	S	S	L	S	S	S	S	S	S	S	N	S	S	S

CORE 24	COMPUTATIONAL SOFTWARE IN CHEMISTRY - LABORATORY COURSE	L	T	P	C
		0	0	4	2

Objectives:

- *To impart skills on use of various chemistry tools that are essential for any student with chemistry as a major course.*
- *To learn the techniques of molecular simulations which will enhance the students' employability in academia and industry.*

UNIT I - BASICS

Basic idea of Molecular Modelling – A brief introduction about computational methods and their applications in chemistry – Basic terminologies used in computational methods (relevant to the exercises given in UNIT II). Computing software - introduction and stepwise approach to Chemdraw, ACD/Chemsketch, Argus Lab, AVOGADRO, Molinspiration, preADMET, SwissADME, SwissDock, 1 – Click online server, Autodock, and Crystal Explorer.

Lectures include entire process of downloading and installation of the software.

UNIT II - HANDS ON EXERCISES

The experiments are related to the topics covered in B.Sc - M.Sc Chemistry courses. The students must do the following exercises depending on the availability of time and suitable computational chemistry software.

A. Drawing the structures of organic molecules and reaction schemes using **Chemdraw** or **ACD/Chemsketch**.

B. For the following experiments, **Argus Lab** or **ACD/Chemsketch** or **Avogadro Molecular Editor** or **Gaussian software** can be used. Minimum of six experiments is required to be carried out in this section.

1. Geometry optimization and single point energy calculations of simple organic molecules.
2. Calculation of energy gap between HOMO and LUMO in simple molecules and visualization of molecular orbitals.
3. Calculation of dipole moment in polar organic molecules.
4. Calculation of electrostatic charges of atoms in organic molecules using population analysis.
5. Calculation of Resonance energy of aromatic compounds.

6. Prediction of the stability of *ortho*, *meta*, *para* products of nitration of aromatic ring using computational chemistry calculations.
7. Calculation of IR stretching frequencies of groups and visualization of normal modes of vibration in organic molecules.
8. Calculation of dimerization energy of carboxylic acids.
9. Perform the conformational analysis of butane using potential energy scan.
10. Find the transition state of simple organic reactions and plot the reaction profile.
11. Determination of heat of hydration of organic molecules.
12. Find the Gibbs free energy of simple gaseous phase reactions and calculate equilibrium constant.
13. Spectral analysis (UV, IR and NMR) of simple organic molecules.
14. Calculation of pKa of simple organic molecules and compare it with experimental values.
15. Calculation of electrophilicity index in hard-soft acids and bases.

C. Prediction of molecular properties, bioactivity and molecular docking of drug molecules.

1. Calculation of molecular properties and bioactivity of the simple drug molecules like aspirin, paracetamol, and the drugs of your choices using the online server **molinspiration.**

2. Prediction of drug likeliness, ADME and Toxicity of the drug classes like antibiotics, antihistamines, anesthetics and drug molecules of your choice using online servers **preADMET** or **SwissADME** or **SwissDock.**

3. Perform molecular docking of your choice using **1-click docking online server tool** at mcule.com. Website: https://mcule.com/. First register at the site and perform molecular docking. Similarly, Autodock tools or Autodock Vina or Argus Lab can be used for molecular docking.

D. Learn to generate Hirshfeld surfaces, study the interaction energies and draw the electrostatic potential map using **Crystal Explorer** Software.

LINKS TO DOWNLOAD SOFTWARE

ACD/Chemsketch : https://www.acdlabs.com/resources/freeware/chemsketch/index.php

Molinspiration : https://www.molinspiration.com/

PreADMET : https://preadmet.bmdrc.kr/

SwissADME : http://www.swissadme.ch/index.php

Crystal Explorer: https://crystalexplorer.scb.uwa.edu.au/

1-click docking online server: https://mcule.com/

Autodock Tools Link: http://mgltools.scripps.edu/downloads

Autodock Vina Link: http://vina.scripps.edu/

Discovery Studio Visualizer: https://www.3dsbiovia.com/products/co..

Avogadro Molecular Editor : https://avogadro.cc/

ArgusLab : http://www.arguslab.com/arguslab.com/ArgusLab.html

REFERENCE BOOKS

1. Jan H. Jensen, *Molecular Modelling Basics*, CRC Press, 2010.
2. Waren J. Hehre, Alan J. Shusterman and Janet E. Nelson, *The molecular modelling workbook for organic chemistry*, Wavefunction Inc., 1998.
3. James B. Foresman and Eleen Frisch, *Exploring Chemistry with Electronic Structure Methods*, Gaussian Inc., Second Edition, 1996.
4. James B. Foresman and Eleen Frisch, *Exploring Chemistry with Electronic Structure Methods*, Gaussian Inc., Third Edition, 2015.
5. Donald W. Rogers, H*eats of Hydrogenation: Experimental and Computational Hydrogen Thermochemistry of Organic compounds*, World scientific Publishing Co, 2006.

COURSE OUTCOMES (COs)

On completion of the course, the students will be able to

CO Nos	CO Statement	Cognitive Level
CO1	Use chemical software for drawing chemical structures, reaction schemes and generation of their names.	K3
CO2	Perform molecular docking in structural molecular biology and computer assisted drug design which enhance their employability in academia and industry.	K4, K6
CO3	Calculate the single point energy, energy gap, dipole moment, resonance energy, equilibrium constant, electrophilicity index, dimerisation energy etc.	K5
CO4	Interpret spectral data (UV, IR, NMR spectrum)	K4
CO5	Investigate intermolecular interactions and packing in crystalline materials using Hirshfeld surface analysis.	K4, K5

MAPPING OF COURSE OUTCOMES WITH POs AND PSOs

CO	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PSO1	PSO2	PSO3	PSO4	PSO5	PSO6	PSO7	PSO8	PSO9
CO1	M	S	S	S	S	S	S	S	S	S	S	M	S	N	S	S	S
CO2	M	S	S	S	S	S	S	S	S	S	S	S	S	N	S	S	S
CO3	M	S	S	S	S	S	S	S	S	S	S	M	S	N	S	S	S
CO4	M	S	S	S	S	S	S	S	S	S	S	M	S	N	S	S	S
CO5	M	S	S	S	S	S	S	S	S	S	S	M	S	N	S	S	S

CORE 25	PROJECT	L	T	P	C
		0	0	7+5*	6

Objectives:

- *This course is designed to reinforce the concepts with analytical techniques.*
- *It provides a platform for students to have a hands-on experience with instruments and present a project report on a research topic.*

Students will do the project work on a title approved by the respective project supervisor. Students will maintain daily records and present oral reports while doing the project. All the above process will be duly assessed by the project supervisor. They will submit the project report at the end of the semester.

COURSE OUTCOMES (COs)

After completing the course, the students will be able to

CO Nos	CO Statement	Cognitive Level
CO1	Identify research problem, carry out literature survey and use of different experimental/spectroscopic techniques.	K1, K2, K3, K4
CO2	Develop interdisciplinary solutions to a variety of chemical problems.	K3
CO3	Communicate research findings efficiently in written (report) and verbal (viva-voce) forms.	K4, K5, K6
CO4	Use terminology appropriate to the field of study correctly and contextually.	K3
CO5	Motivate themselves and acquire basic knowledge for carrying out research work.	K6, K2

MAPPING OF COURSE OUTCOMES WITH POs AND PSOs

CO	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PSO1	PSO2	PSO3	PSO4	PSO5	PSO6	PSO7	PSO8	PSO9
CO1	S	S	S	S	M	M	S	S	S	S	S	S	S	S	S	S	S
CO2	S	S	S	S	S	L	S	S	S	S	S	S	S	N	S	S	S
CO3	M	S	S	M	M	S	S	S	S	S	S	S	S	S	S	S	S
CO4	M	S	M	M	L	L	S	S	S	S	S	S	S	S	S	S	S
CO5	S	S	M	S	M	L	S	S	S	S	S	S	S	S	S	S	S