Appendix

DEPARTMENT OF APPLIED CHEMISTRY

Scheme of Examination and Syllabus for the

Five Year Integrated M.Sc. Chemistry Approved by the Combined Board of Studies in Physical and Mathematical Sciences and

Chemical and Biological Sciences on 27-11-2025

(2023 admission)

PSO

PSO 1: Systematic and coherent awareness in fundamentals and its applications in problem solving, and analytical and critical rationalizations.

PSO 2: A firm grip on the basic principles of experimental/instrumental methods of analysis, and to execute them suitably for an in-depth analysis of chemical problems.

PSO 3: Skills to design and perform scientific experiments and to accurately record and analyze the experimental results.

PSO 4: Overall core competency in the subject and acquire skills for employment in academia and industry.

PSO 5: Knowledge relevant to the needs of present day society in regional, national and international development.

PSO 6: Professional skills to undertake chemical research in any societally relevant areas by inculcating the spirit of teamwork, innovation and entrepreneurship.

SEMESTER: 1

Semester Credit: 22 (Core: 19; Elective: 3) Cumulative Credit: 22

Course Code	Course Name	Course Type	Credits	L-T-P	CE	ESE	Total Marks
ENG10101	English - I	Core (AEC 1)	2	2-0-0	50	50	100
	Language						
MAL10101 HIN10101 GER10101	Malayalam - I Hindi - I German-I	Core (AEC 2)	2	2-0-0	50	50	100
CHE10101	General Chemistry I	Core* (MDC)	3	3-1-0	50	50	100
CHE10102	Quantitative Analysis Lab	Core*	2	0-0-4	100	-	100
CHE10103	Chemistry in Everyday Life	Core	2	2-1-0	50	50	100
MAT10101	Calculus I	Interdepartmental Core	3	3-1-0	50	50	100
PHY10101	General Physics I	Interdepartmental Core	3	3-1-0	50	50	100
PHY10102	Physics Lab I (Mechanics)	Interdepartmental Core	2	0-0-4	100	-	100
BIO10103	General Biology	MDC**	3	3-1-0	50	50	100
CSP10101	Computer Science I	MDC**	3	3-1-0	50	50	100
MAT10103	Mathematical Methods I	MDC**	3	3-1-0	50	50	100
STAT10101	Statistical Methods for Data	MDC**	3	3-1-0	50	50	100

AEC – Ability enhancement Course; MDC – Multidisciplinary Course; VAC – Value Added Course; SEC – Skill Enhancement Course

- Student shall select any one language- Malayalam/Hindi/German
- Will also be offered as an interdepartmental core/MDC
- ** Student shall select any one MDC

Total Credits in Major (Chemistry) -7

SEMESTER: 2

Semester Credit: 22 (Core: 19; Elective: 3) Cumulative Credit: 44

Course Code	Course Name	Course Type	Credits	L-T-P	CE	ESE	Total Marks
ENG10201	English - II	Core (AEC 3)	2	2-0-0	50	50	100
	Language						
MAL10201 HIN10201 GER10201	Malayalam - II Hindi – II German-II	Core (AEC 4)	2	2-0-0	50	50	100
CHE10201	General Chemistry II	Core* (MDC)	3	3-1-0	50	50	100
CHE10202	Inorganic Qualitative Analysis Lab	Core*	2	0-0-4	100	-	100
CHE10203	Industrial applications of petrochemicals and petroleum products	Core	2	2-1-0	50	50	100
MAT10201	Calculus II	Interdepartmental Core	3	3-1-0	50	50	100
PHY10201	General Physics II	Interdepartmental Core	3	3-1-0	50	50	100
PHY10202	Physics Lab II (Waves and Optics)	Interdepartmental Core	2	0-0-4	100	-	100
BIO10203	Biophysical Chemistry	MDC**	3	3-1-0	50	50	100
CSP10201	Computer Science II	MDC**	3	3-1-0	50	50	100
MAT10203	Mathematical Methods II	MDC**	3	3-1-0	50	50	100
STA10201	Probability and Distribution	MDC**	3	3-1-0	50	50	100

SEMESTER: 3

Semester Credit: 22 (Core: 19; Elective: 3) Cumulative Credit: 66

Course Code	Course Name	Course Type	Credits	L-T-P	CE	ESE	Total Marks
CHE10301	General Chemistry III	Core* (MDC)	3	3-1-0	50	50	100
CHE10302	Organic Qualitative Analysis Lab	Core*	2	0-0-4	100	-	100
CHE10303	Chemical Kinetics and Surface Chemistry	Core	2	2-1-0	50	50	100
PHY10301	General Physics III	Interdepartmental Core	3	3-1-0	50	50	100
PHY10302	Physics Lab III (Electricity and Magnetism)	Interdepartmental Core	2	0-0-4	100	-	100
MAT10301	Calculus III	Interdepartmental Core	3	3-1-0	50	50	100
YYY10301	Environmental Science	Interdepartmental Core (VAC I)	4	4-1-0	50	50	100
BIO10303	Human Disease and Health Care	MDC**	3	3-1-0	50	50	100
CSP10301	Computer Science III	MDC**	3	3-1-0	50	50	100
MAT10303	Matrix Theory and Graph Theory	MDC**	3	3-1-0	50	50	100
STA10301	Statistical Inference	MDC**	3	3-1-0	50	50	100

SEMESTER: 4

Semester Credit: 23 (Core: 20; Elective: 3) Cumulative Credit: 89

Course Code	Course Name	Course Type	Credits	L-T-P	CE	ESE	Total Marks
23-808-0401	Inorganic Chemistry I (Inorganic Main Group and Nuclear Chemistry)	Core	4	4-1-0	50	50	100
23-808-0402	Organic Chemistry I	Core	4	4-1-0	50	50	100
23-808-0403	Physical Chemistry I (Equilibrium Thermodynamics)	Core	4	4-1-0	50	50	100
23-808-0404	Theoretical Chemistry I (Introductory Quantum Mechanics)	Core	4	4-1-0	50	50	100
23-808-0405	Inorganic Chemistry Lab I	Core	2	0-0-4	100	-	100
23-808-0406	Physical Chemistry Lab I	Core	2	0-0-4	100	-	100
23-808-0407	Skill Enhancement Course# (SEC I)	Elective	3	0-0-3	100	-	100

Student shall select the course from a bouquet of courses offered by various departments

Total Credits in Major (Chemistry) -41

SEMESTER: 5

Semester Credit: 23 (Core: 16; Elective: 7) Cumulative Credit: 112

Course Code	Course Name	Course Type	Credits	L-T-P	CE	ESE	Total Marks
23-808-0501	Inorganic Chemistry II (Coordination & Bioinorganic Chemistry and Polyhedral Boranes)	Core	4	4-1-0	50	50	100
23-808-0502	Organic Chemistry II (Reaction Mechanism, Rearrangements and Spectroscopic Techniques in Organic Chemistry)	Core	4	4-1-0	50	50	100
23-808-0503	Physical Chemistry II (Electrochemistry and Solid State Chemistry)	Core	4	4-1-0	50	50	100
23-808-0504	Organic Chemistry Lab I	Core	2	0-0-4	100	-	100
23-808-0505	Inorganic Chemistry Lab II	Core	2	0-0-4	100	-	100
23-808-0506	Elective	Elective	4	4-1-0	50	50	100
23-808-0507	Skill Enhancement Course# (SEC II)	Elective	3	2-0-2	100	-	100

Student shall select the course from a bouquet of courses offered by various departments

Total Credits in Major (Chemistry) - 57

SEMESTER: 6 *Semester Credit: 23 (Core: 16; Elective: 7) Cumulative Credit: 135*							
Course Code	Course Name	Course Type	Credits	L-T-P	CE	ESE	Total Marks
23-808-0601	Inorganic Chemistry III (Group Theory and Concepts in Inorganic Chemistry)	Core	4	4-1-0	50	50	100
23-808-0602	Organic Chemistry III (Organic Chemistry Reactions, Reagents, Photochemistry & Pericyclic Reactions)	Core	4	4-1-0	50	50	100
23-808-0603	Physical Chemistry III (Chemical Kinetics and Statistical Thermodynamics)	Core	4	4-1-0	50	50	100
23-808-0604	Organic Chemistry Lab II	Core	2	0-0-4	100	-	100
23-808-0605	Physical Chemistry Lab II	Core	2	0-0-4	100	-	100
23-808-0606	Advanced Photochemistry and Photophysics	Elective	4	3-1-0	50	50	100
23-808-060X	Skill Enhancement Course# (SEC III)/Minor Project	Elective	3	2-0-2	100	-	100

Exit with BSc Chemistry – Total Credit required - 135

Total Credits in Major (Chemistry) – 73 (54%)

SEMESTER: 7

Semester Credit: 22 (Core: 18; Elective: 4) Cumulative Credit: 157

Course Code	Course Name	Course Type	Credits	L-T-P	CE	ESE	Total Marks
23-808-0701	Inorganic Chemistry IV (Reaction Mechanism and Organometallic Chemistry)	Core	4	4-1-0	50	50	100
23-808-0702	Organic Chemistry IV (Natural Products, Dyes and Pigments)	Core	4	4-1-0	50	50	100
23-808-0703	Theoretical Chemistry II (Approximations and Chemical Bonding)	Core	4	4-1-0	50	50	100
23-808-0704	Spectroscopy	Core	4	4-1-0	50	50	100
23-808-0705	Industrial Chemistry Lab	Core	2	0-0-4	100	-	100
23-808-0706	Professional and Career Development in Chemistry	Audit	0	2-0-0	-	-	-
23-808-070x	Elective	Elective	4	4-1-0	50	50	100

Total Credits in Major (Chemistry) -91

BSc Honors with Research

SEMESTER: 8 *Semester Credit: 20 (Core: 16; Elective: 4) Cumulative Credit: 177*							
Course Code	Course Name	Course Type	Credits	L-T-P	CE	ESE	Total Marks
23-808-0801	Elective	Elective (Online MOOC Course-SWAYAM, NPTEL, CUSAT)	4	4-1-0	50	50	100
23-808-0802	Project	Core	16	-	-	300	300

Total Credits in Major (Chemistry) -107 (60%)

Exit with BSc Chemistry Honours (Research) – Total Credit required - 177

BSc Honors

SEMESTER: 8							
			Semester Credit: 20 (Core: 16; Elective: 4) Cumulative Credit: 177				
Course Code	Course Name	Course Type	Credits	L-T-P	CE	ESE	Total Marks
23-808-0801	Advanced Analytical and Instrumentation Techniques I	Core	4	4-1-0	50	50	100
23-808-0802	Advanced Physical Chemistry	Core	4	4-1-0	50	50	100
23-808-0803	Advanced Organic Chemistry I	Core	4	4-1-0	50	50	100
23-808-0804	Computational Chemistry Lab	Core	2	0-0-4	100	-	100
23-808-0805	Open ended Lab	Core	2	0-0-4	100	-	100
23-808-0806	Elective	Elective	4	4-1-0	50	50	100

Total Credits in Major (Chemistry) – 107 (60%)

Exit with BSc Chemistry Honours – Total Credit required - 177

SEMESTER: 9

Semester Credit: 20 (Core: 16; Elective: 4) Cumulative Credit: 177

Course Code	Course Name	Course Type	Credits	L-T-P	CE	ESE	Total Marks
23-808-0901	Advanced Analytical and Instrumentation Techniques II	Core	4	4-1-0	50	50	100
23-808-0902	Instrumentation Lab	Core	4	0-0-8	100	-	100
23-808-0903	Mini Project	Core	4	0-0-8	-	100	100
23-808-0904	New Methods and Strategies in Organic Synthesis and Dynamic Stereochemistry	Elective	4	4-1-0	50	50	100
23-808-0905	Advanced Organic Chemistry II	Elective	4	4-1-0	50	50	100

Total Credits in Major (Chemistry) - 125

SEMESTER: 10							
			Semester Credit: 18 (Core: 18; Elective: 0) Cumulative Credit: 215				
Course Code	Course Name	Course Type	Credits	L-T-P	CE	ESE	Total Marks
23-808-1001	Project Dissertation and Viva Voce	Core	16	-	-	300	300
23-808-1002	Course Viva	Core	2	-	-	-	-

Total Credits in Major (Chemistry) – 141 (65%)

Total Credits Required for Integrated M. Sc. in Chemistry - 215

LIST OF ELECTIVE COURSES

Course Code	Course Name	Course Type	Credits	L-T-P	CE	ESE	Total Marks
23-808-0506	Introduction to Photochemistry and Photophysics	Elective	4	4-1-0	50	50	100
23-808-0606	Advanced Photochemistry and Photophysics	Elective	4	3-1-0	50	50	100
23-808-0707	Supramolecular Chemistry and Materials	Elective	4	4-1-0	50	50	100
23-808-0806	Materials Chemistry	Elective	4	4-1-0	50	50	100
23-808-0904	New Methods and Strategies in Organic Synthesis and Dynamic Stereochemistry	Elective	4	4-1-0	50	50	100
23-808-0905	Advanced Organic Chemistry II	Elective	4	4-1-0	50	50	100

LIST OF SKILL ENHANCEMENT COURSES

Course Code	Course Name	Course Type	Credits	L-T-P	CE	ESE	Total Marks
23-808-0407	Science Communications	Elective	3	2-0-1	100	-	100
23-808-0507	Industrial Chemistry	Elective	3	2-0-2	100	-	100
23-808-0607	Visualization and Computing	Elective	3	2-0-2	100	-	100
23-808-0608	Spectroanalytical Chemistry	Elective	3	2-0-2	100	-	100

CHE10101

GENERAL CHEMISTRY I

Credit 3 **54 hours**

Course Outcome After the completion of the course, the student will be able to	**Cognitive Level**
C.O. 1: Appreciate the evolution of quantum mechanics and correlate the concepts to modern atomic structure	Apply
C.O. 2: Analyze the structure and bonding in simple molecules by applying the concepts of MOT	Analyze
C.O. 3: Understand the different chemical bonding in organic molecules and reactive intermediates	Understand
C.O. 4: Perform a statistical analysis of experimental data	Analyze

Course Outcome	Program Specific Outcome					
	P.S.O. 1	P.S.O. 2	P.S.O. 3	P.S.O. 4	P.S.O. 5	P.S.O. 6
C.O. 1	3	3	0	3	3	1
C.O. 2	3	2	0	2	1	1
C.O. 3	3	2	1	2	1	1
C.O. 4	3	3	2	3	3	1

UNIT I	**10 hrs**
Atomic structure I - Blackbody emission and temperature, Photoelectric effect, Double slit experiment, Line spectrum of elements, Rutherford's experiment, Bohr's atomic model, Failure of Classical mechanics, Evolution of quantum mechanics - Heisenberg's uncertainty principle and its significance, wave particle duality, de Broglie equation.	
UNIT II	**10 hrs**
Atomic Structure -II - Quantum atomic model, hydrogen atomic orbitals and quantum numbers, atomic orbital equations (no derivation required), Sign of wave functions. Radial and angular wave functions. Radial and angular distribution curves. Shapes of s, p, d and f orbitals. Contour boundary and probability diagrams.	
UNIT III	**12 hrs**
Ionic bond: General characteristics, types of ions, size effects, radius ratio rule and its limitations. Packing of ions in crystals. Born-Lande equation with derivation and importance of Kapustinskii expression for lattice energy. Madelung constant, Solvation energy, Covalent bond, Valence Bond theory, Resonance and resonance energy, Molecular orbital theory. bonding, non- bonding, antibonding molecular orbitals (concept only) elementary pictorial approach of homo- and hetero-diatomic molecules H_2, B_2, C_2, O_2, N_2, CO, NO and CO_2, H_2O etc.	

UNIT IV	**10 hrs**
Localized and delocalized chemical bonding, the concept of aromaticity, writing proper Lewis structures, hybridization, reactive intermediates (carbynes, carbenes, carbocation, carbanion, radicals, arynes, nitrenes), Introduction to stereoisomerism. “Symbolism” in Organic Chemistry.	
UNIT V	**12 hrs**
Titrimetric analysis and calculations: Different types of titrations - neutralization, redox (permanganometry, dichrometry, iodometry, iodimetry), complexometric (EDTA titrations) and precipitation titrations – Principle of all types of titrations, titration curves, indicators. Significant figures, Accuracy, Precision, Error, Types of errors- Determinate and Indeterminate errors, Distribution of random errors, Mathematical Expression for error- Absolute and Relative error, Methods to reduce error, Statistical tools for expressing precision- Standard deviation, Relative standard deviation, Variance, Comparison of results- Students t test, f test, Criteria for rejecting a value-Q test, Confidence interval.	

Recommended Text Books:

1. Shriver, D. F., Atkins, P. W. and Langford, C. H. Inorganic Chemistry, 4th Ed., W.H. Freeman & Company, 2006.
2. Housecroft, C. and Sharpe, G., Inorganic Chemistry, 4th Edn., Pearson, 2012.
3. Atkins, P.W. and Paula, J. Physical Chemistry, 8th Edn., Oxford Press, 2006
4. Lee, J.D. Concise Inorganic Chemistry, 5th Edn., John Wiley & Sons, 1999.
5. Douglas, B.E. and Mc Daniel, D.H., Concepts & Models of Inorganic Chemistry, 3rd Ed., Oxford, 1994.
6. Day, M.C. and Selbin,J. Theoretical Inorganic Chemistry, 2nd Edn., ACS Publications, 2002.
7. McMurry, J. Organic Chemistry, 5th Edn., Brooks/Cole, 2000.
8. Carroll, F.A. Perspectives on Structure and Mechanism in Organic Chemistry, 2nd Edn., Wiley, 2010.
9. March, J., Smith, D., March's Advanced Organic Chemistry: Reactions, Mechanisms and Structure, 7th Edn., Wiley, 2013.
10. Skoog, West, Holler, Crouch, Fundamentals of Analytical Chemistry, Wiley, 9th Edn.
11. Fifield, F. W., Kealey, D., Principles and Practice of Analytical Chemistry, Academic Press, 5th Edn.
12. Robinson, J. W., Skelly Frame, E. M., Frame, G. M., II, Undergraduate Instrumental Analysis, Prentice Hall, 2009.
13. Vogel’s Textbook of Quantitative Chemical Analysis, 6th Edn, ELBS, 1998.

CHE10102

QUANTITATIVE ANALYSIS LAB

Credit 2 **36 hours**

Course Outcome After the completion of the course, the student will be able to	**Cognitive Level**
C.O. 1: Understand basic concepts of quantitative volumetric analysis	Understand
C.O. 2: Estimate the amount of a given substance by acidimetry, alkalimetry and permanganometry	Apply

Course Outcome	Program Specific Outcome					
	P.S.O. 1	P.S.O. 2	P.S.O. 3	P.S.O. 4	P.S.O. 5	P.S.O. 6
C.O. 1			3	3		
C.O. 2			3	3		

1.	**Acidimetry and Alkalimetry:** Strong acid -Strong base, Strong acid-weak base, Weak acid-Strong base, Estimation of hardness of water.
2.	**Redox Titrations:** Permanganometry- Estimation of oxalic acid, ferrous ion, MnO_2 in pyrolusite

Recommended Text Books:

1. Vogel's Textbook of Quantitative Chemical Analysis, 6th Ed., Pearsons Education Ltd.

CHE10103

CHEMISTRY IN EVERYDAY LIFE

Credit 2 **36 hours**

Course Outcome After the completion of the course, the student will be able to	**Cognitive Level**
C.O. 1: Understand the importance and the role of chemistry in everyday life	Understand
C.O. 2: Learn about chemicals that lay the foundation for life	Understand
C.O. 3: Understand the type of chemicals used in house hold activities, cosmetics and medicine	Apply
C.O. 4: Apply knowledge of chemistry to improve the quality of life	Apply

Course Outcome	Program Specific Outcome					
	P.S.O. 1	P.S.O. 2	P.S.O. 3	P.S.O. 4	P.S.O. 5	P.S.O. 6
C.O. 1	3	0	0	2	3	2
C.O. 2	3	0	0	2	3	2
C.O. 3	3	0	0	2	3	2
C.O. 4	3	0	0	2	3	2

UNIT I **6 hrs**
Molecules of Life - Cellular and chemical foundations of life, water unique properties, Carbohydrates and their sources, monosaccharides and disaccharides, examples, Lipids, Amino acids, Nucleic acids, Vitamins, Nutrients, Enzymes, Hemoglobin, structure and function, effect of CO, chlorophyll.
UNIT II **8 hrs**
Chemistry for food: chemicals used in kitchen, Butter and edible oils, composition, importance, properties, saturated and unsaturated fatty acids, hydrogenated oils, milk and dairy products, chemistry of cooking, chemical and physical changes during cooking, microwave cooking, nutrients and their stability during cooking, food preservation, colouring and flavouring agents, Beverages, food adulteration, food poisoning.
UNIT III **6 hrs**
Chemistry for cleaning: Soaps, chemical composition, preparation, cleaning action, synthetic detergents, bleaching, other household cleaning agents, toothpaste, mouthwash, sanitizers, shaving cream, shampoo, disinfectants and antiseptics.
UNIT IV **8 hrs**
Chemistry for cosmetics: Basic concepts-composition and classification, Skin chemistry, deodorants, antiperspirants, perfumes fragrances, effect of sunlight on skin, vitamin D, skin burns, sun screens, skin and hair care products, talcum powder, lipstick, moisturizers, colouring and bleaching agents, cosmetic formulations, baby care products.

UNIT V	**8 hrs**
Chemistry for medicines: Contribution of chemistry to human health and historical developments in medicine, Classification and nomenclature, Structure and function of: Analgesics – aspirin, paracetamol, Anthelmintic drug: mebendazole, Antiallergic drug: Chlorpheniramine maleate, Antibiotics: Penicillin V, Chloromycetin, Streptomycin. Sulfa drugs, Anti-inflammatory agent: Oxypheno-butazone, Antimalarials: Primazuine phosphate & Chloroquine, tranquilizer, antidepressants, antihistamines, drugs for chemotherapy, Generic and brand names.	

Recommended Text Books:

1. Chemistry in Daily Life by KIRPAL SINGH, PHI Learning Pvt Ltd.
2. Chemistry Connection, The Chemical Basis of Every day Phenomena, Karukstis, Kerry K. and Van Hecke, Gerald R, Harcourt/Academic Press (2003).
3. Chemistry in the Marketplace (5th ed.) Harcourt Brace (1998).
4. Introduction to Industrial Chemistry, B. K. Sharma: Goel Publishing, Meerut (1998).
5. Medicinal Chemistry by Asthoush Kar.
6. Drugs and Pharmaceutical Sciences Series, Marcel Dekker, Vol.II, INC, New York.
7. Foods – Facts and Principles. N. Shakuntala Many and S. Swamy, 4th ed. New Age International (1998).

CHE10201

GENERAL CHEMISTRY II

Credit 3 **54 hours**

Course Outcome After the completion of the course, the student will be able to	**Cognitive Level**
C.O. 1: Correlate the physical and chemical properties of elements based on their periodic classification	Understand
C.O. 2: Understand the basic concepts of acid-base theory and compare the strength of various acids and bases	Apply
C.O. 3: Assign the nomenclature of simple organic molecules following IUPAC rules and identify various functional groups in organic chemistry	Understand
C.O. 4: Differentiate the properties of real gases from those of a perfect gas	Analyze
C.O. 5: Predict changes in thermodynamic parameters during a process and predict the spontaneity	Apply

Course Outcome	Program Specific Outcome					
	P.S.O. 1	P.S.O. 2	P.S.O. 3	P.S.O. 4	P.S.O. 5	P.S.O. 6
C.O. 1	3	2	1	1	1	1
C.O. 2	3	2	1	2	1	1
C.O. 3	3	1	0	2	2	1
C.O. 4	3	0	0	2	1	1
C.O. 5	3	0	0	2	1	1

UNIT I **10 hrs**
Periodic Properties: Atomic weights, Development of periodic law, The modern periodic table, Basis of periodic classification, orbital types and periodic table, Commonality in electronic configurations, Atomic sizes, ionization energy, Electron negativity, Electron Affinity, Polarizability and polarizing power, Relative orbital energies and overlap, Trends associated with properties – Physical and chemical, Anomalies in periodic properties.
UNIT II **12 hrs**
Acid Base concepts: Theories of acids and bases- Arrhenius Theory, Bronsted-Lowry definition, pH, PKa , PKb, Lux Flood Definition, Solvent system definition, Lewis Definition, Usanovich Definition, Generalized concept. Ionic product of water, Common ion effect, Solubility product, Acid strength, Degree of hydrolysis of salts, Buffer solutions, Mechanism of buffer action, Henderson equation.
UNIT III **10 hrs**
Nomenclature and functional groups in organic molecules: Rules of IUPAC system of nomenclature, naming of common organic compounds. Introduction to organic functional groups- alcohols, ethers, halides, amines, nitro compounds, nitriles, aldehydes, ketones, carboxylic acids and derivatives.

UNIT IV	10 hrs
Gaseous State: Kinetic Theory of gases, Maxwell Boltzmann distribution of molecular velocities (Qualitative approach), Different types of velocities, Gas Laws, Ideal gas equation, Real gases- Deviation from ideal behavior- Compressibility factor, Van der Waals equation, Virial equation, PV isotherms, Continuity of states, Law of corresponding states, Critical phenomena and critical constants. Transport properties.	
UNIT V	**12 hrs**
Thermodynamics: State functions, Reversible and irreversible processes, Isothermal and adiabatic processes, Concepts of work, heat, Internal energy, enthalpy, Heat capacity, entropy, Gibbs energy, Helmholtz energy, Work done in isothermal and adiabatic reversible and irreversible processes, First, second and third laws of thermodynamics, Entropy and free energy as criteria for spontaneity and equilibrium, Unattainability of absolute zero. Standard states. Entropy and free energy changes during isothermal and adiabatic processes, Changes in entropy and free energy with Temperature and pressure, Gibbs-Helmholtz equation, Maxwell's relations, Joule Thomson effect- Inversion temperature, Application of J. T. effect - Liquefaction of gases.	

Recommended Text Books:

1. Mingos, D. M. P., Essential trends in inorganic chemistry, Oxford University press, 1998.
2. Wulfsberg, G., Inorganic Chemistry, VIVA, 2002.
3. Greenwood, N. N., Earnshaw, A., Chemistry of Elements, Maxwell Macmillan, International Edition, Pergamon Press, 1989.
4. Cotton, F.A., Wilkinson, G, Advanced Inorganic Chemistry. Wiley-VCH, 1999.
5. Huheey, J. E., Keiter, E. A., Kieter, R. L., Medhi, O. K., Inorganic Chemistry Principles, Structure and Reactivity, Pearson Education, 4th edition, 2009.
6. Shriver, D. F., Atkins, P. W. and Langford, C. H. Inorganic Chemistry, 4th Ed., W.H.Freeman & Company, 2006.
7. F. Daniels and R. A. Alberty, Physical Chemistry, Wiley Publishers, 4th Edn 2004
8. J. G. Smith, Organic Chemistry, 3rd edn., 2011.
9. J. Clayden, N. Green, S. Warren, P. Wothers, Organic Chemistry, 2nd edn., Oxford, University Press, 2012.
10. P.W Atkins, Julio De Paula, Physical Chemistry, Oxford University Press, 10th/11th edn, 2017/2018.
11. Ira.N.Levine, Physical Chemistry, Tata Mc Graw Hill, 6th edn (Indian) 2011.
12. R.A.Alberty & R.J.Silbey, Physical Chemistry, Wiley Publishers, 4th edn, 2004.
13. T. Engel and P. Reid, Physical Chemistry, Pearson, 3rd Edn, 2013.
14. K J Laidler, J.H Meiser, Physical Chemistry, 4th edn 2003.

CHE10202

INORGANIC QUALITATIVE ANALYSIS LAB

Credit 2 **36 hours**

Course Outcome After the completion of the course the student will be able to	**Cognitive Level**
C.O. 1: Understand basic concepts of inorganic qualitative analysis	Understand
C.O. 2: Identify acid radicals and basic radicals from a given sample mixture	Apply

Course Outcome	Program Specific Outcome					
	P.S.O. 1	P.S.O. 2	P.S.O. 3	P.S.O. 4	P.S.O. 5	P.S.O. 6
C.O. 1		3	3			
C.O. 2		3	3			

1.	Systematic qualitative analysis of mixtures containing two acid and two basic radicals from the list given below by semi micro method. Pb^{2+}, Cu^{2+}, Bi^{2+}, Cd^{2+}, Fe^{2+}, Fe^{3+}, Al^{3+}, Zn^{2+}, Mn^{2+}, Co^{2+}, Ni^{2+}, Ca^{2+}, Sr^{2+}, Ba^{2+}, Mg^{2+}, NH_4^+, CO_3^{2-}, SO_4^{2-}, NO_3^-, F^-, Cl^-, $C_2O_4^{2-}$, CH_3COO^-, PO_4^{3-}.

Recommended Text Books:

1. A.I. Vogel, A Text Book of Qualitative Inorganic Analysis, Longman, 1966

CHE10203

INDUSTRIAL APPLICATIONS OF PETROCHEMICALS AND PETROLEUM PRODUCTS

Credit 2 **36 hours**

Course Outcome After the completion of the course, the student will be able to	**Cognitive Level**
C.O. 1: Explain the chemistry and application of the basic building block chemicals derived from fossil sources.	Understand
C.O. 2: Discuss methods of synthesis and the environmental impact of industrial polymers.	Understand

Course Outcome	Program Specific Outcome					
	P.S.O. 1	P.S.O. 2	P.S.O. 3	P.S.O. 4	P.S.O. 5	P.S.O. 6
C.O. 1	3	0	0	3	3	3
C.O. 2	3	0	0	3	3	3

UNIT I **6 hrs**
Chemistry, use, and the environmental and economic impact of basic building block chemicals derived from fossil sources such as petroleum and coal. Fermentation industry. Introduction to unit processes and operations.
UNIT II **8 hrs**
Petroleum refining and important petrochemicals. Ethylene, acetylene, propylene, butadiene and butenes, aromatic hydrocarbons (benzene, toluene, xylenes-BTX), methane and other alkanes cracking and reforming processes.
UNIT III **8 hrs**
Chemicals from C2, C3 and C4 streams: Chemicals from Propylene. Polymerization to polypropylene, addition reactions, conversion to acrolein and acrylonitrile, cumene hydroperoxide, phenol and acetone. Butadiene-polymerization, Diels-Alder reaction, 1,4-additions, adiponitrile and hexamethylenediamine for nylon production.
UNIT IV **8 hrs**
Chemicals from BTX stream: Chemicals from Benzene, Toluene and Xylene (BTX Process)- Review of electrophilic substitution reactions, phenol-formaldehyde resins, reduction of benzene to cyclohexane, oxidation to adipic acid (nylon 6,6 and nylon 6), caprolactam from cyclohexanone oxime, Beckmann rearrangement, reactions of toluene, benzyl chloride, benzoic acid, benzaldehyde, xylene to phthalic anhydride (plasticizers).
UNIT V **6 hrs**
General introduction to synthetic high polymers- inputs and methods of polymerization. Resins, plastics and elastomers.

Recommended Text Books:

1. Szmant, H.H. "Organic Building Blocks of the Chemical Industry", Wiley & Sons, 1989.
2. J. Clayden, N. Green, S. Warren, P. Wothers, Organic Chemistry, 2nd edn., Oxford University Press, 2012.
3. Speight, James G. Handbook of Petroleum Refining. CRC press, 2016.
4. M. Sami, L. F. Hatch. Chemistry of Petrochemical Processes. 2nd edn., Elsevier, 2001.
5. V.R. Gowariker, N.V. Viswanathan, J. Sreedhar, Polymer Science, New Age International, 2011.
6. F.W. Billmeyer Jr., Text book of Polymer Science, 3rd edn., John Wiley & Sons, 1984.

CHE10301

GENERAL CHEMISTRY III

Credit 3 **54 hours**

Course Outcome After the completion of the course, the student will be able to	**Cognitive Level**
C.O. 1: Apply the basic concepts of kinetics to various processes/reactions	Apply
C.O. 2: Understand the basic surface phenomena and extended application to adsorption	Apply
C.O. 3: Develop an insight into the importance of organic chemistry in life	Understand
C.O. 4: Describe the different types of organic reactions	Understand

Course Outcome	Program Specific Outcome					
	P.S.O. 1	P.S.O. 2	P.S.O. 3	P.S.O. 4	P.S.O. 5	P.S.O. 6
C.O. 1	3	0	0	2	1	1
C.O. 2	3	0	0	2	1	0
C.O. 3	3	2	1	2	1	2
C.O. 4	3	2	3	3	2	3

UNIT I	**9 hrs**
Chemical Kinetics: Rate laws, Order and molecularity, Zero, first, second and third order reactions- Integration of rate equations, Half-life period, Arrhenius equation.	
UNIT II	**9 hrs**
Adsorption: Physical and chemical adsorption, adsorption isotherms- Langmuir (kinetic derivation), Freundlich and BET (No derivation) isotherms, Determination of surface area using Langmuir and BET isotherms, Catalysis- Homogeneous and heterogeneous, Enzyme catalysis.	
UNIT III	**10 hrs**
Stereochemistry: Configuration and conformation- Concept of configuration, classification of stereoisomers, optical isomerism, chirality, wedge formula, Fischer projection, Newman projection, perspective formula. Relative and absolute configurations, sequence rules, D & L, R & S systems of nomenclature. Enantiomers, meso form, diastereoisomers, epimers, anomers. Geometrical Isomerism: E-Z notation. Conformational analysis: Strain in molecules, acyclic molecules, cyclohexane, substituted cyclohexanes- A values.	
UNIT IV	**12 hrs**
Basics of reaction mechanism: Classification and an overview of organic reactions. Electron pushing diagrams. Basics of reaction coordinate diagrams, intermediates, transitions states, exothermic and endothermic reactions, activation energy, rates of reactions and rate determining step. Nucleophilic substitutions - S_N1, S_N2, substitutions on aromatic carbon, Addition reactions - polar and nonpolar	

addition - addition of Bromine and hydrogen halides to double bonds - Markownikoff's rule and peroxide effect., Elimination - E1, E2, E1CB, pyrolytic elimination.
UNIT V **14 hrs**
Biomolecules (structure and function): General introduction to carbohydrates, ring-chain tautomerism, glycocidic linkage, classification, monosaccharides, disaccharides, oligosaccharides, polysaccharides, reducing and nonreducing sugars, structure of aldohexoses, fructose and ribose, "sugar-like" artificial sweetners, basic introduction to amino acids, proteins and nucleic acids.

Recommended Text Books:

1. P.W Atkins, Julio De Paula, Physical Chemistry, Oxford University Press, $10^{th}/11^{th}$ edn, 2017/2018.
2. Ira.N.Levine, Physical Chemistry, Tata Mc Graw Hill, 6^{th} edn (Indian) 2011.
3. R.A.Alberty & R.J.Silbey, Physical Chemistry, Wiley Publishers, 4^{th} edn, 2004.
4. T. Engel and P. Reid, Physical Chemistry, Pearson, 3^{rd} Edn, 2013.
5. K J Laidler, J.H Meiser, Physical Chemistry, 4^{th} edn 2003.
6. 1. Clayden J., Greeves, N. Warren, S., Organic Chemistry, 2^{nd} edn. Oxford University Press, 2001.
7. Bruice, P.Y. Organic Chemistry, 7^{th} edn., Prentice Hall Inc., 2013.
8. March, J., Smith, D., March's Advanced Organic Chemistry: Reactions, Mechanisms and Structure, 7^{th} edn., Wiley, 2013.
9. F. A. Carey, R. J. Sundberg, Advanced Organic Chemistry (parts A and B), 5^{th} edn., Springer, 2008.
10. J. McMurry, Organic Chemistry, 5^{th} edn., Brooks/Cole, 2000.
11. P. Sykes, Guidebook to Mechanism in Organic Chemistry, 6^{th} edn., Prentice Hall, 1986.

CHE10302

ORGANIC QUALITATIVE ANALYSIS LAB

Credit 2 **36 hours**

Course Outcome After the completion of the course, the student will be able to	**Cognitive Level**
C.O. 1: Identify the functional group(s) present in a given organic compound	Understand
C.O. 2: Categorize the unknown organic compound based on functional group analysis and prepare the corresponding derivative	Analyze

Course Outcome	Program Specific Outcome					
	P.S.O. 1	P.S.O. 2	P.S.O. 3	P.S.O. 4	P.S.O. 5	P.S.O. 6
C.O. 1	3	3	3	3	0	3
C.O. 2	3	3	3	3	0	3

1.	Identification of simple organic compounds
2.	Preparation of derivatives

Recommended Text Books:

1. Pavia, D.L. Lampman, G.M. Kriz, G.S. and Engel, R.G. Introduction to Organic Laboratory Techniques: A small scale Approach, 2nd Ed., 2007.
2. Dey, B.B. Sitaraman, M.V. and Govindachari, T.V. Laboratory Manual of Organic Chemistry, 3rd Ed., Viswanathan, 1957.
3. Furniss, B.S. Hannaford, A.J. Smith, P.WG. Tatchell, A.R. Vogel's Textbook of Practical Organic Chemistry, 5th Ed., Longman, 1989.

CHE10303

CHEMICAL KINETICS AND SURFACE CHEMISTRY

Credit 2 **36 hours**

Course Outcome After the completion of the course the student will be able to	**Cognitive Level**
C.O. 1: Apply the laws of chemical kinetics and photochemistry to calculate rate/ rate constants/quantum yield of different types of reactions	Apply
C.O. 2: Apply theory of reaction rates to chemical reactions/processes	Apply
C.O. 3: Understand the surface properties and applications of interfaces	Apply

Course Outcome	Program Specific Outcome					
	P.S.O. 1	P.S.O. 2	P.S.O. 3	P.S.O. 4	P.S.O. 5	P.S.O. 6
C.O. 1	3	0	0	2	1	0
C.O. 2	3	0	0	2	1	0
C.O. 3	3	0	0	2	1	0

UNIT I	**8 hrs**
Complex Reactions -Consecutive, Parallel and Opposing reactions (elementary concepts), Steady state approximation. Chain reactions, Branched chain reactions (basic concepts).	
UNIT II	**8 hrs**
Theories of Reaction rate- Collision Theory, Transition state theory (elementary concepts), Unimolecular reactions- Lindemann mechanism.	
UNIT III	**6 hrs**
Photochemistry: Photochemical laws, Beer-Lambert Law, Quantum yield, Photophysical and photochemical processes- Jablonski Diagram, Fluorescence, Phosphorescence-, Chemiluminescence, Bioluminescence, Photosensitisation.	
UNIT IV	**6 hrs**
Surfaces and Interfaces: Surface free energy and Surface tension, Contact angles and Wetting, Surface films. capillarity, vapour pressure of droplets. Kelvin equation. pressure difference across curved surface -Laplace equation, Surface wetting- hydrophilicity and hydrophobicity.	
UNIT V	**8 hrs**
Colloids: Lyophilic and Lyophobic colloids, Preparation of colloids, Kinetic, optical and electrical properties, Electrical double layer Models for double layer: Helmholtz, Gouy- Chapman and Stern models, Zeta potential. Stability of colloids, Protective colloids- Gold number, Flocculation, Hardy Schulze rule, Surfactants, micelles, Donnan membrane equilibrium, Dorn effect, Sedimentation potential and streaming potential, Emulsions, Gels, Sols.	

Recommended Text Books:

1. P.W Atkins, Julio De Paula, Physical Chemistry, Oxford University Press, 10^{th}/11^{th} Edn, 2017/2018.
2. Ira.N.Levine, Physical Chemistry, Tata Mc Graw Hill, 6^{th} Edn (Indian) 2011.
3. R.A.Alberty & R.J.Silbey, Physical Chemistry, Wiley Publishers, 4^{th} Edn, 2004.
4. T. Engel and P. Reid, Physical Chemistry, Pearson, 3^{rd} Edn, 2013.
5. K J Laidler, J.H Meiser, Physical Chemistry, 4^{th} Edn 2003.
6. K. J. Laidler, Chemical-Kinetics, Paperback Edn., 2018.
7. M. R. Wright, An Introduction to Chemical Kinetics, Wiley, 2004.

23-808-0401

INORGANIC CHEMISTRY I

(Inorganic Main Group and Nuclear Chemistry)

Credit 4 **72 hours**

Course Outcome After the completion of the course, the student will be able to	**Cognitive Level**
C.O. 1: Interpret the types of bonding and structure based on the electronic configuration	Apply
C.O. 2: Explain the reactivity and physicochemical properties based on the type of bonding	Analyze
C.O. 3: Explain the properties of transition metals and lanthanides	Apply
C.O. 4: Compare the structure, bonding and reactivity of the compounds of main group elements	Analyze
C.O. 5: Describe the radioactivity phenomena and its applications	Apply

Course Outcome	Program Specific Outcome					
	P.S.O. 1	P.S.O. 2	P.S.O. 3	P.S.O. 4	P.S.O. 5	P.S.O. 6
C.O. 1	2	1	1	3	2	2
C.O. 2	2	1	1	3	2	2
C.O. 3	3	1	1	3	2	2
C.O. 4	3	1	1	3	2	2
C.O. 5	3	1	1	3	2	2

UNIT I **12 hrs**
s- Block elements- Hydrogen, Hydrogen Bonding, Hydrates, Hydrogen ions, acids and bases, Group 1 elements - General Behavior, Occurrence and abundance, Electronic Configuration and types of bonding, Flame colors and spectra, Color of compounds, Alkali metals in liquid ammonia and other solvents, Oxides, hydroxides, hydrides, alkoxides, amido complexes, Ionic salts and M^+ ions in solution, Alkali metal complexes, Organolithium compounds.
UNIT II **12 hrs**
Group 2 elements – General Behavior, Occurrence and abundance, Electronic Configuration and types of bonding, Elemental Beryllium, Binary Compounds, Coordination compounds with oxygen and nitrogen ligand, organoberyllium compounds, Compounds of Magnesium, Calcium, Strontium- oxides, halides, hydrides, carbides, ionic salts and complexes, alkoxides. Grignard reagents – preparation and properties.

UNIT III	**18 hrs**
General periodic trends of d and f block elements, Metallic property, Chemistry of variable oxidation states, properties of d configuration - d0 to d10, Type of compounds. physical and chemical properties of transition elements; Difference between first row and other rows, Double salts and coordination compounds. Introduction to coordination compounds; coordination numbers and geometries in transition metal complexes; nomenclature; isomerism in transition metal complexes – structural, geometrical and optical isomerism. Lanthanides and Actinides- Stable oxidation states, lanthanide and actinide contraction, Occurrence and recovery; Separation of Lanthanides; difference between 4f and 5f orbitals, Industrial importance of lanthanides. Actinides: Comparison with lanthanides and general characteristics.	
UNIT IV	**16 hrs**
Types of oxides, Chemical properties of Dioxygen, Singlet oxygen, ozone, Peroxo compounds, Superoxide. Nitrogen compounds- Nitrides, Ammonia, Hydrazine, Oxides of Nitrogen, Oxo acids and anions. Sulphur-Nitrogen compounds: Tetrasulphur tetranitride, disulphur dinitride and polythiazyl. SxNy compounds. S-N cations and anions. Sulphur-phosphorus compounds: Molecular sulphides such as P_4S_3, P_4S_7, P_4S_9 and P_4S_{10}. Phosphorus-nitrogen compounds: Phosphazenes and poly phosphazenes. Interhalogen compounds, Structure, hybridization and reactivity of ClF_3, ICl_3, IF_5 and IF_7, Compounds of Xe, Kr and Rn.	
UNIT V	**14 hrs**
Nuclear radius, Nuclear Forces, Nuclear Spin, Magnetic dipole moment, Elementary Particles, Binding Energy, Nuclear models – Shell model- magic number, periodicity in nuclear properties, Liquid drop model – Fission and Fusion, Nuclear Stability, Exchange theory, n/p ratio, Nuclear Radiations, Nuclear reactions, Types of nuclear reactions, Decay Kinetics, Half-life, Radioactive disintegration series. Fission: Fission products and Fission yield curve, Fission energy, theory of nuclear fission, nuclear reactor, breeder reactor - nuclear reactors in India. Fusion reactions, hydrogen bomb and energy of sun. Radio carbon dating principles.	

Recommended Text Books:

1. Mingos, D. M. P., Essential Trends in Inorganic Chemistry, Oxford University Press 1998.
2. Wulfsberg G., Inorganic Chemistry, VIVA, 2002.
3. Greenwood, N. N., Earnshaw, A., Chemistry of the Elements, Maxwell Macmillan International Edition, Pergamon Press, 1989.
4. Cotton, F.A., Wilkinson, G, Advanced Inorganic Chemistry. Wiley-VCH, 1999

5. Huheey, J. E., Keiter, E. A., Kieter, R. L., Medhi, O. K., Inorganic Chemistry Principles Structure and Reactivity, Pearson Education, 4th edition, 2009.
6. Lee, J. D., A New Concise Inorganic Chemistry, ELBS, 1998
7. Miessler, G.L. & Tarr, D. A. Inorganic Chemistry, 5th Ed., Pearson Publication, 2013.
8. Arnikar, H. J., Essentials of Nuclear Chemistry, Wiley Eastern Ltd., New Delhi, 1982.

23-808-0402

ORGANIC CHEMISTRY I

Credit 4 **72 hours**

Course Outcome After the completion of the course the student will be able to	**Cognitive Level**
C.O. 1: Apply the concepts of isomerism and analyse the conformation and configuration of organic molecules.	Apply
C.O. 2: Illustrate the mechanism involved in various reactions	Apply
C.O. 3: Describe bonding properties in organic molecules	Understand
C.O. 4: Explain the molecular structure and stereochemistry of carbohydrates	Apply
C.O. 5: Explain the molecular structure of amino acids and proteins	Apply

Course Outcome	Program Specific Outcome					
	P.S.O. 1	P.S.O. 2	P.S.O. 3	P.S.O. 4	P.S.O. 5	P.S.O. 6
C.O. 1	2	1	1	1	3	2
C.O. 2	3	2	1	2	1	1
C.O. 3	3	1	1	1	1	1
C.O. 4	3	2	1	2	2	1
C.O. 5	1	3	2	2	1	2

UNIT I **16 hrs**

Stereochemistry:

Geometrical & Optical isomerism: the origin of chirality, chiral centres and configuration, axes and planes, helicity. Prochiral centres and faces. Topicity relationships, enantiotopic and diastereotopic groups and faces. Symmetry, stereochemistry and time scale. Allenes, cumulenes, biphenyls, and spirans. Compounds containing chiral atoms other than carbon.

Strain, types of strain including B, F, I, Pitzer strain and Baeyer strain. Acyclic sp^3–sp^3, sp^3-sp^2 systems, structure and stability of small, medium, and large rings, cyclohexane, substituted cyclohexanes, cyclohexenes, decalins, and bicyclic systems.

UNIT II **16 hrs**

Carbohydrates: General introduction to carbohydrates, classification, monosaccharides, disaccharides, oligosaccharides, polysaccharides, mutarotation, glyoxal, stepping up and stepping down, reducing and nonreducing sugar, open chain and closed chain structures of monosaccharides glycosidic linkage, O & N glycosides. Isomers, Fischer projection, D/L notation, Howarth projection, three-dimensional representation of Dglucose, epimers, anomers, enantiomers.

UNIT III **12 hrs**
Amino acids: classification-essential and non-essential amino acids, unnatural amino acids, acid-base behaviour, protein and nonprotein amino acids, Zwitter ions. Strecker synthesis of amino acids. Proteins classification based on i) shape and solubility and ii) increasing complexity of structure. Structure of proteins- primary, secondary, tertiary and quaternary. Biological significance. Concept of isoelectric point and its significance.
UNIT IV **14 hrs**
Substitutions on Aliphatic carbon: –saturated and unsaturated systems – Mechanism of nucleophilic substitution – SN2, SN1 – ion pairs, SET, Neighbouring group participation – non classical carbocations, SNi, Tetrahedral mechanism. Electrophilic substitution – SE2, SEi, SE1. Free radical substitution. Reactivity – Effect of substrate structure, nature of reagents, solvents and stereochemistry on the outcome of these reactions. Ambident nucleophiles and substrates. Typical reactions involving substitution.
UNIT V **14 hrs**
Additions and eliminations: Mechanisms of polar addition – electrophilic, nucleophilic and free radical addition. Nonpolar additions (excluding pericyclic reactions) - Reactivity and orientation. Eliminations - E2, E1 and E1CB mechanisms, reactivity and orientation. Pyrolytic syn eliminations, α - eliminations, elimination vs substitution. Typical reactions involving addition and elimination.

Recommended Text Books:

1. J. Clayden, N. Green, S. Warren, P. Wothers, Organic Chemistry, 2nd ed., Oxford University Press, 2012.
2. March, J., Smith, D., March's Advanced Organic Chemistry: Reactions, Mechanisms and Structure, 7th ed., Wiley, 2013.
3. Bruice, P.Y. Organic Chemistry, 7th ed., Prentice Hall Inc., 2013.
4. F. A. Carey, R. J. Sundberg, Advanced Organic Chemistry (parts A and B), 5th ed., Springer, 2008.
5. J. McMurry, Organic Chemistry, 5th ed., Brooks/Cole, 2000.
6. P. Sykes, Guidebook to Mechanism in Organic Chemistry, 6th ed., Prentice Hall, 1986.
7. E. L. Eliel and S. H. Wilen, Stereochemistry in Organic Compounds, John Wiley, 1994.
8. P. S. Kalsi, Stereochemistry, Conformation and Mechanism, 10th ed., New Age Publications, 2019.

9. E. V. Anslyn, D. A. Dougherty, Modern Physical Organic Chemistry. University Science Books, 2006.
10. Bruckner, R. Advanced Organic Chemistry: Reaction Mechanisms, 1st edn., Academic Press, 2001.

23-808-0403

PHYSICAL CHEMISTRY I

(Equilibrium Thermodynamics)

Credit 4 **72 hours**

Course Outcome After the completion of the course, the student will be able to	**Cognitive Level**
C.O. 1: Predict the dependence of physical and chemical equilibrium on pressure, temperature and concentration	Apply
C.O. 2: Describe the significance of chemical potential in physical and chemical processes	Apply
C.O. 3: Understand the thermodynamics of phase transitions and interpret the phase diagram of a given system	Analyze
C.O. 4: Predict the dependence of chemical equilibrium on pressure, temperature and concentration	Apply

Course Outcome	Program Specific Outcome					
	P.S.O. 1	P.S.O. 2	P.S.O. 3	P.S.O. 4	P.S.O. 5	P.S.O. 6
C.O. 1	3	0	0	3	2	1
C.O. 2	3	0	0	3	2	1
C.O. 3	3	0	0	3	2	1
C.O. 4	3	0	0	3	2	1

UNIT I **14 hrs**
Basic concepts: Review of first, second and third laws, Entropy and free energy changes during isothermal and adiabatic processes, Changes in entropy and free energy with Temperature and pressure, Gibbs Helmholtz equation, Maxwells Relations. Thermochemistry- Enthalpy of physical and chemical changes, Temperature dependence of reaction enthalpies, Hess's law.
UNIT II **14 hrs**
Physical Transformation of substances: Molar Gibbs energy, Phase stability and transitions, phase equilibria of pure substances, Clausius Clapeyron equation, Solid-liquid, liquid-vapor and solid-vapor equilibria, phase rule, phase diagrams of one-component systems, Ehrenfest Classification of Phase transitions.
UNIT III **14 hrs**
Thermodynamics of Mixtures: Partial molar quantities, Chemical potential, Thermodynamics of mixing, Excess function, Chemical potential of liquids, Gibbs Duhem Equation and Duhem Margules Equation. Ideal solutions, Deviations from ideality, Concepts of fugacity and activity, Ideal dilute solutions, Henry's and Raoult's laws, Colligative properties, Regular solutions.

UNIT IV	**14 hrs**
Phase Equilibria of Binary and ternary Systems: Vapor pressure-composition diagrams, Temperature-composition diagrams, Liquid-liquid systems – Completely miscible, Partially miscible and Immiscible, Azeotropes and Azeotropic distillation, Steam distillation. Nernst Distribution Law. Three-component systems.	
UNIT V	**16 hrs**
Chemical Equilibria: Chemical Equilibria and free energy, Equilibrium Constant, Applications of free energy function to physical and chemical changes- Le Chateliers Principle. Effect of temperature and pressure on the chemical equilibrium- van't Hoff reaction isotherm and isochore.	

Recommended Text Books:

1. P.W Atkins, Julio De Paula, Physical Chemistry, Oxford University Press, 10^{th}/11^{th} Edn, 2017/2018.
2. Ira.N.Levine, Physical Chemistry, Tata Mc Graw Hill, 6^{th} Edn (Indian) 2011.
3. R.A.Alberty & R.J.Silbey, Physical Chemistry, Wiley Publishers, 4^{th} Edn, 2004.
4. T. Engel and P. Reid, Physical Chemistry, Pearson, 3^{rd} Edn, 2013.
5. K J Laidler, J.H Meiser, Physical Chemistry, 4^{th} Edn 2003.
6. D.A McQuarrie, J.D Simon, Molecular Thermodynamics, Viva Student Edn. 2010.
7. L. K. Nash, Elements of Chemical Thermodynamics, Addison Wesley, 2^{nd} Edn, 2013.
8. F.W Sears, Introductions to Thermodynamics, Kinetic Theory of Gases and Statistical Mechanics, Addision Wesley Pub. Cambridge, 1998.
9. F.C. Andrews, Equilibrium to Statistical Mechanics, John Wiley, New York, 2002.
10. L.K. Nash, Statistical Thermodynamics, Addison Wesley, New York, 1999.
11. D. A. McQuarrie, Physical Chemistry- A Molecular Approach, South Asian Edn., 2008.
12. D. A. McQuarrie, Statistical Thermodynamics, South Asian Edn., 2008.
13. M. Dole, Introduction to Statistical Thermodynamics, Prentice Hall, London, 1997.

23-808-0404

THEORETICAL CHEMISTRY – 1

(Introductory Quantum Mechanics)

Credit 4 **72 hours**

Course Outcome After the completion of the course the student will be able to	**Cognitive Level**
C.O. 1: Describe and justify the importance of Quantum Mechanics	Analyze
C.O. 2: Understand and apply various postulates in deriving property operators and Schrodinger equation	Apply
C.O. 3: Apply the postulates of quantum mechanics to simple systems of chemical interest, such as the particle-in-a-box, harmonic oscillator, and rigid rotor	Analyze
C.O. 4: Interpret the solutions and appreciate the quantization concept	Analyze

Course Outcome	Program Specific Outcome					
	P.S.O. 1	P.S.O. 2	P.S.O. 3	P.S.O. 4	P.S.O. 5	P.S.O. 6
C.O. 1	3	1		2	1	
C.O. 2	3	1		2	1	
C.O. 3	3	1		2	2	
C.O. 4	3	2	1	2	3	

UNIT I	**18 hrs**
Basics: Evolution of quantum mechanics, Heisenberg's matrix mechanics- commutator relationships, position representation, coordinate- Cartesian, cylindrical and spherical polar and their interconversion, Complex number and their representation in various coordinate systems. Operators, Algebra of operators, Linear and Hermitian operators, Eigenvalue equation, Significance, well-behaved functions, Time dependent Schrodinger equation, conservative and non-conservative systems.	
UNIT II	**12 hrs**
Solving the Schrodinger equation-Particle in a box: Quantum mechanical postulates, construction of various operators – kinetic energy, angular momentum. Translational motion- free particle, particle in one, two and three-dimensional box (rectangular and cubical), separation of variables, concept of degeneracy, introduction to quantum mechanical tunneling.	
UNIT III	**14 hrs**
Solving the Schrodinger equation-Simple Harmonic oscillator: Vibrational motion, 1-D Harmonic oscillator, Method of power series, Hermite equation and Hermite Polynomials, Recursion formula,	

wave function and energy. Transition moment integral, selection rules, Extension of the results to 3D-SHO.
UNIT IV **10 hrs**
Solving the Schrodinger equation-Planar Rigid Rotor: Rigid rotator, Conversion of laplacian opertor into spherical polar coordinates, Particle on a ring, phi equation, Angular momentum operator L^2 and Lz, quantization, polar plots.
UNIT V **18 hrs**
Solving the Schrodinger equation-Non-planar RR: Theta equation and solutions Lagendre equation and Lagendre polynomials, Restriction of ml values, Spherical harmonics, Angular momentum operator L^2 and Lz, Space quantization, polar plots of spherical harmonics.

Recommended Text Books:

1. Atkins, P.W. and Paula, J. Physical Chemistry, 8th Ed., Oxford Press, 2006.
2. Szabo, A.; Ostlund, N. S. “Modern Quantum Chemistry: Introduction to Advanced Electronic Structure theory”, Dover Publications, 1996.
3. Levine, I. N. "Quantum Chemistry", 7th Ed., Pearson Education Inc., 2014.
4. McQuarrie, D. A., "Quantum Chemistry", 2nd Ed.,University Science Books, 2008.
5. Pillar, F. L. “Elementary Quantum Chemistry”, 2nd Ed., Dover Publication, 2001.
6. Chandra, A. K., "Introduction to Quantum Mechanics", 4th Ed, Tata McGraw-Hill, New Delhi, 2003.
7. Prasad, R. K., “Quantum Chemistry”, 4th Ed, New Age International, 2009.

23-808-0405

INORGANIC CHEMISTRY LAB -I

Credit 2 **36 hours**

Course Outcome After the completion of the course, the student will be able to	**Cognitive Level**
C.O. 1: Estimate the amount of a given metal ion by complexometric reactions	Apply
C.O. 2: Identify the cation from the given mixture	Apply

Course Outcome	Program Specific Outcome					
	P.S.O. 1	P.S.O. 2	P.S.O. 3	P.S.O. 4	P.S.O. 5	P.S.O. 6
C.O. 1	3	3	3	2	2	1
C.O. 2	3	3	3	2	2	1

1.	Complexometry: Estimation of Zinc, Magnesium, Calcium, Determination of hardness of water, Estimation of different metal ions from a mixture – use of masking agents.
2.	Analysis of less common ions: Separation and identification of two less familiar metal ions such as Tl, W, Se, Mo, Ce, Th, Ti, Zr, V, U and Li from a mixture of salts.

Recommended Text Books:

1. J. Mendham, R. C. Denney, J. D. Barnes, M. Thomas, Vogel's Textbook of Quantitative Chemical Analysis, 6th Edn., Pearson Education, Noida, 2013.
2. A.I. Vogel, G. Svehla, Vogel's Qualitative Inorganic Analysis, 7th edition., Longman, 1996.
3. V.V. Ramanujam, Inorganic Semimicro Qualitative Analysis, The National Pub.Co., 1974.

23-808-0406

PHYSICAL CHEMISTRY LAB -I

Credit 2 **36 hours**

Course Outcome After the completion of the course, the student will be able to	**Cognitive Level**
C.O. 1: execute and perform experiments based on thermodynamic and kinetic principles	Evaluate

Course Outcome	Program Specific Outcome					
	P.S.O. 1	P.S.O. 2	P.S.O. 3	P.S.O. 4	P.S.O. 5	P.S.O. 6
C.O. 1	3	3	3	3	2	3

1.	Chemical Kinetics: Determination of rate constant of acid hydrolysis of ester. Determination of kinetic parameters.
	Phase diagrams:
2.	CST: Phenol-water system, Determination of CST, Analyse the effect of KCl and succinic acid on CST.
3.	Solid-Liquid Equilibria: Simple Eutectic systems- Construction of phase diagrams, Determination of Molal Depression constant of a solvent and molecular weight of solute by Rast method.
4.	Transition temperature: Determination of transition temperature of a salt hydrate-water system and molecular weight of a solute.
5.	Three component systems: Construction of phase diagram.
6.	Adsorption: Verification of the validity of Langmuir and Freundlich adsorption isotherms.

Recommended Text Books:

1. J. N. Gurtu, and A. Gurtu Advanced Physical Chemistry Experiments, 6th Edn., Pragati Prakashan, 2014.
2. J. B. Yadav, Advanced Practical Physical Chemistry, 36th Ed., 2016.
3. D.P Shoemaker, G.W Garland, J.W Nibler, Experiments in Physical Chemistry, 5th Edn. McGraw Hill.

23-808-0501

INORGANIC CHEMISTRY-II

(Coordination & Bioinorganic Chemistry and Polyhedral Boranes)

Credit 4 **72 hours**

Course Outcome After the completion of the course, the student will be able to	**Cognitive Level**
C.O. 1: Describe and explain the structure, bonding and magnetism of metal complexes using CFT.	Analyze
C.O. 2: Describe the metal-ligand interactions in terms of sigma and pi bonding and covalency using LFT and MO theory	Evaluate
C.O. 3: Understand the importance of metal ions in living systems	Analyze
C.O. 4: Predict the stability and topology of different polyhedral boranes and related compounds	Analyze

Course Outcome	Program Specific Outcome					
	P.S.O. 1	P.S.O. 2	P.S.O. 3	P.S.O. 4	P.S.O. 5	P.S.O. 6
C.O. 1	3	2	1	1	1	1
C.O. 2	3	2	1	2	1	1
C.O. 3	3	1	1	3	2	1
C.O. 4	3	1	1	3	2	1

UNIT I **12 hrs**

Werner's theory, Effective atomic number, Bonding in coordination compounds.

Valence bond description and its limitations. valence bond theory (inner and outer orbital complexes).

Crystal Field Theory (CFT). d-orbital splitting in octahedral and tetrahedral geometries, measurement of 10 Dq (Δ_o), crystal field stabilization energy, CFSE in weak and strong fields, effect of pairing energy, factors affecting the crystal-field parameters.

Crystal field splitting of square planar, trigonal bipyramidal, trigonal planar and linear geometries.

UNIT II **12 hrs**

Application of crystal filed theory, colour and spectral behaviours. magnetism of first-row transition metal complexes, lattice energies, ionic radii, site preferences in spinels. Spectrochemical series, Demerits of CFT.

Octahedral vs. tetrahedral coordination, tetragonal distortions from octahedral geometry, Jahn-Teller theorem, Jahn–Teller effect in octahedral and tetrahedral complexes, square planar geometry. Stabilization of unusually low and high oxidation states of metals.

UNIT III	**16 hrs**
Molecular Orbital Theory: construction of molecular orbital diagrams (using group theory-qualitative idea only), qualitative MO diagrams for octahedral, tetrahedral and square planar complexes, effect of π-bonding, experimental evidence for π-bonding, spectrochemical series. Ligand field theory, Effect of π-donor and π-acceptor ligands in LFSE, back bonding.	
UNIT IV	**14 hrs**
Metal ions in biological systems - Biochemistry of iron – Haemoglobin and myoglobin - O_2 and CO_2 transportation (Elementary idea of structure and oxygen binding), Structure and mechanism of action of sodium potassium pump - Biochemistry of Ca, Zn and Co – Toxicity of metal ions (Pb, Hg and As). Anticancer drugs: Cis-platin, oxaliplatin and carboplatin– Structure and significance. Non-Heme Iron Proteins: Iron storage and transfer – ferritin, transferrin; electron transfer (Iron-sulfur protein) – rubredoxin, ferredoxin; O_2 transport – hemerythrin Copper proteins and Enzymes–Hemocyanin, superoxide dismutase, ceruloplasmin, cytochrome C oxidase; Zinc and Cobalt enzymes carbonic anhydrase, carboxypeptidase, interchangeability of zinc and cobalt enzymes; Vitamin B12; Photosynthesis and N_2 fixation.	
UNIT V	**18 hrs**
Electronic structure and allotropes of boron, boron halides, boron heterocycles, borazine Structure and bonding in polyhedral boranes and carboranes, styx notation; electron count in polyhedral boranes; Wade's rule; topological approach to boron hydride structure. Importance of icosahedral framework of boron atoms in boron chemistry. Closo, nido and arachno structures. Synthesis of polyhedral boranes; electron counting in polycondensed polyhedral boranes, mno rule. Carboranes, metallocarboranes.	

Recommended Text Books:

1. Purcell, K.F & Kotz, J.C. Inorganic Chemistry, 2nd Ed., W.B. Saunders Co, 1991.
2. Huheey, J. E., Keiter, E. A. and Keiter, R. L. Inorganic Chemistry, Principle and structure and reactivity, 4th Ed., Harper Collins College Publishers, New York, 1993.
3. Miessler, G.L. & Tarr, D. A. Inorganic Chemistry, 5th Ed., Pearson Publication, 2013.
4. C. E. Housecroft, A. G. Sharpe, Inorganic Chemistry, 5th ed., Pearson, 2018.
5. Cotton, F.A. & Wilkinson, G, Advanced Inorganic Chemistry. 6th Ed., Wiley- Interscience, 1999.
6. Shriver, D. F., Atkins, P. W. and Langford, C. H. Inorganic Chemistry, 4th Ed., W.H. Freeman & Company, 2006.
7. Lippard, S.J. & Berg, J.M. Principles of Bioinorganic Chemistry 2nd Ed., University Science Books, 1994.

8. Greenwood, N.N. & Earnshaw A., Chemistry of the Elements, 2nd Ed. Butterworth-Heinemann, 1997.
9. Sharpe, A.G. Inorganic Chemistry, 4th Indian Reprint, Pearson Education, 2005.
10. Douglas, B. E.; McDaniel, D.H. and Alexander, J.J. Concepts and Models in Inorganic Chemistry 3rd Ed., John Wiley and Sons, NY, 1994.
11. W. L. Jolly, Modern Inorganic Chemistry, McGraw-Hill International, 2nd Edition, New York, 1991.

23-808-0502

ORGANIC CHEMISTRY II

(Reaction Mechanism, Rearrangements and Spectroscopic Techniques in Organic Chemistry)

Credit 4 **72 hours**

Course Outcome After the completion of the course, the student will be able to	**Cognitive Level**
C.O. 1: Illustrate the mechanism involved in various reactions	Apply
C.O. 2: Illustrate the mechanistic pathway of different rearrangement reactions and identify the products	Apply
C.O. 3: Explain the basic principle of spectroscopy in particular IR, Raman, UV-Visible and NMR spectroscopy	Understand
C.O. 4: Identify structures of simple organic compounds based on the data from UV- Vis, IR, Mass Spectrometry, ^{1}H NMR and ^{13}C NMR spectroscopy	Apply

Course Outcome	Program Specific Outcome					
	P.S.O. 1	P.S.O. 2	P.S.O. 3	P.S.O. 4	P.S.O. 5	P.S.O. 6
C.O. 1	3	1	1	2	1	2
C.O. 2	3	1	1	2	1	2
C.O. 3	2	3	3	1	2	3
C.O. 4	1	3	3	2	1	3

UNIT I **16 hrs**

The study of reactions and the methods of studying reaction mechanisms:– Classification of reactions according to IUPAC conventions. Reaction mechanism: guidelines on Pushing of electrons. Reactive intermediates: Formation, stability and general reactivity. Methods of determining reaction mechanisms (kinetic and non kinetic methods): The Hammond postulate, reactivity vs selectivity principle, the Curtin-Hammett principle, microscopic reversibility, kinetic vs thermodynamic control. Isotope effects: Primary, secondary and Equilibrium isotope effects, Tunneling effects, solvent isotope effects and heavy atom Isotope effects. Linear free energy relationships: Hammett and Taft parameters, Solvent effects (Grunwald-Winstein plots and Schleyer adaptation), nucleophilicity and nucleofugality. Isokinetic and Isoequilibrium temperature, Enthalpy – entropy compensation. Experimental techniques to determine reaction mechanisms: identification of intermediates by trapping and competition experiments, crossover experiments, isotope scrambling, radical clocks and traps, matrix isolation.

UNIT II	**14 hrs**
Substitutions on aromatic carbon: Mechanism of electrophilic, nucleophilic and free radical substitutions - orientation and reactivity. Typical reactions involving aromatic substitution. Rearrangements: Wagner-Meerwein, Pinacol, Demyanov, dienone-phenol, Favorskii, Wolff, Hofmann, Curtius, Lossen, Schmidt, Beckmann, benzidine, and Hofmann-Loffler, Fries, Baeyer-Villiger rearrangements. Fritsch-Buttenberg-Wiechell rearrangement, Corey-Fuchs reaction, Wittig rearrangement.	
UNIT III	**14 hrs**
Nature of electromagnetic radiation, its interaction with matter, intensity and width of spectral lines, Classical and quantum chemical approach to absorption of radiation by molecules. Energy levels in molecules. UV-visible Spectroscopy: Types of electronic transitions, Chromophores and Auxochromes, Bathochromic and Hypsochromic shifts, Intensity of absorption; Effect of structure on absorption characteristics, Application of Woodward Rules for calculation of λmax for the following systems: α,β-unsaturated aldehydes and ketones, λmax for polyenes, aromatic aldehydes, ketones, esters. IR spectroscopy: Fundamental and non-fundamental molecular vibrations; IR absorption positions of O and N containing functional groups; Effect of H-bonding, concentration, temperature, conjugation, resonance and ring size on IR absorptions; Fingerprint region and its significance; application in functional group analysis. Fourier transform IR, group frequencies, fundamental frequencies and overtones, combination tones, Fermi Resonance. Basic introduction to Raman spectroscopy.	
UNIT IV	**16 hrs**
NMR Spectroscopy: Basic principles of Proton Magnetic Resonance, chemical shift and factors influencing it; Spin–Spin coupling and coupling constant; Anisotropic effects in alkene, alkyne, aldehydes and aromatics, Interpretation of NMR spectra of simple compounds. Proton decoupled Carbon-13 NMR, introduction to polarization transfer and NOE.	
UNIT V	**12 hrs**
Mass spectrometry – Introduction. EI ionization. Fragmentation modes and determination of molecular mass by MS. Soft ionization techniques, ion separation and analysis, and hyphenated techniques. HRMS and molecular formula. Problems based on the combined application of various spectroscopic techniques.	

Recommended Text Books:

1. E. V. Anslyn, D. A. Dougherty, Modern Physical Organic Chemistry. University Science Books, 2006.

2. F. A. Carey, R. J. Sundberg, Advanced Organic Chemistry (parts A and B), 5th ed., Springer, 2008.
3. Brian S. Furniss, Antony J. Hannaford, Peter W. G Smith, Austin R.Tatchell, Vogel's Textbook of Practical Organic Chemistry, 5th Edition, Longman Scientific and Technical, 1989.
4. D.L.Pavia, G.M. Lampman, G.S.Kriz, Introduction to Spectroscopy, A Guide for Students of Organic Chemistry, 3rd ed., Thomson. 2004.
5. R. M. Silverstein, G.C. Bassler, T. C. Morril, Spectroscopic identification of organic compounds, John Wiley, 1991.
6. D. H. Williams, I. Fleming, Spectroscopic Methods in Organic Chemistry, Tata McGraw Hill. 1988.
7. W. Kemp, Organic Spectroscopy, 2nd ed., ELBS-Macmillan, 1987.
8. Spectral databases (RIO DB of AIST, for example)
9. C. N. Banwell, Fundamentals of Molecular Spectroscopy, 4th ed., Tata McGraw Hill, 1996.
10. J. Clayden, N. Green, S. Warren, P. Wothers, Organic Chemistry, 2nd ed., Oxford University Press, 2012.
11. March, J., Smith, D., March's Advanced Organic Chemistry: Reactions, Mechanisms and Structure, 7th ed., Wiley, 2013
12. Bruice, P.Y. Organic Chemistry, 7th ed., Prentice Hall Inc., 2013.

23-808-0503

PHYSICAL CHEMISTRY II

(Electrochemistry and Solid State Chemistry)

Credit 4 **72 hours**

Course Outcome After the completion of the course, the student will be able to	**Cognitive Level**
C.O. 1: Describe the theories and mechanism of ionic and electronic conductance and apply the concepts	Apply
C.O. 2: Explain the basic theory of electroanalytical techniques	Apply
C.O. 3: Understand basic properties and symmetry of solids	Understand

Course Outcome	Program Specific Outcome					
	P.S.O. 1	P.S.O. 2	P.S.O. 3	P.S.O. 4	P.S.O. 5	P.S.O. 6
C.O. 1	3	3	1	3	3	1
C.O. 2	3	3	2	3	3	1
C.O. 3	3	2	1	3	3	1

UNIT I **14 hrs**

Introduction- Electrochemical Cells, Electrodes, Types of electrodes- Standard hydrogen electrode, Calomel electrode, Quinhydrone electrode. Electrolytes, Half Reactions, Electrochemical Work, Electrodics: Equilibrium electrochemistry- Half- reactions and electrodes, Standard Electrode potential, Nernst Equation. EMF and free energy. Types of cells. Electrochemical series. Liquid junction potential. Ion–Solvent, Ion–Ion Interactions, Ionic and Electronic Conductance, Conductance Measurement, Equivalent Conductance, Kohlrausch's Law, Ostwalds dilution law, Ionic Mobility, Walden's rule, abnormal conductance, Transport Number- Factors Influencing, measurement- Hittorf's and moving boundary methods.

UNIT II **16 hrs**

Electrode–Ion interface, liquid junction potential, Electrical Double Layer, Electrode and Electrolyte polarization. Overpotential. Butler Volmer Equation. Tafel Plot. Mass transfer control, Charge transfer at electrode-electrolyte interface. Double layer. Electrocapillarity. Hydrogen and Oxygen overvoltage. Activity and Activity Coefficients, Debye-Huckel Theory, Limitations. Extension, Bjerrum ion pair formation. Ionic Atmosphere, Relaxation, Mechanism of Electrolytic Conductance, Debye Huckel Onsager equation for strong electrolytes.

UNIT III **12 hrs**

The electromotive force, Standard potentials, Applications of standard potentials, Determination of solubility product and activity co-efficient, Activity and Activity Coefficient of Electrolytes.

Corrosion of metals- different forms of corrosion and prevention. Electrochemical Theory of corrosion – methods of prevention. Porbaux and Evans diagram. Fuel Cell, Batteries: Basic theory and types (Elementary idea).

UNIT IV **14 hrs**

Electroanalytical Techniques: pH determination, Redox indicators principle. Conductometric and potentiometric titrations. Cyclic voltammetry, Square wave, and linear sweep voltammetry, Chronoamperometry, Chronopotentiometry, Impedance. Coulometry and Polarography, Spectroelectrochemistry (Basic Principles).

UNIT V **16 hrs**

Crystal structures and symmetry, Crystallographic point groups, space group, unit cells, Miller indices, Seven crystal systems and Bravais lattices, Simple, body centered and face centered systems, Packing in solids- packing diagrams, close packing,- hcp and ccp structures, XRD, Braggs equation – derivation, Powder and rotating crystal technique. Identification of cubic crystals based on interplanar ratio.

Ionic solids with formula MX (CsCl, NaCl, Zinc Blende and Wurtzite Structures), MX_2 (Fluorite and Antfluorite Structures, Cadmium Halides, CaF_2, Rutile, Anti-rutile, betacristobalite), other crystal systems (Bismuth tri-iodide, Corundum, Rhenium Trioxide etc.), Mixed oxides (Spinel, Perovskite, Ilmenite). The properties of solids, Mechanical properties Electrical properties, Impact on nanoscience: Nanowires, Optical properties, Magnetic properties.

Point Defects in crystals- stoichiometric and non-stoichiometric defects, Line defect, surface defects, Liquid Crystals- Classification and Application.

Recommended Text Books:

1. J. Bockris and A.K.N. Reddy, Modern Electrochemistry, 2nd Edn., Wiley, New York, 1998
2. R. Crow, Principles and Applications of Electrochemistry, Paper back edn, 4th edn, 1994.
3. S. Glasstone, An Introduction to Electrochemistry, Paperback Edn., 2007.
4. Skoog, West, Holler, Crouch, Fundamentals of Analytical Chemistry, Wiley, 9th Edn.
5. L.V. Azaroff, Introduction to Solids, Mc Graw Hill, 1960.
6. A. R. West, Solid State Chemistry, Wiley Student (Indian) Ed., (2014)
7. A.K. Galwey, Chemistry of Solids, Chapman and Hall, London, 1967. 35
8. Lesley Smart and Elaine Moore, Solid State Chemistry, Chapman and Hall, 1995
9. H. V. Keer, Principles of the Solid State Wiley Eastern Ltd, New Delhi, 1993.
10. C. N. R. Rao and J. Gopalakrishnan, New Directions in Solid State Chemistry. 2nd Edn, Cambridge Uty Press, 1997.

23-808-0504

ORGANIC CHEMISTRY LAB -I

Credit 2 **36 hours**

Course Outcome After the completion of the course, the student will be able to	**Cognitive Level**
C.O. 1: Prepare organic compounds through one step synthesis and purify and recrystallize the product	Analyze
C.O. 2: Plan and perform synthetic procedures, chromatographic separation and purification of organic compounds	Understand
C.O. 3: Separate organic compounds from the organic binary mixture and identify the functional group(s) present	Analyze

Course Outcome	Program Specific Outcome					
	P.S.O. 1	P.S.O. 2	P.S.O. 3	P.S.O. 4	P.S.O. 5	P.S.O. 6
C.O. 1	3	3	3	3	2	1
C.O. 2	3	3	3	2	2	0
C.O. 3	2	2	3	2	1	0

1.	Separation and identification of the components of organic binary mixtures.
2.	One step synthesis of Organic Compounds
3.	General methods of separation and purification of Organic compounds such as 1) Solvent extraction 2) Thin layer chromatography and paper chromatography 3) column chromatography.

Recommended Text Books

1. Pavia, D.L. Lampman, G.M. Kriz, G.S. and Engel, R.G. Introduction to Organic Laboratory Techniques: A small scale Approach, 2nd Ed., 2007.
2. Mann, F.G. Saunders, B.C. Practical Organic Chemistry, 4th Ed., Pearson Education India, 2009.
3. Furniss, B.S. Hannaford, A.J. Smith, P.WG. Tatchell, A.R. Vogel's Textbook of Practical Organic Chemistry, 5th Ed., Longman, 1989.

23-808-0505

INORGANIC CHEMISTRY LAB -II

Credit 2 **36 hours**

Course Outcome After the completion of the course, the student will be able to	**Cognitive Level**
C.O. 1: Apply the concepts of qualitative and quantitative aspects in inorganic preparation	Apply
C.O. 2: Estimate the amount of any given substance gravimetrically	Apply
C.O. 3: Synthesize metal complexes and characterize them by various physicochemical methods	Apply

Course Outcome	Program Specific Outcome					
	P.S.O. 1	P.S.O. 2	P.S.O. 3	P.S.O. 4	P.S.O. 5	P.S.O. 6
C.O. 1	3	2	2	2	2	2
C.O. 2	3	2	2	2	2	2
C.O. 3	3	2	2	2	2	2

1.	Gravimetric analysis: Estimation of Barium, sulphate, Calcium, iron, nickel.
2.	Inorganic preparations: Preparation of Tris(oxalato)manganese(III), Tetrapyridinesilver(II) peroxidisulphate, Tris(acetylacetonato) iron(III), Bis(N,N-diethyldithiocarbamato)nitrosyliron(I), Optical isomers of tris(ethylenediamine)cobalt(III)chloride, Nitropentamminecobalt(III) chloride, Tri(acetylacetonato)manganese(III), Tris(thiourea) copper(I) sulphate, Phenyl lithium, Tetraphenyl lead, Ferrocene, Phosphonitrilic chloride.

Recommended Text Books:

1. A.I. Vogel, A Text Book of Quantitative Inorganic Analysis, Longman, 1966
2. G. Pass, H. Sutcliffe. Practical Inorganic Chemistry 2nd edition, Chapman & Hill. 1974.
3. J. Mendham, R. C. Denney, J. D. Barnes, M. Thomas, Vogel's Textbook of Quantitative Chemical Analysis, 6th Edn., Pearson Education, Noida, 2013.

23-808-0601

INORGANIC CHEMISTRY – III

(Group Theory and Concepts in Inorganic Chemistry)

Credit 4 **72 hours**

Course Outcome After the completion of the course, the student will be able to	**Cognitive Level**
C.O. 1: Analyze the symmetry of any given molecule and assign the point group	Analyze
C.O. 2: Apply the principles of symmetry and group theory in structure, bonding and spectral characteristics of molecules	Apply
C.O. 3: Identify the structure-activity relationship of simple molecules based on their qualitative molecular orbitals	Apply
C.O. 4: Assess the strength of various acids and bases and their reactivity	Evaluate
C.O. 5: Explain behavior of different non-aqueous solvent systems towards different reactions	Apply

Course Outcome	Program Specific Outcome					
	P.S.O. 1	P.S.O. 2	P.S.O. 3	P.S.O. 4	P.S.O. 5	P.S.O. 6
C.O. 1	3	2	2	2	1	1
C.O. 2	3	2	2	2	1	1
C.O. 3	3	3	2	2	1	2
C.O. 4	3	2	1	2	1	1
C.O. 5	3	2	1	2	1	1

UNIT I **18 hrs**

Matrix representation of symmetry operations, similarity transformation and classes, Symmetry classification of molecules into point groups (Schoenflies symbol)- Reducible and Irreducible representations - Great Orthogonality theorem and its consequences (statement only, proof not needed), Character tables, Reduction formula, construction of character tables for point groups with order ≤6-, Interpretation of character tables. Wave functions as bases for irreducible representations, Direct product. Application of symmetry to predict polar and chiral compounds

UNIT II **18 hrs**

Application of Group theory to Hybridization of atomic orbitals: Construction of hybrid orbitals for AB_3(planar), $AB_4(T_d)$, $AB_5(D_3h)$ and $AB_6(O_h)$ type of molecules.

Application of group theory to Molecular Orbital Theory: LCAO and Huckel approximations. Symmetry adapted linear combinations, Projection operators, Application of projection operators to pi-bonding in ethylene, cyclopropenyl systems, benzene and naphthalene. Application of projection operators to sigma bonding in ethylene and $PtCl_4^{2-}$. Molecular orbitals for tetrahedral and octahedral

molecules, Applications of Group theory for molecular vibration, symmetry of group vibrations. Selection rules and applications to IR, Raman and electronic spectra.
UNIT III **12 hrs**
Qualitative molecular orbital theory, symmetry of molecular orbitals, MOs for homo and heteronuclear diatomic molecules, H_2 to F_2, HF, CO, NO, BeH_2, CO_2, H_2O, BH_3, NH_3, B_2H_6. Importance of frontier molecular orbitals, Shape, energy and reactivity of molecules.
UNIT IV **12 hrs**
Relative strength of acids, Pauling rules, Lewis concept, Generalized acid-base concept, Measurement of acid base strength, Lewis acid –base interactions, steric and solvation effects, acid–base anomalies, Pearson's HSAB concept, acid-base strength and hardness and softness, Symbiosis, theoretical basis of hardness and softness, electronegativity and hardness.
UNIT V **12 hrs**
Chemistry in non-aqueous solvents reactions in NH_3, liquid SO_2, solvent character, reactions in SO_2, acetic acid, solvent character, reactions in H_2SO_4 and some other solvents. Molten salts, Green solvent: supercritical CO_2, Ionic liquids and deep eutectic solvents.

Recommended Text Books:

1. F. A. Cotton, Chemical Applications of Group theory, Wiley Eastern, Singapore, 2nd ed., 1992.
2. V. Ramakrishnan, M. S. Gopinathan, Group theory in Chemistry, Vishal Pub. New Delhi, 1996.
3. Alan Vincent, Molecular Symmetry and Group Theory: A Programmed Introduction to Chemical Applications, 2nd ed., Wiley, 2013.
4. Robert L. Carter, Molecular Symmetry and Group Theory, Wiley, 2009.
5. Kieran C. Molloy, Group Theory for Chemists: Fundamental Theory and Applications, 2nd edition, Woodhead publishing, 2010.
6. G.L. Miessler, P.J. Fischer, D.A. Tarr, Inorganic Chemistry, 5th ed., Pearson, 2014.
7. E. Huheey, E. A. Keiter, R. L. Keiter, Inorganic Chemistry: Principles of Structure and Reactivity, 4th ed., Harper Collin College Publishers, 1993.
8. F. A. Cotton, G. Wilkinson, C. A, Murillo, M. Bochmann, Advanced Inorganic Chemistry, 6th ed., Wiley- Interscience: New York, 1999.
9. D. F. Shriver, P. W. Atkins, C. H. Langford, Inorganic Chemistry, 3rd ed., ELBS, 1999.
10. B. Douglas, D. McDaniel, J. Alexander, Concepts and Models of Inorganic Chemistry, 3rd ed., Wiley, 1994.
11. N. N. Greenwood, A. Earnshaw, Chemistry of the Elements, 2nd ed., Butterworth-Heinemann, 1997.
12. C.E. Housecroft, A.G. Sharpe, Inorganic Chemistry, 5th ed., Pearson, 2018.

23-808-0602

ORGANIC CHEMISTRY III

(Organic Chemistry Reactions, Reagents, Photochemistry & Pericyclic Reactions)

Credit 4 **72 hours**

Course Outcome After the completion of the course the student will be able to	**Cognitive Level**
C.O. 1: Interpret the differences in reactivity of various reducing, oxidizing agents, organometallic and organo-nonmetallic reagents with mechanistic illustrations	Apply
C.O. 2: Analyze the reagents and conditions for the synthesis of specific target molecules	Analyze
C.O. 3: Identify the mechanism and the product in a given reaction under photochemical conditions	Apply
C.O. 4: Apply the concepts of Frontier orbital theory in the study of pericyclic reactions	Apply

Course Outcome	Program Specific Outcome					
	P.S.O. 1	P.S.O. 2	P.S.O. 3	P.S.O. 4	P.S.O. 5	P.S.O. 6
C.O. 1	3	1	3	3	1	2
C.O. 2	2	2	3	2	1	2
C.O. 3	1	2	2	1	1	1
C.O. 4	1	2	1	1	1	2

UNIT I **16 hrs**

Reagents for oxidation and reduction: Chromium reagents, activated DMSO, osmium tetroxide, selenium dioxide, singlet oxygen, peracids, hydrogen peroxide, periodic acid, lead tetraacetate, ozonolysis, Woodward and Prevost hydroxylation, Wacker process, Oppenauer oxidation, Sharpless, Shi and Jacobsen asymmetric epoxidations. Catalytic hydrogenations (heterogeneous-Palladium/Platinum/Rhodium and Nickel, homogeneous-Wilkinson), metal hydride reduction-$LiAlH_4$, DIBAL-H, Red-Al, $NaBH_4$ and $NaCNBH_3$. Selectrides, trialkylsilanes and trialkyl stannane. Birch reduction, hydrazine and diimide reduction. Meerwein-Ponndorf-Verley reaction, Enzymatic reduction using Baker's yeast.

UNIT II **14 hrs**

Synthetic applications of organometallic and organo-nonmetallic reagents: Hydroboration reactions, Sakurai allylation, Gilman's reagent, Ullmann and Glaser coupling reactions. Suzuki coupling, Sonogashira coupling, Heck reaction, Buchwald–Hartwig coupling, Negishi coupling and Stille coupling. Metathesis processes of electrophilic carbene complexes (first- and second-generation Grubbs catalyst), ROMP, Dötz reaction and methylenation of carbonyls.

Reagents such as NBS, DCC, DMAP, DEAD, DDQ. Phase transfer catalysts. Chemistry of Nucleophilic Heterocyclic Carbenes (NHCs), multicomponent reactions such as Ugi reaction, Passerini reaction, Biginelli reaction. Click reaction.
UNIT III **16 hrs**
Chemistry of carbonyl compounds: Reactivity of carbonyl groups in aldehydes, ketones, carboxylic acids, esters, acyl halides and amides. Substitution at carbonyl carbon, mechanisms of ester hydrolysis, substitution at α-carbon, aldol and related reactions. Grignard reaction, Reformatsky reaction, Claisen, Darzen, Dieckmann, Knoevenagel and Stobbe condensations. Perkin, Prins, Mannich, Stork-enamine reactions. Conjugate additions, Michael additions and Robinson annulation. Favorskii reaction, Julia olefination, Peterson olefination. Preparation of 1,2-, 1,3-, 1,4- and 1,5-diketones from simple ketones. Reaction with phosphorous and sulfur ylides.
UNIT IV **14 hrs**
Photochemistry: Unimolecular and bimolecular processes in the excited states, mechanism of important photochemical reactions, Paterno-Buchi reaction, Norrish Type I and Type II fragmentation, di-pi- methane rearrangement, Barton reaction, photochemistry of olefins, arenes, cyclohexadienones; photoreduction and photo-oxygenation.
UNIT V **12 hrs**
Pericyclic reactions: Study of the principle of conservation of orbital symmetry: Orbital symmetry diagrams for cycloaddition and electrocyclic reactions. Aromatic Transition State Theory and The Generalized Woodward – Hoffmann rule applied to cycloaddtions, Electrocyclic reactions, Sigmatropic rearrangements and Chelotropic reactions. Pericyclic Reactions in Organic Synthesis: Stereochemistry and Regiochemistry of Cycloaddtions. Substituent and medium effects, Secondary Orbital Interactions in [4+2] cycloadditions, Intramolecular Diels–Alder reactions. Stereochemistry of Electrocyclic Reactions and Sigmatropic rearrangements. Cope rearrangement, Claisen rearrangement and ene-reaction. Pericyclic reactions in Organic synthesis – case studies.

Recommended Text Books:

1. M. B. Smith, Organic Synthesis, 2nd ed., McGraw-Hill, 2000.
2. M. B. Smith, March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure, 7th ed., Wiley, 2013.
3. F. A. Carey, R. J. Sundberg, Advanced Organic Chemistry (parts A and B), 5th ed., Springer, 2008.
4. J. Clayden, N. Green, S. Warren, P. Wothers, Organic Chemistry, 2nd ed., Oxford University Press, 2012.
5. N. J. Turro, V. Ramamurthy, J. C. Scaiano, Modern Molecular Photochemistry of Organic Molecules, University Science Books, 2010.

6. E. V. Anslyn, D. A. Dougherty, Modern Physical Organic Chemistry. University Science Books, 2006.
7. H. R. Crabtree, The Organometallic Chemistry of the Transition Metals, 6th ed., John Wiley & Sons, 2014.
8. S. D. Burke, R. L. Danheiser, Handbook of Reagents for Organic Synthesis, John Wiley & Sons, 1999.

23-808-0603

PHYSICAL CHEMISTRY III

(Chemical Kinetics and Statistical Thermodynamics)

Credit 4 **72 hours**

Course Outcome After the completion of the course the student will be able to	**Cognitive Level**
C.O. 1: Interpret the basic reaction dynamics and kinetics of various reactions and obtain the rate constants for reactions in gaseous state and solutions	Analyze
C.O. 2: Calculate the thermodynamic parameters from kinetic data	Apply
C.O. 3: Explain the different types of statistics and calculate the thermodynamic probability of any given thermodynamic system	Apply
C.O. 4: Apply the principles of statistical thermodynamics to ideal gases/solids and calculate thermodynamic properties from spectroscopic data	Apply

Course Outcome	Program Specific Outcome					
	P.S.O. 1	P.S.O. 2	P.S.O. 3	P.S.O. 4	P.S.O. 5	P.S.O. 6
C.O. 1	3	0	0	2	2	2
C.O. 2	3	0	0	2	2	2
C.O. 3	3	0	0	2	2	2
C.O. 4	3	0	0	2	2	2

UNIT I **14 hrs**
Complex Reactions: Parallel, Consecutive and Opposing reactions, Steady state Approximation, Kinetics of chain reactions - Photochemical reactions H_2-Cl_2 and H_2-Br_2 reaction, Organic decomposition reactions-Rice Herzfield mechanism (acetaldehyde and ethane), Branched Chain Reactions, Explosions-Somenoff Hinshelwood mechanism (H_2-O_2 reaction), Termolecular reactions.
UNIT II **16 hrs**
Molecular reaction dynamics: Reactive encounters, Theories of reaction rates-Collision Theory recap), Activated Complex Theory- Potential energy surface, Erying equation, Comparative evaluation of collision and transition state theory, Thermodynamic treatment of reaction rates. Theory of unimolecular reactions- Lindemann Mechanism, Modifications to Lindemann mechanism-Hinshelwood, RRK and RRKM model. Termolecular reactions. Molecular beam methods, Stripping and rebound mechanism.
UNIT III **16 hrs**
Reactions in Solutions: Cage effect, Transition state theory for reactions in solutions, Effect of ionic strength, dielectric constant and Internal pressure. Primary and secondary salt effect. Diffusion

controlled reactions. Isotope effects: Equilibrium isotope effects. Primary and Secondary kinetic isotope effects.
UNIT IV **14 hrs**
Maxwell Distribution of molecular velocities, Thermodynamic probability, microstate and macrostate, entropy and probability, most probable distribution, residual entropy and its calculation. Ensembles, Maxwell - Boltzman statistics. Quantum statistics: Bose - Einstein statistics, Fermi - Dirac statistics, Dilute Systems.
UNIT V **12 hrs**
Partition function and its relation to thermodynamic properties: Translational, rotational and Vibrational partition function. Molecular partition function for delocalized systems, Calculation of equilibrium constant using partition functions. Heat capacity of gases and solids, Electron gas concept.

Recommended Text Books:

1. W. J. Moore and R. G. Pearson, Kinetics and Mechanism, Wiley, New York.
2. K. J. Laidler, Chemical-Kinetics, McGraw Hill, New York.
3. M. R. Wright, An Introduction to Chemical Kinetics, Wiley, 2004.
4. Richard Masel, Chemical kinetics and Catalysis, Wiley Interscience.
5. P. W. Atkins, Physical Chemistry 8th Edn., Wiley, New York.
6. Christian Reichardt, Solvents and Solvent effects in Organic Chemistry, Wiley VCH 2003.
7. sF.W. Sears, Introductions to Thermodynamics, Kinetic Theory of Gases and Statistical Mechanics, Addision Wesley Pub. Cambridge, 1998.
8. F.C. Andrews, Equilibrium to Statistical Mechanics, John Wiley, New York, 2002.
9. L.K. Nash, Statistical Thermodynamics, Addison Wesley, New York, 1999.
10. P.W Atkins, Julio De Paula, Physical Chemistry, Oxford University Press, 10th/11th edn, 2017/2018
11. D. A. McQuarrie, Physical Chemistry- A Molecular Approach, South Asian Edn., 2008.
12. M. Dole, Introduction to Statistical Thermodynamics, Prentice Hall, London, 1997.
13. D. A. McQuarrie, Statistical Thermodynamics, South Asian Edn., 2008.

23-808-0604

ORGANIC CHEMISTRY LAB II

Credit 2 **36 hours**

Course Outcome After the completion of the course, the student will be able to	**Cognitive Level**
C.O. 1: Plan and perform synthetic procedures, chromatographic separation and purification of organic compounds	Understand
C.O. 2: Use Chemical Abstracts, Scopus, Organic Synthesis collective volumes on web etc. to search, analyse and collect chemical information	Apply
C.O. 3: Use software to Draw the structures and schemes of organic molecules and reactions	Apply

Course Outcome	Program Specific Outcome					
	P.S.O. 1	P.S.O. 2	P.S.O. 3	P.S.O. 4	P.S.O. 5	P.S.O. 6
C.O. 1	3	3	3	3	2	1
C.O. 2	2	2	2	2	0	3
C.O. 3	1	1	1	1	0	0

1.	Preparation of Organic compounds by multistep reactions, purification of products and characterisation using UV-Vis, FTIR and NMR.
2.	Use Chemical Abstracts, Scopus, Organic Synthesis collective volumes on web etc., to search, analyse and collect chemical information.
3.	Drawing the structures of organic molecules and reaction schemes by Proprietary and open source computer software.
	*Progress of the reactions should be followed by spectroscopic and chromatographic methods (UV- Vis, TLC, GC, HPLC, etc.

Recommended Text Books:

1. A. I. Vogel, A. R. Tatchell, B. S. Furnis, A. J. Hannaford, P. W. G. Smith, Vogel's Textbook of Practical Organic Chemistry, 5th ed., John Wiley, 1989.
2. D. L. Pavia, G. M. Lampman, G. S. Kriz, Introduction to Organic laboratory Techniques,
3. L. W. Harwood, C. J. Moody, Experimental Organic Chemistry-Principles and Practice, Blackwell Science Publications

23-808-0605

PHYSICAL CHEMISTRY LAB II

Credit 2 **36 hours**

Course Outcome After the completion of the course, the student will be able to	**Cognitive Level**
C.O. 1: Execute and perform experiments based on pH metry, potentiometry, conductometry and colorimetry	Evaluate

Course Outcome	Program Specific Outcome					
	P.S.O. 1	P.S.O. 2	P.S.O. 3	P.S.O. 4	P.S.O. 5	P.S.O. 6
C.O. 1	3	3	3	2	2	2

1.	pH Metry: Acid-base titrations involving strong and weak acids/bases.
2.	Conductometry: Acid-base titrations involving strong and weak acids/base, Determination of degree of ionization of weak electrolytes.
3.	Potentiometry: Acid-base titrations involving strong and weak acids/base, Determination of degree of ionization of weak electrolytes. Redox titrations.
4.	Colorimetry: Verification of Beer-Lambert Law, Estimation of ferric iron by colorimetry, Estimation from real samples.

Recommended Text Books:

1. Gurtu, J. N., Gurtu, A., Advanced Physical Chemistry Experiments, 6th Ed.,Pragati Prakashan,2014.
2. Yadav, J. B., Advanced Practical Physical Chemistry, 36th Ed., Krishna Prakashan, 2016.
3. D.P Shoemaker, G.W Garland, J.W Nibler, Experiments in Physical Chemistry, 5th Edn., McGraw Hill.

23-808-0701

INORGANIC CHEMISTRY – IV

(Reaction Mechanism and Organometallic Chemistry)

Credit 4 **72 hours**

Course Outcome After the completion of the course, the student will be able to	**Cognitive Level**
C.O. 1: Understand the basic concepts and applications of organometallics	Apply
C.O. 2: Evaluate the structure, bonding and reactions of organometallic compounds and metallocenes	Evaluate
C.O. 3: Predict the stability of organometallic compounds and metal clusters	Apply
C.O. 4: Explain the application of reactions of organometallic complexes in homogeneous catalytic processes	Apply
C.O. 5: Explain the stability of transition metal complexes, their reactivity, and the mechanisms of ligand substitution	Apply

Course Outcome	Program Specific Outcome					
	P.S.O. 1	P.S.O. 2	P.S.O. 3	P.S.O. 4	P.S.O. 5	P.S.O. 6
C.O. 1	1	1	1	2	2	1
C.O. 2	3	1	1	3	3	3
C.O. 3	3	1	1	3	3	2
C.O. 4	3	3	1	3	3	2
C.O. 5	3	3	1	3	3	2

UNIT I **14 hrs**

Organometallic Chemistry. Compounds with transition metal to carbon bonds: eighteen electron rule; classification of ligands, nomenclature, metal-metal multiple bonding, Concept of hapticity of organic ligands. Metal carbonyls: 18 electron rule, EAN rule as applied to carbonyls, electron count of mononuclear, polynuclear and substituted metal carbonyls of 3d series. Preparation and structure of mononuclear and binuclear carbonyls of Cr, Mn, Fe, Co and Ni. π-acceptor behaviour of CO, synergic effect and use of IR data to explain extent of back bonding.

UNIT II **14 hrs**

σ donor ligands – metal alkyl, aryl complexes; σ donor/π acceptor ligands, – metal alkenyls, alkynyls, carbenes, carbynes, isocyanide, phosphines, fluxionality of ligands – structure, bonding, spectra, preparation and reactions.

σ, π donor/π acceptor ligands – olefin complexes, alkyne, allyl, enyl complexes

Metallocene- ferrocene, titanocene, zircanocene, arene complexes, cycloheptatriene, cyclooctatetraene, cyclobutadiene complexes, fluxionality of ligands – structure, bonding, preparation, reactions and spectroscopy.

UNIT III **14 hrs**

Metal–Metal bonds and Transition metal clusters; preparation, properties and spectroscopy. Parallels with nonmetal chemistry- isolobal analogy. Application of Wade-Mingos-Lauher rules in predicting the structure of organometallic clusters Organo-lithium aluminium, magnesium, zinc and titanium compounds – their preparations, properties, reactions, bonding and applications.

Spectral analysis and characterization of organometallic complexes.

UNIT IV **14 hrs**

Reactions of organometallic complexes – Ligand cone angle, oxidative addition, reductive elimination, insertion, nucleophilic and electrophilic attack of coordinated ligands. Homogeneous catalysis using organometallic compounds: olefin hydrogenation, hydroformylation, Wacker process, Ziegler-Natta polymerisation, cyclo oligomerisation, olefin isomerisation, olefin metathesis, Monsanto acetic acid synthesis, Fischer-Tropsch process, hydrosilylation, coupling reactions in organic chemistry.

UNIT V **16 hrs**

Reaction Mechanism: Thermodynamic and kinetic consideration, formation constant and rate constant, inert and labile complexes, factors affecting the stability and lability of complexes.

Ligand substitution in octahedral complexes, mechanism of substitution reactions in octahedral complexes, dissociative, associative and interchange mechanism, energy profile of reactions, acid and base hydrolysis, factors affecting the rate of substitution reactions in octahedral complexes.

Ligand substitution in square planar complexes, mechanism of substitution reactions in square planar complexes, energy profile of reactions, the trans effect and its applications, theories for explaining trans effect, factors affecting the rate of substitution reactions in square planar complexes.

Electron Transfer Reactions: inner sphere and outer sphere mechanism, Marcus theory, photochemical

reactions.

Recommended References:

1. Ch. Elschenbroich, A. Salzer, Organometallics – A Concise Introduction, VCH Publishers, 1989.
2. B. D. Gupta, A. J. Elias, “Basic Organometallic Chemistry”, University Press, 2010.
3. P. Powell, Principles of Organometallic Chemistry, 2nd ed., ELBS, 1991.
4. J. E. Huheey, E. A. Keiter, R. L. Keiter, Inorganic Chemistry: Principles of structure and Reactivity, 4th ed., Harper Collin College Publishers, 1993.

5. Basolo, F, and Pearson, R.C., Mechanisms of Inorganic Chemistry, 2nd Ed., John Wiley & Sons, NY, 1967.
6. Crabtree, Robert H. The Organometallic Chemistry of the Transition Metals. 6th Ed., New York, NY: John Wiley, 2014.
7. Miessler, G.L. & Tarr, D. A. Inorganic Chemistry, 5th Ed., Pearson Publication, 2013.
8. D. F. Shriver, P. W. Atkins, C. H. Langford, Inorganic Chemistry, 3rd ed., ELBS, 1999.

23-808-0702

ORGANIC CHEMISTRY IV

(Natural Products, Dyes and Pigments)

Credit 4 **72 hours**

Course Outcome After the completion of the course the student will be able to	**Cognitive Level**
C.O. 1: Devise synthesis scheme for heterocyclic aromatic and nonaromatic organic compounds	Analyze
C.O. 2: Elucidate structure and device synthesis for important natural products	Apply
C.O. 3: Explain the chemical properties, structure and application of organic dyes and pigments	Understand

Course Outcome	Program Specific Outcome					
	P.S.O. 1	P.S.O. 2	P.S.O. 3	P.S.O. 4	P.S.O. 5	P.S.O. 6
C.O. 1	1	3	3	2	2	2
C.O. 2	1	1	3	1	3	2
C.O. 3	1	1	1	1	3	2

UNIT I **16 hrs**

Heterocyclic compounds: Nomenclature of three to seven-membered aliphatic heterocyclic compounds containing one heteroatom (N, O). Five and six-membered heteroaromatic compounds containing one to four heteroatoms (N, O, S). Indole, quinoline and isoquinoline. Structure and general preparations. Alkaloids: Isolation and classification, isolation, and structure elucidation based on degradative reactions (quinine and atropine). Biosynthesis of quinine and papaverine.

Basic introduction to flavonoids and anthocyanin: Structure, properties and biological functions.

UNIT II **14 hrs**

Dyes and pigments: structure and properties of dyes and pigments, natural and synthetic dyes, classification, azodyes, triarylmethane dyes, anthraquinone dyes, indigoid dyes, cyanine dyes, sulfur dyes, nitro and nitroso dyes. Edible dyes (food colours) with examples, dyes for electro-optical application, textile colourants and cosmetic colourants, porphyrins, chlorins, bactereochlorins and phthalocyanines.

UNIT III **16 hrs**

Terpenoids: Classification, biosynthesis. Structure elucidation and synthesis of abietic acid.

Steroids: classification, biosynthesis. Structure elucidation of cholesterol, conversion of cholesterol to progesterone, androsterone and testosterone. Fatty acids: structure, biosynthesis. Prostaglandins-classification, structure, biosynthesis and synthesis.

UNIT IV	**14 hrs**
Lipids: Classification, biological functions, fatty acids -omega 3 and omega 6 fatty acids, extraction and refining of oils and fats. Carbohydrates: Structure of ribose, glucose, fructose, maltose, sucrose, lactose, starch cellulose and cyclodextrins. Preparation of alditols, glycosides (O, C, and N), deoxysugars. Synthesis of Vitamin C from glucose.	
UNIT V	**12 hrs**
2D NMR spectroscopy, emission and chiroptical spectroscopy.	

Recommended Text Books:

1. I. L. Finar, Organic Chemistry Volumes 1 & 2, 6th ed., Pearson Education Asia, 2004.
2. J. Clayden, N. Green, S. Warren, P. Wothers, Organic Chemistry, 2nd ed., Oxford University Press, 2012.
3. N. R. Krishnaswamy, Chemistry of Natural Products; A Unified Approach, Universities Press, 1999.
4. S. P. Bhutani, Chemistry of Biomolecules, 2nd ed., CRC Press, 2020.
5. R. O. C. Norman, Principles of Organic Synthesis, 2nd ed., Chapman and Hall, 1978.
6. J. A. Joule, K. Mills, Heterocyclic Chemistry, 5th ed., Wiley, 1998.
7. A. Gürses, M.Açıkyıldız, K. Güneş , M. S. Gürses, Dyes and Pigments, Springer, 2016.
8. Heinrich Zollinger, Colour Chemistry: Synthesis, Properties and applications of organic dyes and pigments, VCH, Germany, 1987.
9. D.L.Pavia, G.M. Lampman, G.S.Kriz, Introduction to Spectroscopy, A Guide for Students of Organic Chemistry, 3rd ed., Thomson. 2004.
10. R. M. Silverstein, G.C. Bassler, T. C. Morril, Spectroscopic identification of organic compounds, John Wiley, 1991.
11. Spectral databases (RIO DB of AIST, for example)

23-808-0703

THEORETICAL CHEMISTRY – II

(Approximations and Chemical Bonding)

Credit 4 **72 hours**

Course Outcome After the completion of the course, the student will be able to	**Cognitive Level**
C.O. 1: Derive the Schrodinger equation for multielectronic atoms and interpret the results	Apply
C.O. 2: Derive the variational principle and perturbation theory, use them to calculate properties for simple systems of chemical interest	Analyze
C.O. 3: Explain Hartree-Fock Theory and semiempirical Huckel MO treatment and its application to polyelectronic molecules	Analyze
C.O. 4: Classify various basis sets and justify its use for a specific problem	Analyze
C.O. 5: Explain different chemical properties of molecules by drawing molecular orbitals	Analyze

Course Outcome	Program Specific Outcome					
	P.S.O. 1	P.S.O. 2	P.S.O. 3	P.S.O. 4	P.S.O. 5	P.S.O. 6
C.O. 1	3	2		2	1	
C.O. 2	3	2	1	2	1	
C.O. 3	2	3	1	3	2	1
C.O. 4	3	3	1	3	3	3
C.O. 5	3	3	1	3	3	2

UNIT I **16 hrs**
Solving the Schrodinger equation of Hydrogen atom: Separation into three equations and solutions, Theta and phi equations and solutions, Spherical harmonics, Radial equations and solutions, Laguerre equation and Laguerre polynomials. Solutions of wave functions and energies, quantum numbers and their importance, Radial wave function and radial distribution functions, angular wave function, Shapes of s, p, d and f atomic orbitals. Hamiltonian operators, Wave functions and energy of H like systems, Orbital functions, Postulate of electron spin-orbital and spin functions. Zeeman effect. Spin Orbitals and their construction, Antisymmetric wave functions, Pauli's antisymmetry principle.
UNIT II **12 hrs**
Many body problems, Born –Oppenheimer Approximations, Independent particle method, Drawbacks. Variational method – theory, proof and general treatment of linear variational problem- Application to systems such as Hydrogen, Helium and various other cases. Hamiltonian operator for multielectronic atom, Perturbation method: Time Independent perturbation for non- degenerate –first

order, perturbation corrections to energy and wave functions, Application of this to various systems such as particle in a box, helium atom.

UNIT III **8 hrs**

ISelf-Consistent Field approximation- Hartree's proposal, Pauli's antisymm principle, Pauli exclusion

principle, Electron spin, Constructing Antisymmetric spin incorporated wave functions for He, excited state of He – various electronic states, term symbols. Hartree-Fock Self Consistent Field method for multielectronic atoms. The Coulomb and Exchange Operators, The Fock Operator, Koopmans' theorem, Brillouin's theorem, Slater's treatment of complex atoms, Slater orbitals, Slater determinant and wave function.

UNIT IV **18 hrs**

Chemical Bonding- Application to H_2^+, MO and VB treatment of H_2 molecule- Comparison. Concept of σ, σ^*, π, π^* orbitals and their characteristics, hybrid orbitals, calculation of coefficients of AO used in sp, sp^2 and sp^3 hybrid orbitals, interpretation of geometry, Valence bond model of H_2, Hybridisation of H_2O, BF_3, NH_3 and CH_4 Hartree Fock -Roothaan method - LCAO approximation - Restricted HartreeFock (RHF) for closed shell systems, Restricted open HF (ROHF), and Unrestricted HF (UHF) methods, Empirical, Semi empirical and ab initio methods. Basis functions- Slater Type Orbital and Gaussian Type Orbitals. Contracted and primitive. Basis sets. Minimal, multiple zeta, split-valence, polarized and diffused. Pople style basis sets, designation of basis set size –Dunnings correlation consistent basis sets, Relativistic effects - Effective core potential, ECP.

UNIT V **18 hrs**

HMOT: Pi bonding in simple molecules, HMO method for linear conjugated hydrocarbons, linear, cyclic, polycyclic, heterocyclic; ethylene, 1,3-butadiene, allyl radical, cation and anion, aromatic hydrocarbons, cyclopropenyl systems, cyclobutadiene, benzene, naphthalene, thiophene. Calculation of charge distribution, bond orders and reactivity. QMOT: Applications of Molecular Orbital Theory in Understanding reactions and Mechanisms. Qualitative MO theory. Group orbitals. Frontier Orbitals, Substituent effects on frontier orbitals, HSAB concept, Nucleophiles and Electrophiles, Perturbation theory of reactivity. Application of Frontier Orbital theory in studying ionic and radical reactions, Ambident electrophiles, α-effect.

Recommended Text Books:

1. Atkins, P.W. and Paula, J. Physical Chemistry, 8th Ed., Oxford Press, 2006.
2. Szabo, A.; Ostlund, N. S. "Modern Quantum Chemistry: Introduction to Advanced Structure theory", Dover Publications, 1996.
3. Levine, I. N. "Quantum Chemistry", 7th Edition, Pearson Education Inc., 2014.
4. McQuarrie, D. A., "Quantum Chemistry", 2nd Edition, University Science Books, 2008.

5. Pillar, F. L. “Elementary Quantum Chemistry”, 2nd Edition, Dover Publication, 2001.
6. Chandra, A. K., "Introduction to Quantum Mechanics", 4th Ed, Tata McGraw-Hill, New Delhi, 2003.
7. Prasad, R. K., “Quantum Chemistry”, 4th Edition, New Age International, 2009.
8. Cramer, C. J., “Essentials of Computational Chemistry- Theories and Models”, 2nd Edition, Wiley, 2004
9. Jensen, F., “Introduction to Computational Chemistry”, 3rd Edition, Wiley, 2017.
10. Young, D., “Computational Chemistry – A Practical Guide”, Wiley, 2001.
11. Anslyn, E. V.; Dougherty, D. A. Modern Physical Organic Chemistry. University Science Books

23-808-0704

SPECTROSCOPY

Credit 4 **72 hours**

Course Outcome After the completion of the course, the student will be able to	**Cognitive Level**
C.O. 1: Explain the factors affecting the intensity and broadening of lines in spectra and methods to enhance the sensitivity	Understand
C.O. 2: Explain the principles of rotational, vibrational, Raman, electronic, fluorescence, NMR and ESR	Understand
C.O. 3: Calculate energy required for a particular type of energy transition and determine the parameters involved	Apply
C.O. 4: Apply various theoretical aspects to various spectroscopic techniques for prediction of different spectroscopic observations	Analyze
C.O. 5: Identify various d-d transitions and interpret the electronic spectra of any given transition metal complex	Apply
C.O. 6: Interpret the ESR and Mossbauer spectra of given transition metal complex	Evaluate

Course Outcome	Program Specific Outcome					
	P.S.O. 1	P.S.O. 2	P.S.O. 3	P.S.O. 4	P.S.O. 5	P.S.O. 6
C.O. 1	3	3	2	2	3	1
C.O. 2	3	3	2	2	3	1
C.O. 3	3	3	2	2	3	1
C.O. 4	3	3	2	2	3	1
C.O. 5	3	3	2	2	1	1
C.O. 6	3	3	2	2	3	1

UNIT I	**10 hrs**
Population of energy levels. Induced quantum transitions. Integrated absorption coefficient. Einstein's coefficients of absorption. Basis of selection rules, transition moment integral. Beer's Law. Induced absorption and emission of radiation by molecules, Factors affecting the intensity and width of spectral lines, Methods to reduce line broadening.	
UNIT II	**16 hrs**
Rotational and vibrational energies of diatomic molecules. Linear molecules, Symmetric top and asymmetric top molecules. Rotation spectra: Diatomic and polyatomic molecules, Selection rule.	

Vibration spectra of diatomic molecules, Morse potential of real molecules, overtones, combination and hot bands, Fermi resonance, rotational character of vibration spectra. Coupling of rotation and vibration. Parallel and perpendicular bands.

Vibration spectra of polyatomic molecules, Normal modes of vibrations of polyatomic molecules. Raman Spectroscopy. Rotational Raman spectra. Vibrational Raman spectra, Resonance Raman, mutual exclusion principle. Selection rules and applications to IR and Raman spectra, Surface enhanced Raman spectroscopy.

Applications of Group theory for molecular vibration, symmetry of group vibrations. Selection rules and applications to IR and Raman spectra.

UNIT III **18 hrs**

Electronic energy states of molecules. Selection rules for electronic transitions, Vibrational structure of electronic bands. Electronic transitions and absorption bands. Electronic spectra of diatomic and polyatomic molecules, its relation to electronic arrangement and symmetry of molecules. Different types of electronic transitions, Electronic spectra of conjugated systems.

Principle of fluorescence spectroscopy, Quenching of fluorescence, Mechanisms of quenching Magnetic resonance spectroscopy: Theory of nuclear magnetic resonance, Chemical shifts, Factors affecting chemical shifts, First order and second order spectra, relaxation effects. Fourier Transformation in NMR, Measurement of relaxation time, Spin echo, NOE, 2D NMR, NQR Spectroscopy. MRI, Solid state NMR.

Principle of electron spin resonance.

UNIT IV **14 hrs**

Microstates, Atomic term symbols Free ion terms for dn configuration, Splitting of terms in octahedral and tetrahedral octahedral fields, Correlation diagram for d2 configuration in octahedral geometry, d-d transitions, Selection rules for electronic transitions.

Orgel diagram – splitting for d1, d9, high spin d4, d6, splittings for high spin d2, d3, d8 and d7. Calculation of Dq, B and β

Tanabe Sugano diagrams – splittings for low spin dn systems Electronic Spectral interpretation of some coordination compounds

Consequence of Jahn Teller effect on the electronic spectra of coordination compounds

Charge transfer spectra, Electronic spectra of lanthanide and actinide complexes.

UNIT V **14 hrs**

Electronic paramagnetic resonance spectroscopy: Electronic Zeeman effect, Zeeman Hamiltonian and EPR transition energy. EPR spectrometers, presentation of spectra. The effects of electron Zeeman, nuclear Zeeman and electron nuclear hyperfine terms in the

Hamiltonian on the energy of the hydrogen atom. Second order effect. Hyperfine splittings in isotropic systems, spin polarization mechanism and McConnell's relations Anisotropy in g-value,

EPR of triplet states, zero field splitting, Kramer's rule, survey of EPR spectra of first row transition metal ion complexes.

Mossbauer spectra of Fe (II) and Fe (III) cyanides.

Recommended Text Books:

1. G.L. Miessler, P.J. Fischer, D.A. Tarr, Inorganic Chemistry, 5th ed., Pearson, 2014.
2. F. A. Cotton, G. Wilkinson, C. A, Murillo, M. Bochmann Advanced Inorganic Chemistry, 6th ed., Wiley-Interscience: New York, 1999.
3. J.E. Huheey, E. A. Keiter, R. L. Keiter, Inorganic Chemistry: Principles of structure and Reactivity, 4th ed., Harper Collin College Publishers, 1993.
4. D. F. Shriver, P. W. Atkins, C. H. Langford, Inorganic Chemistry, 3rd ed., ELBS, 1999.
5. B. Douglas, D. McDaniel, J. Alexander, Concepts and Models of Inorganic Chemistry, 3rd ed., John Wiley and Sons, 1994.
6. N. N. Greenwood, A. Earnshaw, Chemistry of the Elements, 2nd ed., BH, 1997.
7. R. S.Drago, Physical Methods for Chemists, 2nd ed., Saunders College Publishing, 1992.
8. C. E. Housecroft, A. G. Sharpe, Inorganic Chemistry, 5th ed., Pearson, 2018.
9. W. L. Jolly, Modern Inorganic Chemistry, 2nd ed., McGraw-Hill, New York, 1991.
10. Solid state chemistry: an introduction, Lesley Smart and Elaine Moore, 4th ed. Taylor and Francis, 2012.
11. Earnshaw, A. Introduction to Magnetochemistry, Academic Press, 1968.
12. Carlin, R.L. Magnetochemistry, Spinger-Verlag, Berlin, 1986.
13. P. W. Atkins, Physical Chemistry 8th ed., W. H. Freeman, New York, 2006.
14. R. A. Alberty, Physical Chemistry 8th ed., Wiley, New York, 1994.
15. G. M. Barrow, Introduction to Molecular Spectroscopy, McGraw Hill, New York, 1962
16. C. N. Banwell, Fundamentals of Molecular Spectroscopy, 4th ed., Tata McGraw Hill, 1996.
17. H. Gunther, NMR Spectroscopy, 2nd ed., John Wiley, 2005.

23-808-0705

INDUSTRIAL CHEMISTRY LAB

Credit 2 **36 hours**

Course Outcome After the completion of the course, the student will be able to	**Cognitive Level**
C.O. 1: Prepare and analyze industrially important chemical products	Create
C.O. 2: Prepare and characterize materials for newer energy technologies	Create

Course Outcome	Program Specific Outcome					
	P.S.O. 1	P.S.O. 2	P.S.O. 3	P.S.O. 4	P.S.O. 5	P.S.O. 6
C.O. 1	1	3	3	3	2	3
C.O. 2	1	3	3	3	2	3

1.	Synthesis, purification and characterisation of pharmaceutically relevant compounds (Paracetamol/Aspirin)
2.	Determination of vitamin C content in fruits/vitamin tablets
3.	Preparation of electrode material for Electrochemical water splitting
4.	Preparation of electrode material for batteries/supercapacitors
5.	Preparation of Biogas
6.	Preparation of 3rd generation Solar cells (e.g. DSSC)
7.	Preparation and characterization of nanomaterials
8.	Photocatalytic water purification
9.	Raman spectroscopic study of selected food (quality analysis/pesticide detection)
10.	Electropolymerization
11.	Preparation and characterization of material for CO_2 capture

Recommended Text Books:

1. J. N. Gurtu, and A. Gurtu Advanced Physical Chemistry Experiments, 6th Ed., Pragati Prakashan, 2014.
2. J. B. Yadav, Advanced Practical Physical Chemistry, 36th Ed., Krishna Prakashan, 2016.
3. Visual Observation and Practical Application of Dye Sensitized Solar Cells in High School Energy Education J. Chem. Educ. 2018, 95, 7, 1167–1172
4. Hands-on Experiment for Preparation and Electrochemical Performance Evaluation of Hydrogen Evolution Reaction Electrodes for Undergraduates J. Chem. Educ. 2023, 100, 4, 1641–1647

5. Single Laboratory Experiment Integrating the Synthesis, Optical Characterization, and Nanocatalytic Assessment of Gold Nanoparticles J. Chem. Educ. 2020, 97, 5, 1454–1459
6. Electropolymerized Conducting Polymer as Actuator and Sensor Device-J. Chem. Ed. 2005, 8, 1372.

23-808-0706

PROFESSIONAL AND CAREER DEVELOPMENT IN CHEMISTRY

Credit 0 **32 hours**

Course Outcome After the completion of the course, the student will be able to	**Cognitive Level**
C.O. 1: Skills on subject specific pedagogy, soft skills, ICT tools, research proposal writing, finding scholarships and software for chemistry	Create

Course Outcome	Program Specific Outcome					
	P.S.O. 1	P.S.O. 2	P.S.O. 3	P.S.O. 4	P.S.O. 5	P.S.O. 6
C.O. 1	3	3	2	2	3	3

Soft Skills – Powerpoint, Word, Exel, Reference management software- Mendeley, Origin, Veusz, Research Proposal Writing – Literature review, Components of proposals, ICT – Google Classroom, Moodle, Class Recording, Teach Infinity, OBS, edmondo, QUIZZ Quiz, Document scanner., Subject specific pedagogy – Molecular model kit, ChemDraw, ChemSketch, Finding International Scholarships- MEXT, DAAD, EURAXESS, J-Rec, Funding through embassy Lab safety, research ethics, research methodology

Recommended Text Books:

1. John M. Swales & Christine B. Feak, Academic Writing for Graduate Students 3rd Edition, Michigan Publishing, 2012.
2. Stephen Bailey, Academic Writing, A Handbook for International Student, 5th Edition, Routledge, Taylor & Francis, 2018.

23-808-0801

ADVANCED ANALYTICAL AND INSTRUMENTATION TECHNIQUES I

Credit 4 **72 hours**

Course Outcome After the completion of the course, the student will be able to	**Cognitive Level**
C.O. 1: Understand the basic principles and instrumentation aspects of various electroanalytical, chromatographic, and thermo-analytical techniques	Understand
C.O. 2: Interpret the data obtained from analytical techniques	Evaluate
C.O. 3: Use the electroanalytical, chromatographic, and thermo-analytical techniques for qualitative and quantitative evaluations	Analyze

Course Outcome	Program Specific Outcome					
	P.S.O. 1	P.S.O. 2	P.S.O. 3	P.S.O. 4	P.S.O. 5	P.S.O. 6
C.O. 1	3	2	1	3	3	1
C.O. 2	1	3	2	3	3	1
C.O. 3	1	2	1	3	3	1

UNIT I	**14 hrs**
Potentiometry: different types of indicator electrodes, limitations of glass electrode, applications in pH measurements, other types of ion selective electrodes, solid, liquid, gas sensing and specific types of electrodes, biomembrane, biological and biocatalytic electrodes as biosensors, importance of selectivity coefficients. CHEMFETS- importance of specially designed amplifier systems for ion selective electrode systems. Potentiometric titrations- types and applications.	
UNIT II	**14 hrs**
Electrogravimetry- electrogravimetry without potential control, controlled potential electrogravimetry, applications. Coulometry- constant current and constant potential coulometry, applications- primary and secondary coulometry, advantages of coulometric titrations Conductance measurement – conductometric titrations.	
UNIT III	**14 hrs**
Polarography – current – voltage curve, DME-components of polarographic current, supporting electrolyte, polarographic maxima. Half-wave potential, Applications of Polarography. Voltammetry - different types, Theory and applications. Stripping analysis. Amperometric titrations – Different types and Applications Impedance spectroscopy, Voltammetric sensors – individual and simultaneous analysis-Case study.	
UNIT IV	**12 hrs**
Thermal methods of Analysis TG, DTA and DSC - Instrumentation and Theory – Factors affecting TGA - effect of atmosphere on DTA. TG of copper sulphate pentahydrate and calcium oxalate	

monohydrate. Application of thermal methods for identification of substances.
UNIT V **18 hrs**
Solvent extraction and Solid phase extraction, Basic principles of solvent extraction Distribution law-Liquid-liquid extractions, synergistic extraction, Batch extraction, continuous extraction, Counter current extraction, super critical fluids Chromatography: Basic principles, adsorption, differential migration, effect and choice of stationary and mobile phases, Classification of chromatographic techniques., Thin layer chromatography, Paper chromatography, column chromatography, gas chromatography, ion exchange chromatography, gel permeation chromatography, supercritical fluid chromatography and size exclusion chromatography, Important applications of chromatographic techniques.

Recommended References:

1. J.M. Mermet, M. Otto, R. Kellner, Analytical Chemistry, Wiley-VCH, 2004.
2. D.A. Skoog, D.M. West, F.J. Holler, S.R. Crouch, Fundamentals of Analytical Chemistry, 8th Edn., Saunders College Pub., 2007.
3. J.G. Dick, Analytical Chemistry, R.E. Krieger Pub., 1978.
4. J.H. Kennedy, Analytical Chemistry: Principles, Saunders College Pub., 1990.
5. G.H. Jeffery, J. Bassett, J. Mendham, R.C. Denney, Vogel's Text Book of Quantitative Chemical Analysis, 5th Edn., John Wiley& sons,1989.
6. C.L. Wilson, D.W. Wilson, Comprehensive Analytical Chemistry, Elsevier, 1982.
7. G.D. Christian, J.E. O'Reilly, Instrumental Analysis, Allyn & Bacon, 1986.
8. R.A. Day, A.L. Underwood, Quantitative Analysis, Prentice Hall, 1967.
9. H.A. Laitinen, W.E. Harris, Chemical Analysis, McGraw Hill, 1975.
10. F.W. Fifield, D. Kealey, Principles and Practice of Analytical Chemistry, Blackwell Science, 2000.
11. Contemporary Instrumental Analysis, Kenneth A. Rubinson, Judith F. Rubinson, Prentice Hall, New Jersey, 2000.
12. Wilson & Wilson's, Comprehensive Analytical Chemistry, Volume 47, Modern Instrumental Analysis, Edited by S. Ahuja, N. Jespersen, Reed Elsevier India Private Ltd., Noida, 2006.
13. Journal of Chromatography Library, Volume 3, Liquid Column Chromatography-A Survey of Modern Techniques and Applications, Edited by Z. Deyl, K. Macek, J. Janak, Elsevier Scientific Publishing Company, Amsterdam, 1975.
14. Gas Chromatography, John Willett, John Wiley & Sons, Singapore, 1991.
15. Fundamentals of Analytical Chemistry, Doughlas A. Skoog, Donald M. West, F. James Holler, Stanley R. Crouch, 9th Ed., Cengage Learning, 2014.
16. Allen J. Bard, Larry R. Faulkner, Electrochemical Methods-Fundamentals and Applications, John Wiley & Sons, New York, 1980

23-808-0802

ADVANCED PHYSICAL CHEMISTRY

Credit 4 **72 hours**

Course Outcome After the completion of the course, the student will be able to	**Cognitive Level**
C.O. 1: Apply the principles of statistical thermodynamics to solids and gases	Apply
C.O. 2: Explain the basics of transport phenomena and electrokinetic effects and explain entropy production for physical and chemical processes	Apply
C.O. 3: Apply the principles of acid-base and enzyme catalysis to given kinetic data	Apply
C.O. 4: Explain the fundamentals of photophysical/photochemical processes and energy/electron transfer	

Course Outcome	Program Specific Outcome					
	P.S.O. 1	P.S.O. 2	P.S.O. 3	P.S.O. 4	P.S.O. 5	P.S.O. 6
C.O. 1	3	0	0	2	2	1
C.O. 2	3	0	0	2	2	1
C.O. 3	3	0	0	2	2	1
C.O. 4	3	0	0	2	2	1

UNIT I **16 hrs**
Transport properties- Diffusion, effusion, Viscosity, Thermal conductivity. Heat capacity of solids-Einstein and Debye theory. Application of Bose-Einstein Statistics, Gas degeneration, Application to liquid helium, Bose Einstein Condensation. Application of Fermi-Dirac Statistics to electrons in metals, Extreme Gas Degeneration, Electron gas in metals and its contribution to pressure and heat capacity. Partition function for systems of dependent particles: Configurational integral and configurational partition function.
UNIT II **14 hrs**
Linear Non-equilibrium thermodynamics: General theory, Local entropy production, balance equation for concentration. Energy conservation in open systems. Entropy balance equation. Forces and Fluxes, Steady state and local equilibrium conditions. Linear phenomenological laws. Phenomenological coefficient, Systems with heat, matter and electrical transport, Onsager Reciprocal relation, Application to Diffusion -Thermal diffusion, Thermal Osmosis and electrokinetic effects, Soret Coefficient, Seebeck effect.
UNIT III **16 hrs**

Catalysis: Catalysis and Inhibition, Homogeneous and heterogeneous Catalysis – Transition state theory, General mechanism. General Mechanism of homogeneous catalysis- Arrhenius and vant Hoff intermediates, Acid base catalysis- specific and general acid catalysis, Enzyme catalysis- Michaelis-Menten Mechanism, Competitive and non competitive inhibition. Kinetics of Surface catalysis: Unimolecular and bimolecular Surface reactions. Kinetics of adsorption- Langmuir Hinshelwood mechanism and Rideal-Eley mechanism. Autocatalysis- Oscillatory reactions- Lotka- Volterra, Oregonator, Brussellator
UNIT IV **14 hrs**
Vapour pressure, Surface tension - determination of vapour pressure. Parachor – determination, application to structure elucidation of compounds, Viscosity - determination of molecular mass from viscosity measurements. Refraction – refractive index, molar refraction and optical exaltation– application to structure elucidation, Concept of superhydrophobicity/super-oleophilcity.
UNIT V **12 hrs**
Photochemistry: Photochemistry and photophysics- Applications, Excited state reactivity and life time, Excimers and Exciplex, Energy and electron transfer -Elementary idea, Quenching- Static and Dynamic, Stern Volmer equation, Photocatalysis and photoelectrocatalysis- Elementary principles.

Recommended Text Books:

1. F.W. Sears, Introductions to Thermodynamics, Kinetic Theory of Gases and Statistical Mechanics, Addision Wesley Pub. Cambridge, 1998.
2. F.C. Andrews, Equilibrium to Statistical Mechanics, John Wiley, New York, 2002.
3. L.K. Nash, Statistical Thermodynamics, Addison Wesley, New York, 1999.
4. P.W Atkins, Julio De Paula, Physical Chemistry, Oxford University Press, $10^{th}/11^{th}$ edn, 2017/2018
5. D. A. McQuarrie, Physical Chemistry- A Molecular Approach, South Asian Edn., 2008.
6. M. Dole, Introduction to Statistical Thermodynamics, Prentice Hall, London, 1997.
7. D. A. McQuarrie, Statistical Thermodynamics, South Asian Edn., 2008.
8. I. Prigogine, Introduction to Thermodynamic Irreversible Processes, 3^{rd} ed., Wiley Interscience, 1968.
9. S. R. de Groot, P. Mazur, Non-equilibrium Thermodynamics, Dover Publications, 2011.
10. G. Lebon, D. Jou, J. Casas, Understanding Non-equilibrium Thermodynamics, Springer. 2008.
11. S. Kjelstrup, D. Bedeaux, E. Johannessen, J. Gross, Non-Equilibrium Thermodynamics for Engineers: Second Edition, World Scientific Publishing Company, 2017.
12. D. Kondepudi and I. Prigogine, Modern Thermodynamics: From Heat Engines to dissipative Structures, Wiley, New York.
13. W. J. Moore and R. G. Pearson, Kinetics and Mechanism, Wiley, New York.
14. K. J. Laidler, Chemical-Kinetics, McGraw Hill, New York.

15. M. R. Wright, An Introduction to Chemical Kinetics, Wiley, 2004.
16. Richard Masel, Chemical kinetics and Catalysis, Wiley Interscience

23-808-0803

ADVANCED ORGANIC CHEMISTRY I

Credit 4 **72 hours**

Course Outcome After the completion of the course the student will be able to	**Cognitive Level**
C.O. 1: Analyze the conformational effects on the reactivity of reactions	Apply
C.O. 2: Analyze the reagents and conditions for the synthesis of specific target molecules	Analyze
C.O. 3: Describe strategies for the stereospecific/stereoselective organic transformations towards chiral target molecules	Apply
C.O. 4: Construct a synthetic pathway for simple to complex organic molecules by retrosynthetic approach	Apply

Course Outcome	Program Specific Outcome					
	P.S.O. 1	P.S.O. 2	P.S.O. 3	P.S.O. 4	P.S.O. 5	P.S.O. 6
C.O. 1	3	0	0	2	0	0
C.O. 2	3	0	2	2	0	0
C.O. 3	1	0	2	2	0	0
C.O. 4	3	0	2	2	0	0

UNIT I **16 hrs**

Reaction mechanisms and conformational effects on reactivity - Ester hydrolysis, alcohol oxidations, S_N2 reactions, elimination reactions, epoxidation by intramolecular closure of halohydrins, strain-modulated reactivity, epoxide openings (S_N2), electrophilic additions to olefins, rearrangement reactions, conformational and stereoelectronic effects on reactivity. Stereoselective reactions of cyclic compounds. Reactions on small rings. Stereochemical control in six-membered rings. Stereochemistry of bicyclic compounds. Reactions with cyclic intermediates/transition states.

UNIT II **14 hrs**

Asymmetric Synthesis: Introduction to asymmetric synthesis, principle, general strategies, chiral pool strategy, chiral auxiliaries, chiral reagents – Binol derivatives of $LiAlH_4$, chiral catalysts – CBS catalyst. Stereospecific and stereoselective synthesis, determination of enantiomeric and diastereomeric excess. Stereoselective nucleophilic additions to acyclic carbonyl groups- Cram's Rule, Felkin-Ahn Model, Effect of chelation on selectivity.

UNIT III **12 hrs**

Protecting groups- protection and deprotection of hydroxyl, carboxylic acids, and carbonyls in aldehydes and ketones, amines, alkenes and alkynes. Chemo- & regioselective protection and deprotection. Functional group equivalents, reversal of reactivity (Umpolung).

UNIT IV	**16 hrs**
Disconnection approach-introduction to retrosynthesis, basic principles, synthons, and synthetic equivalents. Monofunctional and bifunctional disconnection, One group C-X and two groups C-X disconnections, one group C-C and two groups C-C disconnections. Computers in organic synthesis – introduction to softwares –SYNTHIA, MAPOS, AiZynthFinder.	
UNIT V	**14 hrs**
Retrosynthetic analysis: Longifoline, Corey lactone, Djerassi - Prelog lactone and D-luciferin. Application of AiZynthFinder to retrosynthetic analysis.	

Recommended Text Books:

1. P.S.Kalsi: Stereochemistry, Conformation and Mechanism, 3rd Edn., New Age Publications.
2. E. L. Eliel and S. H. Wilen: Stereochemistry in Organic Compounds, 1994, John Wiley.
3. J. Clayden, N. Green, S. Warren, P. Wothers, Organic Chemistry, 2nd ed., Oxford University Press, 2012.
4. P. S. Kalsi, Stereochemistry, Conformation and Mechanism, 9th ed., New Age Publications, 2017.
5. T. Tsuji, Transition Metal Reagents and Catalysts: Innovations in Organic Synthesis, John Wiley & Sons, 2000.
6. S. Warren, Organic Synthesis: The Disconnection Approach, 2nd ed., John Wiley, 2008.
7. E. Robert, Gawley, J. Aube, Principles of Asymmetric Synthesis, 2nd ed., Elsevier, 2012.
8. T.W. Greene, P. G. M. Wuts, Protecting Groups in Organic Synthesis, 2nd ed., John Wiley, 1991.

23-808-0804

COMPUTATIONAL CHEMISTRY LAB

Credit 2 **36 hours**

Course Outcome After the completion of the course, the student will be able to	**Cognitive Level**
C.O. 1: Carry out computational chemistry software to perform calculations	Apply
C.O. 2: Analyze the calculated results and interpret the results to solve chemical puzzles	Analyze

Course Outcome	Program Specific Outcome					
	P.S.O. 1	P.S.O. 2	P.S.O. 3	P.S.O. 4	P.S.O. 5	P.S.O. 6
C.O. 1	2	2	3	3	3	3
C.O. 2	2	2	3	3	3	3

	Computational calculations using available programme package:
1.	Constructing molecular structures or models
2.	Molecular geometry optimization
3.	Conformational analysis
4.	Thermodynamic and spectroscopic properties
5.	Molecular orbital analysis
6.	Electron density and electrostatic potential map

Recommended Text Books:

1. Foresman, J. and Frisch, A.," Exploring chemistry with electronic structure methods", Guassian Inc, 2000.
2. Cramer, C. J., "Essentials of Computational Chemistry- Theories and Models", 2nd Edition, Wiley, 2004
3. Jensen, F., "Introduction to Computational Chemistry", 3rd Edition, Wiley, 2017.
4. Young, D., "Computational Chemistry – A Practical Guide", Wiley, 2001.

23-808-0805

OPEN ENDED LAB

Credit 4

Course Outcome After the completion of the course, the student will be able to	**Cognitive Level**
C.O. 1: Identify and hypothesise an independent research problem and write a literature review	Analyze

Course Outcome	Program Specific Outcome					
	P.S.O. 1	P.S.O. 2	P.S.O. 3	P.S.O. 4	P.S.O. 5	P.S.O. 6
C.O. 1	3	3	3	3	3	3

Students will identify a research problem and carry out a literature survey on selected topic. A project will be undertaken with guidance from concerned teacher. There will be report submission and evaluation at the end of the semester.

23-808-0901

ADVANCED ANALYTICAL AND INSTRUMENTATION TECHNIQUES II

Credit 4 **72 hours**

Course Outcome After the completion of the course, the student will be able to	**Cognitive Level**
C.O. 1: Gain an in-depth understanding of working principles of advanced analytical and surface characterization techniques	Understand
C.O. 2: Choose and optimize the right techniques and instrumentation configuration for a particular analysis	Evaluate
C.O. 3: Analyse the data for differentiation and quantitative evaluation of analytes and surfaces	Analyze

Course Outcome	Program Specific Outcome					
	P.S.O. 1	P.S.O. 2	P.S.O. 3	P.S.O. 4	P.S.O. 5	P.S.O. 6
C.O. 1	3	3	2	2	3	2
C.O. 2	2	3	2	2	3	1
C.O. 3	2	2	2	3	3	1

UNIT I	**14 hrs**
Gas chromatography – basic instrumental set up-inlets, carriers, columns, detectors and comparative study of TCD, FID, ECD, NPD and MS. Qualitative and quantitative studies using GC, Preparation of GC columns, packet columns and capillary columns, selection of stationary phases of GLC, Choosing the parameters-Temperature, Length of the column, Sample size, Flow rate, CHN analysis by GC, Case study.	
UNIT II	**14 hrs**
Capillary electrophoresis-migration rates and plate heights, instrumentation, sample introduction, detection methods, applications. Capillary gel electrophoresis. Capillary isotachophoresis. Isoelectric focusing. Capillary electrochromatography, packed columns. Micellar electrokinetic Chromatography.	
UNIT III	**16 hrs**
Separation process, Eddy diffusion, Mass transfer, Longitudinal diffusion, Retention parameters in HPLC-Capacity factor, Retention time, Retention volume, Peak width, Total number of theoretical plates, Height equivalent of a theoretical plate, Resolution and retention time, Solvent delivery systems, Detectors, Instrumentation and functioning of HPLC, Types of HPLC - Modes of separation in HPLC- adsorption chromatography, reversed phase chromatography, ion pair chromatography, ion exchange chromatography Solubility and retention in HPLC, Method development in HPLC - Selection of mobile phase and optimization, Preparation of sample, Selection of column and solvent,	

HPLC method validation, HPLC Analysis -Case study Dos and Don'ts in HPLC - Troubleshooting in HPLC.
UNIT IV **14 hrs**
Measurement of alpha, beta, and gamma radiations, neutron activation analysis and its applications. Principle and applications of isotope dilution methods, Radioimmunoassay (RIA), Immunoradiometric assay (IRMA), Enzyme linked immunosorbent assay (ELISA)-Principles and practical aspects.
UNIT V **12 hrs**
Chemical Analysis of surfaces: Surface preparations-ion scattering spectrometry secondary ion scattering microscopy (SIMS)-Auger election spectroscopy-ESCA instrumentation and application. Electron Microscopies, Basic principles of TEM and SEM, Elemental analysis, XRD, Scanning probe microscopies an overview, Basic principles of AFM and STM, Case study.

Recommended References:

1. J.M. Mermet, M. Otto, R. Kellner, Analytical Chemistry, Wiley-VCH, 2004.
2. D.A. Skoog, D.M. West, F.J. Holler, S.R. Crouch, Fundamentals of Analytical Chemistry, 8th Edn., Saunders College Pub., 2007.
3. J.G. Dick, Analytical Chemistry, R.E. Krieger Pub., 1978.
4. J.H. Kennedy, Analytical Chemistry: Principles, Saunders College Pub., 1990.
5. G.H. Jeffery, J. Bassett, J. Mendham, R.C. Denney, Vogel's Text Book of Quantitative Chemical Analysis, 5th Edn., John Wiley& sons,1989.
6. C.L. Wilson, D.W. Wilson, Comprehensive Analytical Chemistry, Elsevier, 1982.
7. G.D. Christian, J.E. O'Reilly, Instrumental Analysis, Allyn & Bacon, 1986.
8. R.A. Day, A.L. Underwood, Quantitative Analysis, Prentice Hall, 1967.
9. H.A. Laitinen, W.E. Harris, Chemical Analysis, McGraw Hill, 1975.
10. F.W. Fifield, D. Kealey, Principles and Practice of Analytical Chemistry, Blackwell Science, 2000.
11. Contemporary Instrumental Analysis, Kenneth A. Rubinson, Judith F. Rubinson, Prentice Hall, New Jersey, 2000.
12. Wilson & Wilson's, Comprehensive Analytical Chemistry, Volume 47, Modern Instrumental Analysis, Edited by S. Ahuja, N. Jespersen, Reed Elsevier India Private Ltd., Noida, 2006.
13. Journal of Chromatography Library, Volume 3, Liquid Column Chromatography-A Survey of Modern Techniques and Applications, Edited by Z. Deyl, K. Macek, J. Janak, Elsevier Scientific Publishing Company, Amsterdam, 1975.
14. Gas Chromatography, John Willett, John Wiley & Sons, Singapore, 1991.
15. Fundamentals of Analytical Chemistry, Doughlas A. Skoog, Donald M. West, F. James Holler, Stanley R. Crouch, 9th Ed., Cengage Learning, 2014.

23-808-0902

INSTRUMENTATION LAB

Credit 4 **72 hours**

Course Outcome After the completion of the course, the student will be able to	**Cognitive Level**
C.O. 1: Understand the operation principles of various instruments and perform experiments using them	Evaluate

Course Outcome	Program Specific Outcome					
	P.S.O. 1	P.S.O. 2	P.S.O. 3	P.S.O. 4	P.S.O. 5	P.S.O. 6
C.O. 1	2	3	3	3	3	3

1.	REFRACTOMETRY: Variation of refractive index with composition and Determination of unknown composition
2.	Cyclic voltammetry determination oxidation reduction potentials, HOMO and LUMO levels
3.	UV-VIS-NIR spectroscopy: Band Gap Estimation of thin films
4.	Fluorescence spectroscopy: Emission Excitation spectral analysis, Fluorescence quantum yield, fluorescence lifetime, quenching
5.	Synthesis and characterization of Nano-silver
6.	Raman spectroscopy: Vibrational analysis of compounds, Surface Enhanced Raman spectroscopy
7.	TGA-DTA Thermal analysis
8.	Gas Chromatography
9.	Diffused reflectance spectroscopy
10.	Determination of Alkalinity of water; DO and BOD and COD of waste water

Recommended Text Books:

1. J. N. Gurtu, and A. Gurtu Advanced Physical Chemistry Experiments, 6th Edn., Pragati Prakashan, 2014.
2. B. P. Levitt, Findlay's Practical Physical Chemistry, 9th Edn, Longman Group Ltd.
3. Vogel's text book of quantitative chemical analysis, Fifth Edition.

23-808-0903

MINI PROJECT

Credit 4

Course Outcome After the completion of the course, the student will be able to	**Cognitive Level**
C.O. 1: identify and hypothesise an independent research problem	Analyze

Course Outcome	Program Specific Outcome					
	P.S.O. 1	P.S.O. 2	P.S.O. 3	P.S.O. 4	P.S.O. 5	P.S.O. 6
C.O. 1	3	3	3	3	3	3

Students will identify a research problem and carry out an independent project under the supervision of concerned teacher and shall submit a report. There will be an evaluation at the end of the semester.

23-808-1001 and 23-808-1002

PROJECT AND COURSE VIVA

Credit 16+2

1.	The students shall carry out research project in reputed research laboratory for the entire semester.
2.	The students shall submit a project report on the research work carried out.
3.	The students will have to present the results of the research project in a seminar and appear for a comprehensive viva-voce. A course viva will also be conducted along with project evaluation

Elective Courses

23-808-0506

INTRODUCTION TO PHOTOCHEMSITRY AND PHOTOPHYSICS

Credit 4 **64 hours**

Course Outcome After the completion of the course the student will be able to	**Cognitive Level**
C.O. 1: Gain a comprehensive understanding of the basic principles of photochemistry and Photophysics	Understand
C.O. 2: Gain a comprehensive understanding of the interaction between light and matter at the molecular level	Analyze
C.O. 3: Forecast the spectral characteristics of simple molecules under standard ambient conditions	Analyze
C.O. 4: Gain expertise in using spectroscopy techniques to study photophysical and photochemical processes	Apply
C.O. 5: Design molecular systems with functionalities appropriate for photochemical and photophysical applications	Apply

Course Outcome	Program Specific Outcome					
	P.S.O. 1	P.S.O. 2	P.S.O. 3	P.S.O. 4	P.S.O. 5	P.S.O. 6
C.O. 1	3	2	1	2	3	1
C.O. 2	3	1	1	2	3	2
C.O. 3	3	1	1	2	3	2
C.O. 4	3	2	1	2	3	2
C.O. 5	3	2	1	2	3	2

UNIT I **14 hrs**
Interaction of light with matter, absorption of light– theoretical understanding (qualitative), absorption spectra, molecular level understanding w.r.t π-π*, n-π*, d-d, CT, MLCT and LMCT transitions, selection rules, solvent effects, fundamental laws.
UNIT II **12 hrs**
Emission of light – theoretical understanding(qualitative) w.r.t Frank-Condon principle, PES, excited state deactivation, Jablonski diagram, singlet and triplet states, emission spectra, fluorescence, phosphorescence, lifetime, quantum yield, fundamental laws.
UNIT III **12 hrs**
Deactivation of excited states- photophysical process, photochemical process, Electron transfer, Energy transfer, FRET and DET (qualitative), dioxygen, intersystem crossing, solvent and temperature effects, delayed fluorescence, triplet harvesting, kinetics, quenching and sensitization.
UNIT IV **12 hrs**

Spectroscopic techniques – Instrumentation for absorption, emission and lifetime, scope of techniques, Actinometry, Integrated Sphere, UV-DRS, ATR, PV-ATR, UV-SEC and Time-resolved spectroscopy (basics).
UNIT V **12 hrs**
Applications- Photochemistry of semiconductors and nanomaterials, photosynthesis, photocatalysis, solar energy conversion, photo responsive materials and photodynamic therapy.

Recommended Textbooks:

1. Principles of Molecular Photochemistry, Nicholas J. Turro, V. Ramamurthy, J.C. Scaiano, University Science Books, 2009.
2. Modern Molecular Photochemistry, Nicholas J. Turro, University Science Books,2015.
3. Organic and inorganic photochemistry, V. Ramamurthy, Kirk S. Schanze, M. Dekker, 1998.
4. Photochemistry and Photophysics: Concepts, Research, Applications, Vincenzo Balzani, Paola Ceroni, Alberto Juris, Wiley-VCH, 2014.
5. Principles of Fluorescence Spectroscopy, Joseph R. Lakowicz, Springer, 2006.
6. Fundamentals of Photochemistry, K. K. Rohatgi- Mukherjee, New Age International (P) Limited, 2017.
7. Principles and Applications of Photochemistry, Brian Wardle, Wiley, 2009.
8. Physical Chemistry, Peter Atkins, Julio de Paula, James Keeler, Oxford, 2018.
9. Principles of Instrumental Analysis, Douglas A. Skoog, F. James Holler, Stanley R. Crouch, Cengage, 2020.
10. Semiconductor Photocatalysis, Horst Kisch, Wiley-VCH, 2015.

23-808-0606

Advanced Photochemistry and Photophysics

Credit 4 **64 hours**

Course Outcome After the completion of the course the student will be able to	**Cognitive Level**
C.O. 1: Gain a comprehensive understanding of the photochemical and Photophysical processes	Understand
C.O. 2: Gain a expertise the common instrumentation techniques to study photophysical and photochemical processes	Analyze
C.O. 3: Gain a comprehensive understanding of the advanced spectroscopic techniques for in depth analysis advanced photo functional materials	Analyze
C.O. 4: Gain exposure to advanced applications in industry	Understand

Course Outcome	Program Specific Outcome					
	P.S.O. 1	P.S.O. 2	P.S.O. 3	P.S.O. 4	P.S.O. 5	P.S.O. 6
C.O. 1	3	1	1	2	3	1
C.O. 2	1	3	3	2	3	1
C.O. 3	3	3	2	2	3	1
C.O. 4	1	1	1	3	3	3

UNIT I	**14 hrs**
Introduction of photophysical and photochemical process, Mechanisms of Spectral Shift, Solvatochromism, Lippert-Mataga Equation, Photochromism, Excimers, Exciplexes. Fluorescence Quenching, Theories of Static Quenching and Dynamic Quenching, Derivation of Stern-Volmer Equation, Deviations, Energy and Electron Transfer Basic Concepts- Donor-Acceptor Systems, Photoinduced Energy Transfer – Trivial Mechanism, Dexter Mechanism, Forster Mechanism, Efficiency, Distance Measurements, Photoinduced Electron Transfer- Libby's Theory, Marcus Theory.	
UNIT II	**12 hrs**
Instrumentation-Fluorescence Spectrometer, Quantum Yield Measurements, Lifetime Measurement, Light Sources, Monochromators, Optical Filters, Detectors, Polarizers, Ideal Spectrometers, Distortion and Corrections in Measurements, Inner Filter Effects.	
UNIT III	**12 hrs**
Optical Microscopy, Fluorescence Microscopy, Diffraction-limited resolution Confocal microscopy, basic concepts, instrumentation aspects, confocal imaging, concept of two- and multiphoton microscopy, two and multiphoton lithography.	
UNIT IV	**12 hrs**

Ultrafast Dynamics- Pump-Probe technique, Kinetic studies, transient absorption, complimentary techniques, insitu absorption spectroscopy, DRS, Tauc Plot, Mott-Schottky plots, Interface UV-Vis spectroscopy, Photophysics and photochemistry of NPs, SPR, VSC and chemistry under VSC.
UNIT V **12 hrs**
Applications of Photoinduced Process: Singlet Oxygen – Methods of Singlet oxygen generation and Detection – Chemistry of Singlet Oxygen – Photodynamic Therapy of Cancer, Fluorescence Sensors, Artificial Light-Harvesting Systems, Atmospheric Photochemistry, Dye Sensitized Solar Cells - Bulk Heterojunction Solar Cells, Luminescent Solar Concentrator, Organic Light Emitting Devices. Photoresists – Photolithography – Photochromism – Photonic Materials and Lasers.

Recommended Text Books:

1. N. J. Turro, V. Ramamurthy, J. C. Scaiano, Modern Molecular Photochemistry of Organic Molecules, University Science Books, 2010.
2. C.E. Wayne, Photochemistry (Oxford Chemistry Primers), Oxford University Press; 1st ed., 1996.
3. J. R. Lakowicz, Principles of Fluorescence Spectroscopy, Plenum Press, 3rd ed., 2010.
4. A. M. Braun, M.-T. Maurette, Esther Oliveros, Photochemical Technology, John Wiley & Sons, 1991.
5. M. A. Fox, M. Chanon, Photoinduced Electron Transfer Part A, B. C and D, Elsevier Science Publishing Company, 1988.
6. J. Mattay Ed., Photoinduced Electron Transfer 1-5 (Topics in Current Chemistry), Springer, 1st ed., 1990-1993
7. G. J. Kavarnos, Fundamentals of Photoinduced Electron Transfer, 1st ed., Wiley- VCH, 1993.
8. V. Ramamurthy, K. Schanze, Molecular and Supramolecular Photochemistry, Volume 10, Semiconductor Photochemistry and Photophysics, Marcel Dekker, New York, 2003.
9. V. Ramamurthy, Photochemistry in Organized and Confined Media, VCH Publishers, NewYork, 1991.

23-808-0707

SUPRAMOLECULAR CHEMISTRY AND MATERIALS

Credit 4 **72 hours**

Course Outcome After the completion of the course the student will be able to	**Cognitive Level**
C.O. 1: Explain the structural features of any given supramolecular system	Analyze
C.O. 2: Analyze the type of possible interactions in any given host guest assembly	Analyze
C.O. 3: Predict the photochemical and Photophysical behavior in constrained media	Analyze
C.O. 4: Interpret the principle of materials for applications like catalysis, solar energy conversions, drug delivery, etc.	Evaluate
C.O. 5: Explain the theory and applications of magnetic and superconducting materials.	Evaluate

Course Outcome	Program Specific Outcome					
	P.S.O. 1	P.S.O. 2	P.S.O. 3	P.S.O. 4	P.S.O. 5	P.S.O. 6
C.O. 1	3	2	1	2	1	1
C.O. 2	3	2	1	2	1	1
C.O. 3	3	2		2	1	1
C.O. 4	3	2	1	2	1	2
C.O. 5	3	2	1	2	1	2

UNIT I **14 hrs**
Self-assembly and preorganization, Supramolecules non-covalent forces and interactions in supramolecules–Hydrogen bonding, π Effects, dipole interactions, induced dipole interactions, hydrophobic interactions. Solvent Effects, Thermodynamics of binding phenomena.
UNIT II **14 hrs**
Molecular Recognition – Host guest interactions, Macrocycles, Structure, Preparation and Properties of crown ethers, cryptates, cryptands, carcerands, calixarenes, cyclodextrins, fullerenes, dendrimers, rotaxanes, cucurbiturils.
UNIT III **16 hrs**
Complex Architectures – Self-assembly, Complementarity and Reorganization, Coordination driven self-assembly of supramolecular two and three dimensional architectures, COF, MOF and their applications.
UNIT IV **14 hrs**
Photochemistry in constrained media- photophysical, photochemical processes, energy transfer, electron transfer. Effect of structural features and interactions on energy levels. Applications –

photocatalysis, water splitting, solar cell, CO2 reduction, drug delivery, sensors, gas separation and storage.
UNIT V **14 hrs**
Review of different types of magnetic behaviours, magnetic susceptibility, paramagnetism, ferromagnetism, magnetic domains, magnetic materials, antiferromagnetism-transition metal monooxides, molecular magnetism, single molecule magnets, superconductors, magnetic properties of super conductors, Josephson effects, BCS theory, High temperature superconductors.

Recommended Text Books:

1. Jonathan W. Steed, Jerry L. Atwood, Supramolecular Chemistry, Wiley, 2013.
2. J. M. Lehn, Supramolecular Chemistry: Concepts and Perspectives, Wiley, 1995
3. E.V. Ansyln, D. A. Dougherty, Modern Physical Organic Chemistry, University Press, 2006.
4. P. Klan and J. Wirz, Photochemistry of Organic Compounds,
5. Nicholas J. Turro, V. Ramamurthy, J.C. Scaiano, Modern Molecular Photochemistry of Organic Molecules,
6. Christian S. Diercks, Markus J. Kalmutzki, and Omar M. Yaghi, Introduction to Reticular Chemistry: Metal-OrganicFrameworks and Covalent Organic Frameworks, Wiley, 2019.
7. Shengqian Ma, Jason A Perman, Elaboration and Applications of Metal-Organic Frameworks, World Press, 2018.
8. Earnshaw, A. Introduction to Magnetochemistry, Academic Press, 1968.
9. Carlin, R.L. Magnetochemistry, Spinger-Verlag, Berlin, 1986.
10. Introduction to molecular magnetism: From transition metals to lanthanides, C. Benelli, D. Gatteschi, Wiley-VCH, 2015.
11. Solid state chemistry: an introduction, Lesley Smart and Elaine Moore, 4th ed. Taylor and Francis, 2012.

23-808-0806

MATERIALS CHEMISTRY

Credit 4 **60 hours**

Course Outcome After the completion of the course the student will be able to	**Cognitive Level**
C.O. 1: To acquire basic knowledge on various types of materials	Understand
C.O. 2: To gain insight on the structure – property relationship of different materials	Understand
C.O. 3: To get knowledge on various characterization techniques	Analyze
C.O. 4: To get an idea about the materials in advanced technological applications	Apply

Course Outcome	Program Specific Outcome					
	P.S.O. 1	P.S.O. 2	P.S.O. 3	P.S.O. 4	P.S.O. 5	P.S.O. 6
C.O. 1	3	1	1	2	3	2
C.O. 2	3	1	2	3	3	3
C.O. 3	3	3	3	3	3	3
C.O. 4	3	3	3	3	3	3

UNIT I **12 hrs**

Chemistry of Materials. Ionic and covalent solids. Molecular and metallic solids. Amorphous and crystalline materials. Crystalline state. Structural organization of crystalline solids-theories of bonding. Crystal structures. Imperfections in crystal structures.

Semiconductor materials- properties and types of semiconductors. Structure and Bonding of semiconductor materials. Silicon based semiconductors. II-VI (wide band gap) and III-V (narrow band gap) compound semiconductors. Electrical, optical and magnetic properties of semiconductor materials. Preparation and properties of ZnO, ZnS, CdS, CdTe, Ga-As, In-S, Cu-In-S. Application in photovoltaic devices.

UNIT II **10 hrs**

Polymer Materials- classification and nomenclature of polymers. Methods of Polymerization. Structure–property relationships. Plastics and elastomers. Viscoelastic behaviour. Rubber like elasticity. Crystalline and amorphous polymers. Glass transition temperature and crystalline melting. Functional Polymers.

UNIT III **12 hrs**

Nanomaterials. Materials in the nanodomain. Zero, one- and two-dimensional materials. Particle size dependent change in properties of materials. Metals in the nanodomain. Gold and silver nanoparticles. Preparation, properties and applications. Core shell structures. Semiconductor nanoparticles. Quantum dots. ZnO, ZnS, CdS and CdSe quantum dots.

Electrical and optical properties. Nano domains of Carbon-fullerenes, carbon nanostructures, graphene, graphene quantum dots.
UNIT IV **14 hrs**
Characterization of Materials. Optical Microscopy- Principles, instrumentation and application of confocal Raman microscopy, SPM/STM. Electron microscopy- SEM, FESEM, TEM. Principles, instrumentation and applications. Surface and core level techniques- Photoelectron spectroscopy - X-Ray and UV. Thermal methods- TG/DTG, DTA, DSC, DMA. X-Ray Diffraction.
UNIT V **12 hrs**
Materials in Advanced Technology. Organic Polymer Semiconductors, Solid ionic conductors - Advanced materials for energy generation and energy storage. Porous membranes. Optical and photonic materials.

Recommended Text Books:

1. B. D. Fahlman, Materials Chemistry, 2nd ed. Springer, Heidelberg, 2011.
2. Harry R. Allcock, Introduction to Material Chemistry, John Wiley & Sons, Inc., New Jersy, 2008
3. R. Zallen, Physics of Amorphous Solids, Wiley, New York, 1983.
4. R. J. Borg, G. J. Dienes, The Physical Chemistry of Solids, Academic Press, Boston, 1993.
5. D. Kingery, H. K. Bowen, D. R. Uhlmann, Introduction to Ceramics, 2nd ed., Wiley, New York, 1992.
6. J. M. J. Cowie, Polymers. Physics and Chemistry of Modern Materials, 3rd ed., CRC Press, Boca Raton, 2007.
7. S. O. Kasap, Principles of Electronic Materials and Devices, Mc Graw Hill, 2006.

23-808-0904

NEW METHODS AND STRATEGIES IN ORGANIC SYNTHESIS AND DYNAMIC STEREOCHEMISTRY

Credit 4 **64 hours**

Course Outcome After the completion of the course the student will be able to	**Cognitive Level**
C.O. 1: To learn various organic reactions and reagents used in them as tools applied in the art of organic synthesis	Apply
C.O. 2: Analyze the reagents and conditions for the synthesis of specific target molecules	Analyze
C.O. 3: To learn and apply various concepts such as stereochemistry and fundamental principles of stereoselectivity in organic chemistry	Apply
C.O. 4: Analyze the effect of molecular conformation in the outcome of a reaction	Analyze

Course Outcome	Program Specific Outcome					
	P.S.O. 1	P.S.O. 2	P.S.O. 3	P.S.O. 4	P.S.O. 5	P.S.O. 6
C.O. 1	2	3	3	3	2	2
C.O. 2	2	3	3	2	1	2
C.O. 3	3	2	1	1	1	2
C.O. 4	1	3	1	1	3	1

UNIT I **14 hrs**
Chemo-, regio- and stereoselective functional groups interconversions; oxidation and reduction processes and their synthetic utility; metal-free oxidation (boron-, peroxide-, sulfur-, iodine-based) and metal-based (Ru-, Cr-, Mn-, Os-, Pd-) reagents; transfer hydrogenation; enantioselective oxidation and reduction processes.
UNIT II **12 hrs**
Strategic carbon-carbon and carbon-heteroatom bonds formation; carbon-carbon multiple bonds construction processes and corresponding named reactions; functional group transposition; conjunctive reagents; construction of cyclic frameworks; fused and spirocyclic systems.
UNIT III **12 hrs**
Stereochemistry: Geometrical & Optical isomerism: the origin of chirality, chiral centres and configuration, axes and planes, helicity. Prochiral centres and faces. Topicity relationships, enantiotopic and diastereotopic groups and faces. Symmetry, stereochemistry and time scale. Allenes, cumulenes, biphenyls, and spirans. Compounds containing chiral atoms other than carbon.

Strain, types of strain including B, F, I, Pitzer strain and Baeyer strain. Acyclic sp^3–sp^3, sp^3-sp^2 systems, structure and stability of small, medium, and large rings, cyclohexane, substituted cyclohexanes, cyclohexenes, decalins, and bicyclic systems.
UNIT IV **13 hrs**
Stereoselectivity in cyclic molecules: Introduction; Stereochemical control in six-membered rings; Reactions on small rings; Regiochemical control in cyclohexene epoxides; Stereoselectivity in bicyclic compounds; Fused bicyclic compounds; Spirocyclic compounds; Reactions with cyclic intermediates or cyclic transition states.
UNIT V **13 hrs**
Diastereoselectivity: Prochirality; Diastereoselective additions to carbonyl groups without rings; Stereoselective reactions of acyclic alkenes; Stereoselective Aldol reactions; Single enantiomers from diastereoselective reactions.

Recommended Text Books:

1. W. Carruthers, Modern Methods of Organic Synthesis, Cambridge University Press, 1996
2. L. Kuerti and B. Czako, Strategic Applications of named Reactions in Organic Synthesis, Elsevier Academic Press, 2005
3. F. A. Cary and R. I. Sundberg, Advanced Organic Chemistry, Part A and B, 5th Edition, Springer, 2009
4. J. Clayden, N. Greeves, and S. Warren, Organic Chemistry, Oxford University Press, 2nd Edition, 2012
5. L. F. Tietze, G. Brasche, and K. Gericke, Domino Reactions in Organic Synthesis, Wiley, 2006
6. Roderick Bates, Organic Synthesis using Transition Metals, 2nd Edition, Wiley, 2012
7. George S. Zweifel and Michael H. Nantz, Modern Organic Synthesis: An Introduction, W. H. Freeman Publisher, 2007.
8. P.S.Kalsi: Stereochemistry, Conformation and Mechanism, 3rd edn., New Age Publications
9. Peter Sykes, A Guide Book to Mechanism in Organic Chemistry, Pearson Education, New Delhi.
10. Bruckner, R. Advanced Organic Chemistry: Reaction Mechanisms, 1st edn., Academic Press, 2001.

23-808-0905

Advanced Organic Chemistry II

Credit 4 **60 hours**

Course Outcome After the completion of the course the student will be able to	**Cognitive Level**
C.O. 1: Apply organocatalysts for various organic synthesis	Apply
C.O. 2: Design and synthesis suitable heterogeneous catalysts for various synthetic applications	Apply
C.O. 3: Understand biorthogonal chemistry and its applications	Understand
C.O. 4: Design and construct suitable polymers with the required properties for different applications	Apply
C.O. 5: To design and synthesise functional organic materials for specific applications	Apply

Course Outcome	Program Specific Outcome					
	P.S.O. 1	P.S.O. 2	P.S.O. 3	P.S.O. 4	P.S.O. 5	P.S.O. 6
C.O. 1	3	1	3	1	1	1
C.O. 2	3	3	3	1	1	2
C.O. 3	1	1	1	1	2	3
C.O. 4	1	1	1	3	3	1
C.O. 5	1	1	1	2	3	3

UNIT I **10 hrs**
Organocatalysis: Introduction to organo-catalyzed reactions, amine, iminium, enamine and carbene-based catalysis reactions. Organocatalysis for asymmetric synthesis.
UNIT II **12 hrs**
Heterogeneous catalysis: introduction, immobilization and solid supports, metal catalysts (single atoms and nanoclusters), organometallic compounds, magnetically active heterogeneous catalysts.
UNIT III **12 hrs**
Introduction to bioorthogonal chemistry: concept, various ligation strategies viz., 1,3-dipolar cycloaddition of azides with cyclooctynes and nitrones with cyclooctynes; oxime/hydrazone formation from aldehydes and ketones, the tetrazine ligation, the isocyanide-based click reaction, and the quadricyclane ligation.
UNIT IV **13 hrs**
Polymers for advanced technologies: Liquid-crystalline and high-performance polymers, functional polymers, Polymers for drug release and drug carrier systems, Polymeric gels and networks.

Synthesis and applications of conducting polymers: PPVs, polyaniline (PANI) and polythiophene, polycarbazole, polyacetylene-synthesis and applications (sensor and LED). Polymers in solar cell application.
UNIT V **13 hrs**
Functional organic materials: Organic materials for photovoltaic application. Organic electronic luminescent materials. Synthesis of porphyrins and their opto-electrochemical properties. Introduction to nonlinear optics, molecules for NLO and imaging. Organic molecular switches. Design, synthesis and functions of Metal-Organic Framework (MOF) and Covalent Organic Framework (COF).

Recommended Text Books:

1. L. Albrecht, A. Albrecht, L. Dell'Amico, Asymmetric Organocatalysis: New Strategies, Catalysts, and Opportunities, Wiley-VCH, 2022.
2. MacMillan, D. The Advent and Development of Organocatalysis, Nature, 2008, 455, 304–308.
3. W. Y. Teoh, A. Urakawa, Y. H. Ng, P. Sit, Heterogeneous Catalysts: Advanced Design, Characterization and Applications, WILEY-VCH GmbH, 2021.
4. F. Zaera, Molecular Approaches to Heterogeneous Catalysis, 2021, 214179.
5. Scinto, S. L., Bilodeau, D. A., Hincapie, R. et al. Bioorthogonal Chemistry. Nat. Rev. Methods Primers 1, 30 2021.
6. R. E. Bird, S. A. Lemmel, X. Yu, Q. A. Zhou, Bioconjugate Chemistry, 2021, 32, 2457-2479.
7. J. R. Reynolds, B. C. Thompson, T. A. Skotheim, Conjugated Polymers, Perspective, Theory, and New Materials, 4th ed., 2019, Taylor & Francis Group.
8. W. Hou, Y. Xiao, G. Han, J.-Y. Lin, The Applications of Polymers in Solar Cells: A Review. Polymers 2019, 11, 143.
9. V. F. Yusuf, N. I. Malek, S. K. Kailasa, Review on Metal–Organic Framework Classification, Synthetic Approaches, and Influencing Factors: Applications in Energy, Drug Delivery, and Wastewater Treatment, ACS Omega, 2022, 7, 44507-44531.
10. T. J. J. Müller and Uwe H. F. Bunz, Functional Organic Materials- Syntheses, Strategies and Applications, WILEY-VCH, 2007.
11. M. S. Lohse, T. Bein, Covalent Organic Frameworks: Structures, Synthesis, and Applications, Advanced Functional Materials, 2018, 22, 1705553.
12. Introduction to Organic Electronic and Optoelectronic Materials and Devices by Sam-Shajing Sun, Larry R. Dalton, CRC Press, 2008.
13. Organic Optoelectronics by Wenping Hu, John Wiley and Sons, 2013.
14. Organic Electronics Materials and Devices by S. Ogawa, Springer, 2015.
15. A Journey Through the World of Molecular Machines by C. Davis, Create Space, 2010.

16. Molecular Machines and Motors: Recent Advances and Perspectives by A. Credi, S. Silvi and M. Venturi, Topics in Current Chemistry (Springer), 354, 2014.

SKILL ENHANCEMENT COURSES

23-808-0407

Science Communications

Credit 3 **45 hours**

Course Outcome

1. Present data and results of an experiment accurately and effectively.
2. Understand the importance of effective science communication.
3. Identify different target audiences and tailor communication strategies to meet their needs.
4. Develop skills in writing for diverse audiences and purposes.
5. Develop skills in oral presentation and public speaking.
6. Understand the ethical considerations in science communication

Module I (Weeks 1-5)

Good lab practices, Quantifying error in experiments and data analysis, Error propagation, Obtaining good statistical accuracy, Central Limit theorem

Publishing scientific results: The structure of a scientific paper and presentation. Academic ethics & Intellectual property rights.

Module II (Weeks 6-12)

Week 6 – 7: Writing for diverse audiences and purposes, Writing for the web and social media.

Activity: Developing concise science writing skills: Students have to prepare an article for the common man explaining a given scientific research paper/topic to the public.

Week 8 – 10: Preparing and delivering effective speeches, Engaging with the audience.

Activity: Students have to prepare and record a 5-10 min podcast explaining a scientific idea to the public.

Week 11-12: Handling questions and interviews

Activity: Each student takes turns attending a 10 min interview with other students on selected topics.

Module III (Weeks 13 – 16)

Week 14 – 16: Preparing and delivering effective presentations, Using visual aids to communicate science, Principles of data visualization.

Activity: Students have to prepare a 10 min PowerPoint presentation on a given topic.

Week 17 – 18: Final Project: Prepare a scientific report on an experiment the students performed in the lab with abstract, introduction, content, results and references.

Text Books:

1. Science Communication – A Practial Guide for Scientists, L. Bowater, K. Yeoman, Wiley
2. John Durant, and Bina Venkataraman. STS.034 Science Communication: A practical Guide. Fall 2011. Maasachuetts Institute of Technology: MIT Open CourseWare, https://ocw.mit.edu. License: Creative Commons BY-NC-SA
3. Effective Science Communication, S. Illingworth and S. Allen, IOP.
4. The Scientist's Guide to Writing: How to Write More Easily and Effectively throughout Your Scientific Career by Stepen B. Heard

Communicating Science: A Practical Guide by Gavin Brenner and Alan S. J. King

23-808-0507

INDUSTRIAL CHEMISTRY

Credit 3 **60 hours**

Course Outcome After the completion of the course the student will be able to	**Cognitive Level**
C.O. 1: Prepare and analyze industrially important chemical products	Create
C.O. 2: Prepare the treatment methods for conversion of natural resources to value added chemicals	Create

Course Outcome	Program Specific Outcome					
	P.S.O. 1	P.S.O. 2	P.S.O. 3	P.S.O. 4	P.S.O. 5	P.S.O. 6
C.O. 1	1	3	3	3	3	3
C.O. 2	1	3	3	3	3	3

UNIT I	**15 hrs**
Fats and oils general introduction, chemical composition of fats and oils, quality parameters, sources and classification, value added products from vegetable oils. Cleaning products general introduction, Chemistry of cleaning action, classification of cleaning products, Soap and Detergents, chemical composition, principles of preparation, different methods, builders and additives, quality parameters Margarine- Importance, chemical composition, preparation methods, principles of emulsification Biodiesel: energy scenario, consumption pattern, fossil fuel depletion and environmental issues, Alternate solutions, transesterification; FT process, catalysts; biodiesel purification, fuel properties.	
UNIT II	**8 hrs**
Water purification: Concept of Pure Water, Water Contamination, Water Purification Methods, Water quality parameters.	
UNIT III	**7 hrs**
General introduction to essential oils and natural flavours, natural sources, extraction techniques and principles.	
UNIT IV	**10 hrs**
Practice: Preparation, characterization and quality analysis of value added products from vegetable oils (soap, margarine, vanaspati).	
UNIT V	**10 hrs**
Practice: Purification of contaminated water, estimation of quality parameters, pH, conductivity, Total Dissolved Solids, hardness, turbidity, Dissolved oxygen, COD, chloride	
UNIT VI	**10 hrs**
Practice: Extraction and characterization of essential oils and flavours from natural sources.	

Recommended Text Books:

1. Krishna Chattopadhyay and Manas Mandal ANALYTICAL CHEMISTRY SKILL ENHANCEMENT COURSE, CBSCBS Publishers & Distributors, 2022
2. J. N. Gurtu, and A. Gurtu Advanced Physical Chemistry Experiments, 6th Ed., Pragati Prakashan, 2014.
3. J. B. Yadav, Advanced Practical Physical Chemistry, 36th Ed., Krishna Prakashan, 2016.

23-808-0607

VISUALIZATION AND COMPUTING

Credit 3 **60 hours**

Course Outcome After the completion of the course the student will be able to	**Cognitive Level**
C.O. 1: Understand the structures using 3D visualization	Apply
C.O. 2: Build molecule, biomolecules and unit cell	Apply
C.O. 3: Extract structural information from available databases	Analyze
C.O. 4: Calculate and analyse structures and protein ligand binding energies under MM	Analyze

Course Outcome	Program Specific Outcome					
	P.S.O. 1	P.S.O. 2	P.S.O. 3	P.S.O. 4	P.S.O. 5	P.S.O. 6
C.O. 1	3	3		3	3	3
C.O. 2	3	3	2	3	3	3
C.O. 3	3	3	2	3	3	3
C.O. 4	3	3	2	3	3	3

UNIT I	**10 hrs**
Introduction to cheminformatics, Grahical 3D-visualisation of the chemical world using various visualizer tools: Molecules, Biomolecules and Materials. Various file formats, Interconversion of various file formats.	
UNIT II	**15 hrs**
Building molecules, biomolecules and materials using softwares. Internal, Cartesian and fractional coordinate systems. Z-matrix, Unit cell and lattice.	
UNIT III	**10 hrs**
Introduction to databases – Crystallographic databases, Materials project, PDB database – PDB data, Secondary structure prediction, Fold recognition.	
UNIT IV	**10 hrs**
Molecular Mechanics - Force fields - energy calculation, minimization and analysis.	
UNIT V	**15 hrs**
Basics of structure based drug design- Docking - Molecular Recognition, Prediction of Protein-ligand interaction sites.	

Recommended Text Books

1. Leach, A.R. “Molecular Modelling Principles and Application, Longman”, 2001.
2. Haile, J.M. “Molecular Dynamics Simulation Elementary Methods,” John Wiley and Sons, 1997.

3. Satya Prakash Gupta, QSAR and Molecular Modeling, Springer - Anamaya Publishers, 2008.
4. Cramer, C. J., “Essentials of Computational Chemistry- Theories and Models”, 2nd Edition, Wiley, 2004
5. Jensen, F., “Introduction to Computational Chemistry”, 3rd Edition, Wiley, 2017.
6. Young, D., “Computational Chemistry – A Practical Guide”, Wiley, 2001.

23-808-0608

SPECTROANALYTICAL CHEMISTRY

Credit 3 **60 hours**

Course Outcome After the completion of the course the student will be able to	**Cognitive Level**
C.O. 1: Acquire theoretical and practical knowledge in instrumentation aspects of spectroanalytical devices	Apply
C.O. 2: Acquire skill to independently operate the instruments	Apply
C.O. 3: Interpret the data and derive qualitative and quantitative analysis	Apply

Course Outcome	Program Specific Outcome					
	P.S.O. 1	P.S.O. 2	P.S.O. 3	P.S.O. 4	P.S.O. 5	P.S.O. 6
C.O. 1	3	3	1	3	3	2
C.O. 2	1	2	3	3	3	2
C.O. 3	2	2	3	3	3	2

UNIT I **8 hrs**
A brief introduction to analytical methods in chemistry, Qualitative analysis and quantitative analysis, applications in day-to-day life. Introduction to various spectroanalytical techniques, concept of light matter interaction, Jablonski Diagram and origin of different spectroscopies.
UNIT II **10 hrs**
Brief theoretical introduction to colourimetry, absorption spectroscopy, fluorescence spectroscopy, vibrational spectroscopy, refractometry, polarimetry, smartphone spectroscopy.
UNIT III **12 hrs**
Detailed Instrumentation aspects of colourimeter, UV-VIS-NIR spectrometer, Fluorimeter, IR spectrometer, Raman spectrometer, refractometer, smartphone spectrometers.
UNIT IV **10 hrs**
Practice: Colurimetry and UV-VIS spectroscopy: hands on training on the instrument, preparation of stock solutions, verification of Beeer-Lambertz law, Estimation of unknown concentration, establish correlation between molecular structure and spectrum, smartphone spectroscopy and comparison with colorimetry and UV-VIS spectroscopy.
UNIT V **12 hrs**
Practice: vibrational spectroscopy: hands on training on the instrument, preparation of samples, IR and Raman spectroscopic characterization of organic and inorganic samples, assignment of peaks to functional groups, spectral processing, data processing, chemometry and machine learning tools., preparation of nanomaterials of surface enhanced Raman spectroscopy, comparative study of Raman and SERS.

UNIT VI	8 hrs
Practice: Refractometry and Polarimetry: hands on training on the instrument, preparation of stock solutions, estimation of refractive index and optical activity, estimation of unknown concentration, analysis of food samples	

Recommended Text Books:

1. Krishna Chattopadhyay and Manas Mandal, ANALYTICAL CHEMISTRY SKILL ENHANCEMENT COURSE, CBSCBS Publishers & Distributors, 2022.
2. Gurtu, J. N., Gurtu, A., Advanced Physical Chemistry Experiments, 6th Ed.,Pragati Prakashan,2014.