

SRI VENKATESWARA UNIVERSITY::TIRUPATI
S.V.U.COLLEGE OF SCIENCES
DEPARTMENT OF CHEMISTRY

(Syllabus common for SV University College and affiliated by SVU Area)
(Revised Scheme of Instruction and Examination, Syllabus etc., with effect from the
Academic Years 2016-17 for I and II Semesters and 2017-18 for III and IV Semesters)

M.Sc. CHEMISTRY

SCHEME OF INSTRUCTION AND EXAMINATION

Semester	Code	Title of the course	Hrs/week	No. of Credits	Core/Elective	Uni. Exams (Hours)	IA	Semester end exam	Total Marks
FIRST	CHE-101	Inorganic Chemistry -I	4	4	Core	3	20	80	100
	CHE-102	Organic Chemistry-I	4	4	Core	3	20	80	100
	CHE-103	Physical Chemistry	4	4	Core	3	20	80	100
	CHE-104	Inorganic Practical-I	2	2	Practica	--	--	--	50
	CHE-105	Organic Practical-I	2	2	Practica	--	--	--	50
	CHE-106	Physical Practical-I	2	2	Practica	--	--	--	50
	Che-107	General Chemistry-I	2	2	Compul Founda	3	10	40	50
	Che-108	HUMAN VALUES AND PROFESSIONAL ETHICS – I	4	4	Elective founda	3	20	80	100
		TOTAL		24					600

second	CHE-201	INORGANIC CHEMISTRY-II	4	4	Core	3	20	80	100
	CHE-202	ORGANIC CHEMISTRY-II	4	4	Core	3	20	80	100
	CHE-203	PHYSICAL CHEMISTRY-II	4	4	Core	4	--	--	100
	CHE-204P	INORGANIC CHEMISTRY	2	2	Practica	4	--	--	100
	CHE-205P	ORGANIC CHEMISTRY	2	2	Practica	3	20	80	100
	CHE-206P	PHYSICAL CHEMISTRY	2	2	Practica	3	20	80	100
	CHE-207	General Chemistry-II	2	2	Compul Founda	3	20	80	100
	CHE-208	Human Values and Professional Ethics-I	4	4	Elective foundat				
		TOTAL		24					600

M.Sc. ANALYTICAL CHEMISTRY

SEMESTER-III

Semester	Code	Title of the course	Hrs / week	No. of Credits	Core/ Elective	Uni Exams (Hours)	IA	Semester end exam	Total Marks
THIRD	CHE AC-301	INORGANIC SPECTROSCOPY & THERMAL METHODS OF ANALYSIS	4	4	core	3	20	80	100
	CHE AC-302	ORGANIC SPECTROSCOPY	4	4	core	3	20	80	100
	CHE AC-303	Classical Methods of Analysis	4	4	Practical	--		--	100
	CHE AC-304	Instrumental methods of analysis	4	4	Practical	--		---	100
	CHE AC-305 (related to subject)	A): ORGANIC CHEMISTRY - III B): PHYSICAL CHEMISTRY – III C): GREEN CHEMISTRY	4 4	4 4	Generic Electives:*	3 3	20 20	80 80	100 100
	CHE AC-306 Other department	A)Spectral Techniques (or) B)Chromatographic Techniques	4	4	Open Elective	3	20 20	80 80	100 100
					24				600

*Among the generic electives a student shall choose two.

SEMESTER-IV

FOURTH	CHE AC-401	Quality control and General Principles	4	4	core	3	20	80	100
	CHEAC-402	Instrumental Methods of Analysis	4	4	core	3	20	80	100
	CHE AC-403	Instrumental Methods of Analysis-II	8	4	Practical	4		--	100
	CHE AC-404	Project Work	8	4	Practical	4		---	100
	CHE AC-405 (related to subject)	a)Applied and Environmental aspects b) Bioinorganic, Bioorganic & Biophysical Chemistry c) Chemistry of Nanomaterial & Functional materials	4 4	4 4	Generic Elective	3 3	20 20	80 80	100 100
	CHEAC-406 other department	a) Drug Chemistry (Or) b) Electroanalytical Techniques	4 4	4 4	Open Elective	3 3	20 20	80 80	100 100
					24				600

*Among the generic electives a student shall choose two.

M.Sc. ENVIRONMENTAL CHEMISTRY

SEMESTER-III

Semester	Code	Title of the course	Hrs / week	No. of Credits	Core/ Elective	Uni. Exams (Hours)	IA	Semester end exam	Total Marks
THIRD	CHE EC-301	Physical Chemistry -III	4	4	core	3	20	80	100
	CHE EC-302	Spectroscopy Applications	4	4	core	3	20	80	100
	CHE EC-303	Water Analysis	4	4	Pract	--		--	100
	CHE EC-304	Instrumental Methods of Analysis-I	4	4	Practice	--		---	100
	CHE EC-305 (related to subject)	a)Organic Chemistry III B)In organic Spectroscopy & Thermal Methods of Analysis C) Green Chemistry	4 4	4 4	Generic Electives:*	3 3	20 20	80 80	100 100
	CHE EC-306 other department	a)Spectral Techniques or b)Chromatographic Techniques	4	4	Open Elective	3	20 20	80 80	100 100
					24				

*Among the generic electives a student shall choose two.

SEMESTER-IV

FOURTH	CHE EC-401	Water Pollution Monitoring and Environment laws	4	4	core	3	20	80	100
	CHE EC-402	Air Pollution, control Methods- Noise and Thermal pollution	4	4	core	3	20	80	100
	CHE EC-403	Instrumental Methods of analysis-II	8	4	Practica	4		--	100
	CHE EC-404	Project work	8	4	Practica	4		---	100
	CHE EC-405 (related to subject)	a)Energy, Environment and soils b)Bio inorganic, Bioorganic &Biophysical c)Chemistry of Nanomaterials & Functional materials	4 4	4 4	Generic Elective	3 3	20 20	80 80	100 100
	CHE EC-406 other department students	a) Drug Chemistry Or b)Electroanalytical Techniques	4 4	4 4	Open Elective	3 3	20 20	80 80	100 100
					24				

*Among the generic electives a student shall choose two.

M.Sc. INORGANIC CHEMISTRY

SEMESTER-III

Semester	Code	Title of the course	Hrs / week	No. of Credits	Core/ Elective	Uni. Exams (Hours)	IA	Semester end exam	Total Marks
THIRD	CHE IC-301	Inorganic Spectroscopy & Thermal Methods of Analysis	4	4	core	3	20	80	100
	CHE IC-302	Organic Spectroscopy	4	4	core	3	20	80	100
	CHE IC-303	Preparation of Inorganic complexes and characterization	4	4	Pract	--		--	100
	CHE IC-304	Instrumental Methods of Analysis-I	4	4	Practicle	--		---	100
	CHE IC-305 (related to subject)	A) Organic Chemistry-iii b) Physical Chemistry iii c) Green Chemistry	4 4	4 4	Generic Electives:*	3 3	20 20	80 80	100 100
	CHE IC-306 other department	a) Spectral Techniques or b) Chromatographic Techniques	4	4	Open Elective	3	20 20	80 80	100 100
					24				

*Among the generic electives a student shall choose two.

SEMESTER-IV

FOURTH	CHE IC-401	Coordination compounds, Organometallic chemistry & Chemistry of non-transition elements	4	4	core	3	20	80	100
	CHE IC-402	Instrumental Methods of Analysis	4	4	core	3	20	80	100
	CHE IC-403	Instrumental Methods of Analysis-ii	8	4	Practica	4		--	100
	CHE IC-404	Project work	8	4	Practica	4		---	100
	CHE IC-405 (related to subject)	a) Solid state and photo Chemistry b) Bioinorganic, Bioorganic & Biophysical c) Chemistry of Nanomaterials	4 4	4 4	Generic Elective	3 3	20 20	80 80	100 100
	CHE IC-406 other department students	a) Drug chemistry or b) Electroanalytical Techniques	4 4	4 4	Open Elective	3 3	20 20	80 80	100 100
					24				

*Among the generic electives a student shall choose two.

M.Sc. ORGANIC CHEMISTRY

SEMESTER-III

Semester	Code	Title of the course	Hrs / week	No. of Credits	Core/ Elective	Uni. Exams (Hours)	IA	Semester end exam	Total Marks
THIRD	CHE OC-301	Organic Chemistry-III	4	4	core	3	20	80	100
	CHE OC-302	Organic Spectroscopy&Applications	4	4	core	3	20	80	100
	CHE OC-303	Organic Estimations	4	4	Pract	--		--	100
	CHE OC-304	Multistep preparations	4	4	Practicle	--		---	100
	CHE OC-305 (related to subject)	A) In Organic Spectroscopy & Thermal Methods of Analysis b) Physical Chemistry iii c) Green Chemistry	4 4	4 4	Generic Electives:*	3 3	20 20	80 80	100 100
	CHE OC-306 other department	a) Spectral Techniques or b) Chromatographic Techniques	4	4	Open Elective	3	20 20	80 80	100 100
					24				

*Among the generic electives a student shall choose two.

SEMESTER-IV

FOURTH	CHE OC-401	Organic Synthesis-I	4	4	core	3	20	80	100
	CHE OC-402	Organic Synthesis-II	4	4	core	3	20	80	100
	CHE OC-403	Spectral Identification of organic compounds	8	4	Practica	4		--	100
	CHE OC-404	Project work	8	4	Practica	4		---	100
	CHE OC-405 (related to subject)	a) Hetero Cycles & Natural products b) Bioinorganic, Bioorganic & Biophysical Chemistry c) Chemistry of Nanomaterials & Functional materials	4 4	4 4	Generic Elective	3 3	20 20	80 80	100 100
	CHE OC-406 other department	a) Drug chemistry or b) Electroanalytical Techniques	4 4	4 4	Open Elective	3 3	20 20	80 80	100 100
					24				

*Among the generic electives a student shall choose two.

M.Sc. PHYSICAL CHEMISTRY

SEMESTER-III

Semester	Code	Title of the course	Hrs / week	No. of Credits	Core/ Elective	Uni. Exams (Hours)	IA	Semester end exam	Total Marks
THIRD	CHE PC-301	Physical Chemistry-III	4	4	core	3	20	80	100
	CHE PC-302	Organic Spectroscopy	4	4	core	3	20	80	100
	CHE PC-303	Practical-III	4	4	Pract	--		--	100
	CHE PC-304	Practical-III	4	4	Practicle	--		---	100
	CHE PC-305 (related to subject)	a) Organic Chemistry-III b) In Organic Spectroscopy & Thermal Methods of Analysis c) Green Chemistry	4	4	Generic Electives:*	3	20	80	100
			4	4		3	20	80	100
	CHE PC-306 other department students	a) Spectral Techniques or b) Chromatographic Techniques	4	4	Open Elective	3	20	80	100
						20	80	100	
				24				600	

*Among the generic electives a student shall choose two.

SEMESTER-IV

FOURTH	CHE PC-401	Electrochemistry	4	4	core	3	20	80	100
	CHE PC-402	Thermodynamics, Polymers and Solid state Chemistry	4	4	core	3	20	80	100
	CHE PC-403	Practical-I	8	4	Practica	4		--	100
	CHE PC-404	Project work	8	4	Practica	4		---	100
	CHE PC-405 (related to subject)	a) Chemical Kinetics b) Bioinorganic, Bioorganic & Biophysical Chemistry c) Chemistry of Nanomaterials & Functional materials	4	4	Generic Elective	3	20	80	100
			4	4		3	20	80	100
	CHE PC-406 other department students)	a) Drug chemistry or b) Electroanalytical Techniques	4	4	Open Elective	3	20	80	100
4			4	3		20	80	100	
				24				600	

*Among the generic electives a student shall choose two.

FIRST SEMESTER

CHE 101- CORE THEORY: INORGANIC CHEMISTRY-I

UNIT-I: CO-ORDINATION COMPOUNDS

15 Hrs

Introduction to Crystal field Theory, CFSE and its calculation, Pairing energy, Splitting of 'd' orbitals in Trigonal bi pyramidal, square planar, square pyramid and pentagonal bipyramidal geometries, Jahn –Teller effect, Application of CFT, OSSE, site Selection in Spinels, Short comings of CFT, Evidence for covalency –Nephelauxetic effect. MOT of coordinate bonds –M.O. Diagrams for octahedral, tetrahedral and square planar complexes. Experimental evidences for π - bonding – Crystallography, Infrared spectroscopy and Photoelectron spectroscopy.

UNIT-II: CHEMISTRY OF NON-TRANSITION ELEMENTS

15 Hrs

General characteristics of the non- transition elements special features of individual elements ; Synthesis' properties and structure of their Halides and Oxides, Polymorphism of Carbon, Phosphorus and Sulphur, Synthesis, properties and structure of boranes, Carboranes, borazines, Silicates, Carbides, Sulphur-nitrogen compounds. Electron counting in boranes, Wades rules (Poly hedral skeletal electron pair theory), Isopopoly and hetero poly acids.

UNIT-III: REACTION MECHANISMS IN COMPLEXES

15 Hrs

Reactivity of metal complexes. Inert and Labile complexes. Concept of Labile and Inert complexes in terms of Valence bond and Crystal Field theories. Taube's classification of complexes as labile and inert complexes. Dissociative (D) and Dissociative interchange Mechanism (Id) & Associative (A) and Associative interchange Mechanism (Ia). Substitution reactions in octahedral complexes- Acid Hydrolysis -factors affecting Acid Hydrolysis - Base Hydrolysis-conjugate Base Mechanisms - Anation Reactions -Substitution Reactions in Square Planar complexes- Trans effect – Mechanisms of Trans effect: polarization and π -bonding theories. Electron Transfer Reaction-Inner Sphere and outer Sphere Mechanisms- Marcus theory.

UNIT-IV: METAL π COMPLEXES-I

15 Hrs

Nature of π bonding, Classification of π ligands, π donor ligands and π -acceptor ligands.

Metal Carbonyls: Synthesis of metal carbonyls, Structures of metal carbonyls of the types $M(CO)_n$ ($M=Cr, Fe, Ni; n=4-6$), $M_2(CO)_n$ ($M=Co, Fe, Mn; n=8-10$), $M_3(CO)_{12}$ ($M=Fe, Ru$ and Os), $M_4(CO)_{12}$ ($M=Co, Rh, Ir$). IR Spectra of metal carbonyls (i) Detection of bridging and terminal CO ligand, (ii) Synergistic effect, EAN and 18-electron rule. Electron counting methods (i) Oxidation state method and (ii) Neutral Atom method.

Metal Nitrosyls: Synthesis of metal Nitrosyls, bonding, Electron donation by nitric oxide, Models for NO bonding (i) Covalent model and (ii) Ionic models, Structures of metal nitrosyls (1) $[Fe_4S_3(NO)]$ (2) $[Fe_2(NO)_2I_2]$ (3) $[(\phi_3P)_2Ir(CO)Cl(NO)]^+$ (4) $[(\phi_3P)_2Ru(NO)_2Cl]$, Detection of bridging NO ligand, Applications of metal nitrosyls.

Books Suggested

1. F.A.Cotton and G.Wilkinson, Advanced In-organic chemistry VI Edition, 1999. John wiley & sons. Inc., New York.
2. James E. Huheey, Inorganic chemistry- Principles of structure and reactivity, VI Edition 1993. Harper Collins College Publishers, New York.
3. J.D.Lee: Concise Inorganic Chemistry (Blackwell)
4. Gary Wolfsburg: Inorganic Chemistry (5th Ed. (Viva Books)
5. W.L.Jolly: Modern Inorganic Chemistry (McGraw-Hill)
6. B.N Figgis: Introduction to Ligand Fields (John-Wiley)
7. S.F.A.Kettle: Coordination compounds.
8. Coordination Chemistry. Bassalo & Jahson.

CHE 102- CORE THEORY: - ORGANIC CHEMISTRY-I

UNIT-I: Stereochemistry

15 Hrs

Stereoisomerism-Stereoisomers Classification – Configuration and conformation.

Molecular Three dimensional representations: Wedge, Fischer, Newman and Saw-horse formulae, their description and interconversions.

Molecular Symmetry & Chirality: Symmetry operations and symmetry elements (C_n & S_n). Criteria for Chirality. Dissymmetrization.

Optical isomerism: Molecular Symmetry and Chirality-Cahn-Ingold-Prelog rules R, S-nomenclature, stereoisomerism resulting from more than one chiral center, meso and pseudoasymmetric compounds - **Axial Chirality** - Stereochemistry of allenes spiranes - biphenyl derivatives and atropisomerism - **Planar chirality** - Ansa compounds and trans - Cycloalkenes - **Helicity**. Helically chiral compounds

Geometrical isomerism - E, Z - nomenclature - Physical and Chemical methods of determining the configuration of geometrical isomers-Stereoisomerism in 3, 4 and 5-membered cyclic compounds.

UNIT-II: Substitution Reactions

15 Hrs

i) Aliphatic Nucleophilic substitutions: The S_N2 , S_N1 , mixed S_N1 and S_N2 , SET

mechanisms. Reactivity- effects of substrates, attacking nucleophiles, leaving groups and reaction medium. Common carbocation rearrangements – primary, secondary and tertiary.

The neighbouring group participation (NGP) -anchimeric assistance, NGP by σ and π -bonds, phenonium ions, norbornyl and norbornenyl systems, Classical and nonclassical carbocations, NGP by halogens and heteroatoms (O,N,S)

The S_N1 and S_N2' mechanisms. Nucleophilic substitution at an allylic, and vinylic carbons.

ii. Aromatic Nucleophilic Substitution: The S_NAr , S_N1 , benzyne and $S_{RN}1$ mechanisms.

Reactivity - effect of substrate, structure, leaving group and attacking nucleophile. The von Richter, Sommelet - Hauser and Smiles rearrangements.

UNIT-III: Reactive intermediates

15 Hrs

Types of reactions, types of bond cleavage mechanisms, generation, structure, stability and reactivity of carbocations, carbanions, free radicals, carbenes, nitrenes and arynes. Thermodynamic and kinetic requirements, kinetic and thermodynamic control, potential energy diagrams, transition states and intermediates, methods of determining mechanisms, isotope effects.

UNIT-IV: Terpenoids

15 Hrs

Classification of terpenoids, occurrence, isolation, general methods of structure determination. Isoprene and special isoprene rule. Structure determination and synthesis of the following representative molecules: Farnesol, Zingiberine, Cadinene and Abietic acid.

Books Suggested:

1. Advanced Organic Chemistry-Reactions, Mechanism and Structure, Jerry March, John Wiley.
2. Advanced Organic Chemistry, F.A. Carey and R.J Sundberg, Plenum.
3. Structure and Mechanism in Organic Chemistry C.K.Inglod, Cornell University Press.
5. Organic Chemistry, R.T Morrison and R.N. Boyd, Prentice - Hall.
6. Principles of Organic Synthesis, R.O.C Norman and J. M. Coxon, Blackie Academic.
7. Stereochemistry, P.S.Kalsi, Wiley Eastern.
8. Text book of Organic Chemistry, M.C. Murry
9. Organic Chemistry, Vol I, I.L.Finar, ELBS Eds.

CHE 103- CORE THEORY: PHYSICAL CHEMISTRY- I

UNIT-I : Quantum Chemistry-I

15 Hrs

(A) Introduction to Exact Quantum Mechanical Results

Operator algebra, Eigen values and Eigen functions, Operators for momentum and energy, Degeneracy, Linear combination of Eigen functions of an operator, well behaved wave functions, Normalized and orthogonal functions, The schrodinger wave equation and the postulates of Quantum Mechanics, **Applications of Schrodinger wave equation:** Particle in one dimensional and three dimensional box, harmonic oscillator, rigid rotor, hydrogen atom and its applications. Hydrogen like wave function, hydrogen like orbitals and their representation, polar plots, contour plots and boundary diagram. . **Approximate Methods:** The variation Theorem, Linear variation principle, perturbation Theory (first Order and non-degenerate), Application of variation Method and perturbation theory to the helium atom, The Born-Oppenheimer approximation.

UNIT-II: Chemical Dynamics

15 Hrs

(A) **Theories of reaction rates:** Collision theory, steric factor. Theory of Absolute Reaction Rates-Reaction coordinate, activated complex and the transition state. Thermodynamic formulation of reaction rates.

(B) **Unimolecular reactions:** Lindemann, Lindemann-Hinshel wood, and RRKM theories. Termolecular reactions. Complex reactions-Rate expressions for opposing, parallel and consecutive reaction (all first order type)

(C) **Chain reactions:** Dynamic chain, hydrogen-bromine reaction, pyrolysis of acetaldehyde, decomposition of ethane, photochemical reactions- H_2-Br_2 , H_2-Cl_2 reactions, Autocatalysis, H_2-O_2 reaction explosion limits. (D) **Fast Reactions:** Flow system – Temperature and pressure Jump Methods – Relaxation Techniques.

UNIT – III : Thermodynamics

15 Hrs

(A) **Brief review of Thermodynamic concepts:** Enthalpy, entropy, free energy. Concept of Entropy –Entropy as a state function –Entropy change in reversible process and irreversible process – Temperature – Entropy diagrams – Entropy change and phase change – Entropy of mixing – Entropy and disorder.

(B) **Statistical thermodynamics:** Partial molar properties: their significance and determination of partial molar properties, fugacity and its determination. Concept of distribution, thermodynamic probability and most probable Distribution, Ensemble averaging, postulates of ensemble averaging, canonical, grand canonical and micro-canonical ensembles, partition functions, translational, rotational, vibrational and electronic partition functions, Gibbs- Duhem equation, calculation of thermodynamic properties in terms of partition functions, Entropy of monatomic gases (Sackur-Tetrad equation)

UNIT-IV : Electrochemistry I

15 Hrs

(A) Thermodynamic and Kinetic concept of Electrochemistry

Thermodynamic and Kinetic Derivation of Nernst Equation, Chemical and Concentration Cells with and without Transference, Liquid Junction Potential, Derivation of the Expression for Liquid Junction Potentials-its determination and elimination, Applications of EMF Measurements: (i)Solubility product, (ii)pH Determination, (iii) Potentiometric Titrations. ;

(B) Conductivity

Theory of Electrolytic Conductance, Derivation of Debye-Huckle Equation and its Verification, Debye- Falkenhagen Effect, and Wein Effect, Kohlrausch law. Calculation of Solubility of Sparingly soluble Salt from Conductance Measurements.

Conductometric Titrations : Titration of Strong Acid Vs Strong Base (HCl vs NaOH) ; Titration of Weak Acid Vs Strong Base (AcOH vs NaOH); Titration of mixture of Strong and Weak Acids vs Strong Base ; Precipitation Titrations. ; **Electrocatalysis** : Influence of various parameters.

Books Suggested

1. physical chemistry, P. W. Atkins (ELBS)
2. Introduction to quantum chemistry, A. K. Chandra (Tata McGraw Hill)
3. Quantum Chemistry, Ira N. Levine (Prentice Hall)
4. Atomic Structure and Chemical bond, Manas Chandra.
5. Chemical Kinetics, K.J. Laidler (Mc Graw Hill)
6. Kinetics and Mechanism of Chemical Transformations, J. Rajaraman and J. Kuriacose (Mcmilan)
7. Thermodynamics for chemists, S. Glasstone
8. Chemical thermodynamics, I.M. Klotz
9. Statistical Thermodynamics, M. Dole
10. Modern Electrochemistry, Vol. I & II, J.O. M.Bockris and A.K.N.Reddy (pln)
11. An Introduction to Electrochemistry (3rd ed.), S. Glasstone (Affiliated East-West)

FIRST SEMESTER PRACTICALS

CHE-104: CORE PRACTICAL- 1: INORGANIC CHEMISTRY

I Semi Micro Qualitative Analysis:

Qualitative Analysis of a mixture containing four cations including two less common cations (viz., W, Mo, Se, Te, V, Ce, Th, Zr, Li and U).

CHE-105: CORE PRACTICAL - 2: ORGANIC CHEMISTRY

- a) Identification of single organic component by systematic qualitative analysis.
- b. Single step preparations.
 1. Preparation of aspirin
 2. Preparation of p-nitroacetanilide
 3. Preparation of p-bromoacetanilide

CHE-106: CORE PRACTICAL - 3: PHYSICAL CHEMISTRY

1. Calibration of volumetric apparatus and statistical analysis of the data.
2. Determination of critical solution temperature of phenol-water system and study the effect of electrolyte on CST.
3. Determination of Eutectic composition and temperature of binary system
4. Determination of distribution coefficient of benzoic acid between water and benzene.
5. Study the adsorption of acetic acid on charcoal and analysis of the data on the basis of Langmuir and Freundlich adsorption isotherms.
6. Determination of rate constant of acid hydrolysis of an ester and investigate the effect of catalyst concentration, reactant concentration and temperature.

CHE 107: COMPULSORY FOUNDATION: (GENERAL CHEMISTRY-I)

UNIT-I: TREATMENT OF ANALYTICAL DATA

15 Hrs

Precision and accuracy –mean and median values –Standard deviation – coefficient of variation, Types of errors: Determinate and indeterminate errors, confidence limits, significant figures, computations, minimization of errors, statistical evaluation of data –T-test, F-test, and X^2 -test. Correlation coefficient and coefficient of determination; Limit of detection (LOQ); Limit of determination (LOD) Sensitivity and selectivity of an analytical method.

UNIT-II: FLAME EMISSION AND ATOMIC ABSORPTION SPECTROSCOPY 15 Hrs

(a) **Flame Emission Spectroscopy:** Principles, chemical reactions in flames, Interferences, evaluation methods, flame photometer and experimental technique, procedure for determinations, limitations and disadvantages. Applications

(b) **Atomic Absorption Spectroscopy: Flame AAS:** Principle, Instrumentation – Sources of radiation (HCL and EDL), Different types of burners, Interferences- Physical, Chemical, spectral and back ground correction, and methods of minimization

GF AAS: Principle and technique –Comparison between Flame AAS and furnace AAS, Applications of AAS, Comparison between Atomic Absorption & Flame Photometry.

Books Suggested

1. H.W. Willard, LL. Merritt and J.A. Dean: Instrumental Methods of Analysis
2. Vogel's Text book of Quantitative Inorganic Analysis.
3. Analytical Chemistry
4. Instrumental Methods of Analysis H. Kaur

CHE 108: ELECTIVE FOUNDATION (HUMAN VALUES AND PROFESSIONAL ETHICS – I)

Chapter I: Definition and Nature of Ethics – Its relation to Religion, Politics, Business, Law, Medicine and Environment. Need and Importance of Professional Ethics – Goals – Ethical Values in Various Professions.

Chapter II: Nature of Values – Good and Bad, Ends and Means, Actual and Potential Values, Objective and Subjective Values, Analysis of Basic Moral Concepts – Right, Ought, Duty, Obligation, Justice, Responsibility and Freedom, Good Behavior and Respect for Elders, Character and Conduct.

Chapter III: Individual and Society: Ahimsa (Non-Violence), Satya (Truth), Brahmacharya (Celibacy), Asteya (Non Possession) and Aparigraha (Non-stealing). Purusharthas (Cardinal virtues) - Dharma (Righteousness), Artha (Wealth), Kama (Fulfillment Bodily Desires), Moksha (Liberation), Crime and Theories of Punishment – (a) Reformative, Retributive and Deterrent, (b) Views on Manu and Yajnavalkya

Chapter IV: Bhagavad Gita – (a) Niskama Karma, (b) Buddhism – The Four Noble Truths – Arya astanga marga, (c) Jainism - Mahavratas and Anuvratas. Values Embedded in Various Religions, Religious Tolerance, Gandhian Ethics.

Books for study:

1. Johns S Mackenjie: A Manual of ethics
2. "The Ethics of Management" by Larue Tone Hosmer, Richard D. Irwin Inc.
3. Management Ethics – Integrity at work by Joseph A. Petrick and John F. Quinn, Response Books, New Delhi.

4. "Ethics in Management" by S.A. Shelekar, Himalaya Publishing House.
5. Harold H. Titus: Ethics for Today
6. Maitra, S.K: Hindu Ethics
7. William Lilly: Introduction to Ethics
8. Sinha: A Manual of Ethics
9. Manu: Manava Dharma Sastra or the Institute of Manu: Comprising the Indian System of Duties: Religious and Civil (ed) G.C. Haughton.
10. Sasruta Samhita: Tr. KavirajKunjanlal, KunjanlalBrishagratha, Chowkamba Sanskrit Series, Vol I,II and III, Varanasi, Vol I PP, 16-20, 21-32 and 74-77 only.
11. Charaka Samhita: Tr. Dr. Ram Karan Sarma and Vaidya Bhagavan Dash, Chowkambha Sanskrit Series Office. Varanasi I, II, III Vol I PP 183-191.
12. Ethics, Theory and Contemporary Issues. Barbara Mackinnon, Wadsworth/Thomson Learning, 2001.
13. Analyzing Moral Issues, Judith A. Boss, Mayfield Publishing Company, 1999.
14. An Introduction to Applied Ethics (Ed.) John H. Piet and Ayodya Prasad, Cosmo Publications.
15. Text Book for Intermediate First Year Ethics and Human Values, Board of Intermediate Education – Telugu Academy, Hyderabad.
16. I.C. Sharma Ethical Philosophy of India. Nagin& Co Julundhar.

SECOND SEMESTER

(CBCS syllabus of the students admitted from 2016-17)

CHE 201-CORE THEORY: INORGANIC CHEMISTRY-II

UNIT – I: TRANSITION METAL II – COMPLEXES II 15 Hrs

Transition metal π – complexes with unsaturated organic molecules – alkenes, alkynes, diene, dienyl and Cyclopentadienyl complexes and arene complexes-general methods of preparation, properties, nature of bonding and structural features – Important reactions relating to Nucleophilic and Electrophilic attack on ligands and to organic synthesis.

UNIT – II: ELECTRONIC SPECTRA OF COMPLEXES 15 Hrs

Russel-Saunders coupling – Spectroscopic term symbols- Derivation of term symbols of p^2 and d^2 configuration, Hole Formulation, Energy ordering of terms (Hund's Rules), Splitting of energy levels and spectroscopic states in Octahedral field, Selection rules – Break – down of selection rules

Orgel diagrams, Definition and utility–Orgel Diagrams for d^1 to d^9 configurations in Octahedral and tetrahedral fields. Interpretation of electronic spectra of high spin octahedral and tetra hedral complexes of Ti(III), V(III), Cr(III), Mn(III), Mn(II), Fe(II), Fe(III), Co(III), Co(II), Ni(II) and Cu(II) complexes, Calculation of Dq and B^1 parameters for Cr(III) and Ni(II) complexes.

Tanabe – Sugano diagrams, Differences between Orgel diagrams and Tanabe – Sugano diagrams, Tanabe – Sugano diagrams of d^2 to d^6 and d^8 configurations. Charge transfer spectra- LMCT and MLCT.

UNIT – III: MAGNETIC PROPERTIES OF TRANSITION METAL COMPLEXES 15 Hrs

Diamagnetism and paramagnetism-orbital and spin contributions, spin-orbit coupling, Hund's third rule and Energies of J levels – Curie law and Curie – Weiss law- Ferromagnetism and antiferromagnetism – Temperature independent magnetism Magnetic susceptibility and its determination by Gouy's and Faraday methods.

Calculation of magnetic moment from magnetic susceptibility, spin-only formula, Orbital contribution to magnetic moment (Oh and Td Complexes) –Paramagnetism and crystalline fields – Ti (III), V (III), VO^{2+} , Cr (III), Mn (II), Fe (III), Co(II), Ni (II) and Cu (II). Magnetic Exchange in copper acetate and other dimmers – spin cross over in complexes.

UNIT –IV: CATALYSIS 15 Hrs

Homogeneous catalysis, Metal ion catalyzed reactions – Redox potentials and processes – Mechanism of redox processes involving ligands – Factors affecting redox potentials - other types of metal catalyzed reactions – Reactions involving Ag (I) , Cu (II) and Os (VIII) – Reactions of Oxyanions – Factors affecting rate (General discussion only) – Induced reactions – Free radical reactions – Thermal decomposition of peroxy disulphate – Fe(III) – S_2O_8 reactions – chain reactions – H-Br reactions, H_2O_2 – S_2O_8 reactions.

Books Suggested

1. Inorganic Chemistry principles of Structure and Reactivity 6th Edition. James E. Huheey.
2. Organometallic Chemistry: R.C.Mehrotra and Singh.
3. R. S. Drago: Structural methods in Inorganic Chemistry.
4. H. H. Willard, L. L. Merritt, Jr., J. A. Dean and F. A. Settle, Jr.: Instrumental Methods of Analysis (CBS Publishers).
5. R. L. Carlin: Magnetic Chemistry. R. L. Datta and A. Syamal: Elements of Magnetic Chemistry.

CHE 202- CORE THEORY: ORGANIC CHEMISTRY-II

UNIT-I: Reaction mechanism-I 15 Hrs

Electrophilic addition to carbon carbon double bond: Stereoselective addition to carbon carbon double bond; anti addition- Bromination and epoxidation followed by ring opening. Syn addition of OsO_4 and $KMnO_4$.

Elimination reactions Elimination reactions E_2 , E_1 , E_{1CB} mechanisms. Orientation and stereoselectivity in E_2 eliminations. Pyrolytic syn elimination and α -elimination, elimination Vs substitution. Factors influencing the elimination reactions

Determination of reaction mechanism: Determination of reaction mechanism: Energy profiles of addition and elimination reactions, transition states, product isolation and structure of intermediates, use of isotopes, chemical trapping, crossover experiments. Use of IR and NMR in the investigation of reaction mechanism.

UNIT-II: Molecular Rearrangements: 15 Hrs

Rearrangements to electron deficient Carbon atom:

Pinacol-Pinacolone, Wagner-Meerwein, Dienone-Phenol and Demjonoje Rearrangements

Rearrangements to electron deficient Nitrogen atom:

Hofmann, Curtius, Schmidt and Beckmann Rearrangements.

Rearrangements to electron deficient Oxygen atom: Baeyer-Villiger and Dakins Rearrangements

Rearrangements to electron rich Carbon atom: Favorski and Neber Rearrangements

Aromatic and Sigmatropic Rearrangements: Fries and Claisen Rearrangements

UNIT III: Three and four membered heterocycles: 15 Hrs

Systematic nomenclature (Hantzsch-Widmann system) and Replacement nomenclature for monocyclic heterocycles (Three and four membered rings). Synthesis and chemical reactions of aziridines, oxiranes, thiiranes, azetidines, oxetanes, and thietanes.

UNIT-IV: Alkaloids 15 Hrs

Occurrence, isolation, general methods of structure elucidation and physiological action, degradation, classification based on nitrogen heterocyclic ring, structure elucidation and synthesis of the following: Atropine, Papaverine and Quinine.

Books Suggested:

1. Advanced Organic Chemistry-Reactions, Mechanism and Structure, Jerry March, John Wiley.
2. Advanced Organic Chemistry, F.A. Carey and R.J Sundberg, Plenum.
3. Structure and Mechanism in Organic Chemistry C.K.Inglod, Cornell University Press.
4. Organic Chemistry, R.T Morrison and R.N. Boyd, Prentice - Hall.
5. Modern Organic Reactions, H.O. House, Benjamin.
6. Principles of Organic Synthesis, R.O.C Norman and J. M. Coxon, Blackie Academic.
7. Stereochemistry, P.S.Kalsi, Wiley Eastern.
8. Text book of Organic Chemistry, M.C. Murry
9. Text book of Organic Chemistry, Fessendon and Fessendon.
10. Text book of Organic Chemistry, T.W. Solomon,
11. Organic Chemistry, Vol II, I.L.Finar, ELBS Eds.
12. Heterocyclic chemistry T.L Gilchrist, Longman Scientific Technical
13. An Introduction to the Heterocyclic compounds, R M Acheson, John Wiley.

CHE 203: CORE THEORY: PHYSICAL CHEMISTRY-II**UNIT-I: Quantum Chemistry-II** 15 Hrs

(A) Angular momentum: Angular momentum, Rotations and angular momentum, Eigen functions and Eigen values of angular momentum, Ladder operator, addition of angular momenta, spin, antisymmetry and pauli Exclusion principle. Slater determinant. ;

(B) Molecular Orbital Theory

Atomic Orbitals, Simple Molecular Orbitals, Hybrid Atomic Orbitals, Shapes and energies of Molecular Orbital, Systems of Organic Molecules (Ex: Methane, Ethylene, Acetylene). Huckel theory of conjugated systems, Π -bond order and charge density calculations, application of Huckel theory to ethylene, butadiene and benzene.

UNIT-II: Surface Chemistry 15 Hrs

Surface tension, capillary action, pressure difference across curved surface, (Laplace equation), vapour pressure of droplets (Kelvin equation), Gibbs adsorption isotherm, BET adsorption isotherm, derivation of BET equation, limitations of BET equation, estimation of surface area from BET equation, Surface films on liquids. Concept of electric double layer model- Helmholtz perrin, Gouy- Chapman and stern models (no derivation)

Micells: Surface active agents, classification of surface active agents micellisation, hydrophobic interaction, critical micellar concentration (CMC), factors affecting the CMC of surfactants, thermodynamics of micellisation, emulsions, reverse micelles.

UNIT-III: SYMMETRY AND GROUP THEORY

15 Hrs

Definition of a group, rules that are set for a group, sub-group, order of a group, Relation between order of a finite group and its sub-group, conjugacy relation and class of a group, symmetry elements and symmetry operation. Symmetry point group (ML, MS and MS), Schoenflies symbols - Representation of groups by matrices (representation for C_n , C_{nv} , D_{nh} etc. groups to be worked out explicitly), character of a representation, group multiplication tables, reducible - irreducible representations The great orthogonality theorem (without proof) - character tables (H_2O, NH_3) and their use in spectroscopy, Mulliken character tables.

UNIT-IV: ELECTROCHEMISTRY- II

15 Hrs

Irreversible Electrode phenomenon:

Reversibility and irreversibility, Dissolution and deposition potentials, Decomposition voltage, overvoltage, diffusion overvoltage, charge transfer overvoltage, concentration overvoltage-hydrogen and oxygen overvoltages, Tafel plots, Exchange current density and Transfer coefficient, Butler-Volmer equation for one electron transfer processes.

Polarography:

Theory, classification, principle, Instrumentation of Polarography, DME, HMDE diffusion current, Ilkovic equation, DC-Polarography, AC-Polarography, Controlled Potential Electrolysis, Millicoulometry, Equation for half-wave potentials, for reversible system when oxidant alone, reductant alone and both are present.

Books Suggested

1. P.W. Atkins: Physical Chemistry (ELBS).
2. A.K. Chandra: Introduction to quantum Chemistry (Tata Mc Graw Hill).
3. Ira N. Levine: Quantum Chemistry (Prentice Hall).
4. R. Mcweeny: Coulson's Valence (ELBS).
5. J.O.M. Bockris and A.K.N. Reddy, Modern Electrochemistry, vol.I & II (Plenum).
6. S. Glasstone; An Introduction to Electrochemistry (3rd ed.)(Affiliated East-West).
7. V. Moroi: Micelles, theoretical and applied aspects (Plenum).
8. S. Glasstone: A text Book of physical Chemistry (2nd Ed.) (Macmilan).
9. Maron and prutton: principles of physical Chemistry.
10. Silbey, Alberty, Bawendi. Physical Chemistry. Jhon-Wiley & Sons. 4th edition-2006.
11. V.S. Bagotsky. Fundamental of Electrochemistry. Jhon Wiley & sons. 2nd editions-2006.
12. Jack Simons. An Introduction to theoretical chemistry. The press Syndicate of the University of Cambridge.
13. D.N. Bajpai: Advanced physical Chemistry: S. Chand & Company, 1998.

II SEMESTER PRACTICALS

CHE-204 : CORE PRACTICAL: INORGANIC CHEMISTRY

I . Quantitative Analysis:

Separation and determination of two component mixtures:

- (i) Separation of Al(III) and Determination of Fe (III)
- (ii) Separation of Cu(II) and Determination of Zn (II)
- (iii) Separation of Ca(II) and Determination of Mg (II)
- (iv) Separation of Cu(II) and Determination of Ni (II)
- (v) Determination of Ferrocyanide and Ferricyanide

II. Preparation of Metal Complexes:

- (i) Tetra(ammine) copper (II) sulphate.
- (ii) Mercury tetra(thiocyanato) cobaltate(II).
- (iii) Hexa(ammine) Nickel (II) chloride.
- (iv) Tris(acetylacetonato) Manganese (III) chloride.
- (v) Tris (ethylenediammine) Nickel (II) thiosulpha

CHE-205: CORE PRACTICAL: ORGANIC CHEMISTRY

Separation and Identification of two component organic mixture by systematic qualitative analysis.

CHE-206: CORE PRACTICAL: PHYSICAL CHEMISTRY PRACTICALS

1. Conductometry:
 - (a) Determination of cell constant
 - (b) Verification of Onsager equation
 - (c) Determination of dissociation constant of a weak acid
 - (d) Titration of a strong acid with a strong base
 - (e) Titration of a weak acid with a strong base
2. Potentiometry:
 - (a) Titration of a strong acid with a strong base
 - (b) Titration of a weak acid with a strong base
 - (c) Redox titration
3. Coulometry: Estimation of Manganese
4. pHmetry: Strong acid, Strong base titrations.

CHE-207: COMPULSORY FOUNDATION (GENERAL CHEMISTRY-II)

UNIT-I: ELECTRO ANALYTICAL METHODS

15 Hrs

Theory of potentiometry, calculation electrode potential at the equivalence. Finding of equivalence volume, derivative and linear titration plots. Ion-sensitive electrodes –types of ion sensitive electrodes –metal based cation and anion sensitive electrodes, solid membrane electrodes, glass electrodes. Liquid ion-exchange electrodes, gas sensing membrane electrodes, Amperometric titrations - Anodic stripping voltammetry, chronoamperometry, chronopotentiometry, Cyclic Voltammetry, Differential Pulse Polarography, linear sweep voltammetry, square wave voltammetry.

UNIT-II: CHROMATOGRAPHY

15 Hrs

General principles and classifications of chromatographic separations

Thin layer chromatography: Classification, principle, experimental technique, sample application, development of plate, retardation factor.

Gas liquid chromatography: Gas liquid chromatography - instrumentation (columns and detectors), retention time and retention volume. Chromatographic behaviour of solutes, column efficiency and resolution, column processes and band broadening, time of analysis and resolution, Van-Deemter equation.

High performance liquid chromatography: Theory and instrumentation- column performance, gradient elution, delivery system, sample introduction, separation columns, detectors and applications of HPLC.

Books Suggested

1. H.W. Willard, LL. Merrit and J.A. Dean: Instrumental Methods of Analysis. Affiliated East-West).
2. G.H. Jeffery J. Bassett, J. Mendham and R.C. Denny. Vogel's Text Book of Quantitative Chemical Analysis (ELBS).
3. D.A. Skoog and D.M. West: Principles of Instrumental Analysis (Holt, Rinehart and Wilson).
4. J.G. Dick : Analytical Chemistry (McGraw Hill).
5. D. Midgley and K. Torrance : potentiometric Water Analysis (John Wiley).
6. Silbey, Alberty, Bawendi. Physical chemistry. Jhon-Wiley & sons. 4th edition-2006.

CHE 208: ELECTIVE FOUNDATION (Human Values and Professional Ethics – II)

Chapter I: Value Education – Definition – Relevance to present day – Concept of human values - Self introspection – Self esteem. Family values-Components, Structure and responsibilities of family Neutralization of anger – Adjustability – Threats of family life – Status of women in family and society – Caring for needy and elderly – Time allotment for sharing ideas and concerns.

Chapter II: Medical ethics – Views of Charaka, Sushruta and Hippocrates on moral responsibility of medical practitioners. Code of ethics for medical and healthcare professionals. Euthanasia, Ethical obligation to animals, Ethical issues in relation to health care professionals and patients. Social justice in health care, human cloning, problem of abortion. Ethical issues in genetic engineering and Ethical issues raised by new biological technology or knowledge.

Chapter III: Social ethics – Organ trade, Human trafficking, Human rights violation and social disparities, Feminist ethics, Surrogacy/pregnancy. Ethics of media – Impact of Newspapers, Television, Movies and Internet, Business ethics – Ethical standards of business – Immoral and illegal practices and their solutions. Characteristics of ethical problems in management, ethical theories, causes of unethical behavior, Ethical abuses and work ethics.

Chapter IV: Environmental ethics – Ethical theory, man and nature - Ecological crisis, Pest control, Pollution and waste, Climate change, Energy and pollution, Justice and environmental health.

Books for study:

1. Johns S Mackenjie: A Manual of ethics
2. "The Ethics of Management" by Larue Tone Hosmer, Richard D. Irwin Inc.
3. Management Ethics – Integrity at work by Joseph A. Petrick and John F. Quinn, Response Books, New Delhi.
4. "Ethics in Management" by S.A. Shelekar, Himalaya Publishing House.
5. Harold H. Titus: Ethics for Today
6. Maitra, S.K: Hindu Ethics
7. William Lilly: Introduction to Ethics
8. Sinha: A Manual of Ethics
9. Manu: Manava Dharma Sastra or the Institute of Manu: Comprising the Indian System of Duties: Religious and Civil (ed) G.C. Houghton.
10. Sasruta Samhita: Tr. KavirajKunjanlal, KunjanlalBrishagratha, Chowkamba Sanskrit Series, Vol I,II and III, Varanasi, Vol I PP, 16-20, 21-32 and 74-77 only.

11. Charaka Samhita: Tr. Dr. Ram Karan Sarma and Vaidya Bhagavan Dash, Chowkambha Sanskrit Series Office. Varanasi I, II, III Vol I PP 183-191.
12. Ethics, Theory and Contemporary Issues. Barbara Mackinnon, Wadsworth/Thomson Learning, 2001.
13. Analyzing Moral Issues, Judith A. Boss, Mayfield Publishing Company, 1999.
14. An Introduction to Applied Ethics (Ed.) John H. Piet and Ayodya Prasad, Cosmo Publications.
15. Text Book for Intermediate First Year Ethics and Human Values, Board of Intermediate Education – Telugu Academy, Hyderabad.
16. I.C. Sharma Ethical Philosophy of India. Nagin & Co Julundhar.

SEMESTER-III (ORGANIC CHEMISTRY)

CHE-OC-301 Core-Theory Organic Chemistry III

UNIT I: REAGENTS IN ORGANIC SYNTHESIS

15 Hrs

Use of the following reagents in organic synthesis: Anhydrous AlCl₃, Boran trifluoride, N-Bromosuccinimide, Diazomethane, Dicyclohexylcarbodiimide, Lead tetraacetate, Ziegler-Natta catalysts, DDQ, Dithianes, Merrifield resin.

UNIT-II: ORGANOMETALLIC REAGENTS

15 Hrs

Synthesis and applications of Grignard reagents, Organolithium, Zinc, Copper, Mercury, Palladium and Rhodium compounds in Organic Synthesis, Homogeneous catalytic hydrogenation and hydroformylation reactions

UNIT III: ASYMMETRIC SYNTHESIS

15 Hrs

Topocity - Prochirality- Substrate selectivity - Diastereoselectivity and enantioselectivity- Substrate controlled methods-use of chiral substrates - examples

Auxiliary controlled methods-Use of chiral auxiliaries-Chiral enolates-alkylation of chiral imines – Stereoselective Diels-Alder reaction

Reagent controlled methods-Use of chiral reagents-Asymmetric oxidation-Sharpless epoxidation-Asymmetric reduction-Use of lithium aluminium hydride and borate reagents.

UNIT IV: METHODS OF ORGANIC SYNTHESIS

15 Hrs

- i. **Oxidations:** (a) Alcohols to carbonyls-Chromium (iv) oxidants-Dimethyl sulfoxide oxidation, periodate oxidation, Oppenauer oxidation, oxidation with manganese dioxide, oxidation with silver carbonate (b) Alkenes to epoxides-peroxide induced epoxidations. (c) Alkenes to diols-oxidation with potassium permanganate, osmium tetroxide, Prevost reaction (d) Ketones to esters-Bayer-Villiger oxidation (e) Oxidative bond cleavage-cleavage of alkenes by transition metals. (f) Oxidation of alkyl or alkenyl fragments-selenium dioxide and chromium trioxide oxidations.
- ii. **Reductions :** Reduction with lithium aluminium hydride, sodium borohydride, alkoxides, bis-methoxy ethoxy aluminium hydride, Boran aluminium hydride and derivatives-catalytic hydrogenation-dissolving metal reductions, Non-Metallic reducing agents including enzymatic and microbial reductions.

Books suggested:

1. Advanced Organic Chemistry-Reactions, Mechanism and Structure, Jerry March, John Wiley.
2. Advanced Organic Chemistry, F.A. Carey and R.J Sundberg, Plenum.
3. A Guide Book to Mechanism in Organic Chemistry, Peter Sykes, Longman.

4. Structure and Mechanism in Organic Chemistry, C.K.Inglod, Cornell University Press.
5. Organic Chemistry, R.T Morrison and R.N. Boyd, Prentice - Hall.
6. Name reactions and reagents in organic synthesis, B.P. Muway and M.G Ellord, John Wiley.
7. Modern Organic Reactions, H.O. House, Benjamin.
8. Principles of Organic Synthesis, R.O.C Norman and J.M Coxon, Blackie Academic & Professional.
9. Reaction Mechanism in Organic Chemistry, P.S. Kalsi, New Age International.
10. Principles of organometallic chemistry, P. Powell, ELBS.
11. Organo transition metal chemistry-Applications to organic synthesis, S.G. Davis, Pergmon.
12. Stereochemistry to Organic Compounds, E.L. Eliel and others, John Wiley.
13. Stereochemistry to Organic Compounds, D. Nasipuri, New Age International.
14. Stereochemistry, P.S.Kalsi, Wiley Eastern.

CHE 302: CORE THEORY: ORGANIC SPECTROSCOPY AND APPLICATIONS

UNIT-I: ULTRAVIOLET AND VISIBLE SPECTROSCOPY: 15Hrs

Various electronic transitions (185-800 nm), effect of solvent on electronic transitions, ultraviolet bands for carbonyl compounds, unsaturated carbonyl compounds, dienes, conjugated polyenes. Fisher-Woodward rules for conjugated dienes and carbonyl compounds, ultraviolet spectra of aromatic and heterocyclic compounds. Steric effect in biphenyls.

UNIT – II: INFRARED SPECTROSCOPY 15Hrs

Instrumentation and sample handling. Characteristic vibrational frequencies of alkanes, alkenes, alkynes, aromatic compounds, alcohols, ether, phenols and amines. Detailed study of vibrational frequencies of carbonyl compounds (ketones, aldehydes, esters, amides, acids, anhydrides, lactones, lactams and conjugated carbonyl compounds). Effect of hydrogen bonding and solvent effect on vibrational frequencies, overtones, combination bands and fermi resonance, FT-IR

UNIT –III: ¹H NMR spectroscopy: Magnetic properties of nuclei, Principles of NMR. Instrumentation, CW and pulsed FT instrumentation, equivalent and non equivalent protons, enantiotopic and diastereotopic protons, Chemical shifts, factors affecting the chemical shifts, electronegativity and anisotropy, shielding and deshielding effects, Signal integration, Spin-spin coupling: vicinal, germinal and long range, Coupling constants and factors affecting coupling constants.

Applications of ¹H NMR spectroscopy: Reaction mechanisms (cyclic bromonium ion, electrophilic and nucleophilic substitutions, carbocations and carbanions), E, Z isomers, conformation of cyclohexane and decalins, keto-enol tautomerism, hydrogen bonding, proton exchange processes (alcohols, amines and carboxylic acids), C-N rotation. Stereochemistry, hindered rotation, Karplus curve variation of coupling constant with dihedral angle. Simplification of complex spectra, nuclear magnetic double resonance, contact shift reagents, nuclear Overhauser effect (NOE).

¹³C NMR spectroscopy: General considerations, chemical shift (aliphatic, olefinic, alkyne, aromatic, heteroaromatic and carbonyl carbon), coupling constants. Two dimensional NMR spectroscopy-COSY.

UNIT-IV: MASS SPECTROMETRY**15Hrs**

Introduction, ion production, type of ionization, EI, CI, FD, and FAB-factors affecting fragmentation, ion analysis, ion abundance. Mass spectral fragmentation of organic compounds, common functional groups, molecular-ion peak, metastable peak, Mc. Lafferty rearrangement. Nitrogen rule, isotope labeling. High resolution mass spectrometry, Examples of mass spectral fragmentation of organic compounds with respect to their structure determination.

Books suggested:

1. Organic spectroscopy, W. Kemp 5th Ed, ELBS
2. Spectroscopy of organic compounds, RM Silversteen and others, 5th Ed, John Wiley
3. Spectroscopy of organic compounds, P.S. Kalsi, Wiley, 1993.
4. NMR in chemistry-A multi nuclear introduction, William Kemp, Mc Millan, 1986.
5. Spectroscopic methods in Organic chemistry, DH Williams & I Flemmi,

PRACTICALS**CHE-OC-303 Core-Practical Organic Estimations PRACTICAL –I**

- 1) Estimation of phenol
- 2) Estimation of glucose
- 3) Estimation of percentage purity of aspirin
- 4) Estimation of percentage purity of paracetamol.

CHE-OC-304 Core-Practical Multistep preparations PRACTICAL –II

- 1) Preparation of benzilic acid
- 2) Preparation of benzanilide
- 3) Preparation of o-chlorobenzoic acid
- 4) Preparation of symmetric tribromobenzene

CHE –OC-305(A)- GENERIC ELECTIVE INORGANIC SPECTROSCOPY & THERMAL METHODS OF ANALYSIS**UNIT –I: THERMAL METHODS OF ANALYSIS 15 Hrs**

Thermo gravimetry –Principle, Factors affecting the results, instrumentation. Application with special reference to $\text{CuSO}_4 \cdot 5\text{H}_2\text{O}$, $\text{CaC}_2\text{O}_4 \cdot 2\text{H}_2\text{O}$. Different thermal analysis – principle, instrumentation, difference between TG and DTA, applications with special reference to the clays and minerals.

Different scanning calorimetry –principle, and applications to inorganic materials like chlorates and perchlorates, ammonium nitrate.

UNIT –II: MOSSBAUER SPECTROSCOPY and NQR 15 Hrs

Mossbauer spectroscopy: Basic principles, Recoil energy, Doppler shift, Chemical shift, Quadrupole effects, Magnetic effects. Instrumentation, spectral parameters and spectrum display.

Application of the technique to the studies of (1) bonding and structures of Fe^{2+} and Fe^{3+} compounds, (2) Sn^{2+} and Sn^{4+} compounds.

NQR spectroscopy: Basic principles of NQR spectroscopy, quadrupole nuclei, quadrupole moments, electric field gradient, coupling constant and applications.

UNIT –III: ELECTRON SPIN RESONANCE SPECTROSCOPY 15 Hrs

Basic Principles, Hyper fine splitting, Factors affecting the 'g' value. Isotropic and anisotropic hyperfine coupling constants, Hamiltonian and spin densities. Zero field splitting and Kramer's degeneracy, Relaxation process and line widths. Instrumentation and Applications. The EPR spectrum of bis(salicylidimine)-copper(II) complex, study of inorganic free radicals, biological applications of Electron Spin Resonance (Study of free radicals and Iron-sulfur proteins)

UNIT –IV: PHOTO ELECTRON SPECTROSCOPY 15 Hrs

Photoelectric effect, Koopmans's theorem, ionization energy.

X-ray photoelectron spectroscopy (ESCA): Principle, Binding energies, Chemical shift, Applications of XPS to Qualitative analysis, to surface studies and structural analysis.

Ultraviolet photoelectron spectroscopy- Principle, application of UPES in studying the molecular orbitals of O₂ and N₂ molecules.

Block diagram of photoelectron spectrophotometer. Sources of radiation, detectors.

Auger spectra – Principle, Applications of Auger spectra to surface studies and use of Auger spectra as a finger print tool.

Books Suggested

1. F.A.Cotton and G.Wilkinson, Advanced In-organic chemistry VI Edition,1999.John Wiley & sons. Inc., New York.
2. J.E. Huheey, E.A.Keiter and R.L.Keiter: Inorganic Chemsitry, Principles of Structure and Reactivity (4th Ed.) (Addison-Wesley)
3. Gary Wulfsberg: Inorganic Chemistry (5th Ed. (Viva Books)
4. J.D.Lee: Concise Inorganic Chemistry (Blackwell)
5. W.L.Jolly: Modern Inorganic Chemsitry (McGraw-Hill)
6. R.L.Carlin: Magneto-chemsitry (Springer-Verlag)
7. R.L.Dutta and A.Syamal: Elements of Magnetochemsitry (Affiliate East-West).
8. K. Hussain Reddy – Text book of Bioinorganic chemistry

CHE-305 (B): GENERIC ELECTIVE -PHYSICAL CHEMISTRY - III

UNIT-I Applications of Group Theory 15 Hrs

Construction of reducible and irreducible representations, Determination of Character Co ordinate of C_{2v} point group based on 3N Co ordinates. Standard reduction formula, Determination of normal modes of vibrations of SO₂, NH₃, POCl₃, PtCl₄²⁻ ·H₂O₂ molecules. Mutual exclusion Principle, Direct Product, Accidental Degeneracy and Fermi resonance Group Theory and Spectroscopy: IR Spectral activity of NH₃ molecule, selection rules, symmetry Criteria for optical activity, symmetry restrictions on dipole moments, symmetry and stereo isomerism. Prediction of IR and Raman Spectral activity of H₂O and CO₂.

UNIT-II: X-ray Diffraction: 15 Hrs

(A) Solid State Chemistry

Dislocation of Solids, Schottky and Frenkel defects, insulators, a, d semiconductors, Band theory of solids, solid state reactions.

(B) Bragg conditions-Miller Indices- Laue method, Bragg method, Debye Scherrer method of X-ray structural analysis of crystals. Index reflections, identification of unit cells from systematic absences in diffraction pattern- structure of simple lattices and X-ray intensities- structure factor and its relation to intensity and electron density- Description of procedure for X-ray structure analysis (NaCl and KCl)

(C) **Electron Diffraction:** Scattering intensity Vs scattering angle, Wierlequation, and its importance. Measurement techniques, Elucidation of structures of simple gas phase molecules, Low energy electron diffraction (LEED) for the study of surfaces.

UNIT-III: SPECTROSCOPY

15 Hrs

Microwave spectroscopy: classification of molecules, rigid rotator model, effect of isotopic substitution on the transition frequencies, intensities- stark effect.

Infrared spectroscopy: Linear harmonic oscillator, zero point energy, anharmonicity, Mores potential energy diagram, fundamental and overtone transitions, hot bands and combinations bands. Vibration-rotation spectroscopy, PQR branches, selection rules, factors affecting the band positions and intensities for IR region.

Raman spectroscopy: Classical and quantum theories of Raman effect, pure rotational, pure vibrational Raman spectroscopy, selection rules, mutual exclusion principle, resonance Raman spectroscopy and coherent antistokes Raman spectroscopy. Vibrational- rotational Raman spectroscopy.

UNIT-IV: POLYMER SOLUTIONS

15 Hrs

Thermodynamics of polymer dissolution, effect of molecular weight on solubility, solubility of crystalline and amorphous polymer, heat of dissolution, regular solution theory, Hildebrand solubility parameter, Flory-Huggins theory of polymer solutions, conformational entropy, osmotic pressure and viscosity of polymer solutions. Molecular weight determination by light scattering, ultra centrifugation and sedimentation equilibrium method. Liquid Crystals- synthesis and applications

Books Suggested

1. F.A.Cotton : Introduction to Group theory for chemists.
2. Geroage Davidson Elsevier : Introductory Group Theory for Chemists.
3. Gurdeep Raj , Ajay Bhagi&Vinod Jain : Group Theory and Symmetry in Chemistry
4. Instrumental methods of analysis – M.H.Willard, Meritt Jr. and J.A.Dean
5. Principles of instrumental analysis – Skoog and West
6. F. W. Billmeyer, Jr.: Text Book of Polymer Science. Wiley Interscience.
7. V. R. Gowariker, N. V. Viswanathan, JayadevSreedhar.: polymer Science. New Age international Publishers.

CHE-305 (C): GENERIC ELECTIVE - GREEN CHEMISTRY

UNIT-I

Fundamentals and significance of Green Chemistry: Discussion of the current state of chemistry and the environment and the definition of green chemistry. Assessment of the impact of chemistry in the environment and definition of risk hazard. An introduction to the tools of green chemistry and its fundamental principles.

Principles of Green Chemistry: Prevention of waste / by-products , Hazardous products- Designing of safer chemicals- Selection of appropriate solvents and starting materials- Use of protecting groups and catalysis- Designing of biodegradable products.

UNIT-II

Catalysis for Green Chemistry: Use of biocatalysts- Biochemical Oxidation, Biochemical Reduction, Enzyme Catalyzed Hydrolytic Process, Modified biocatalysis- transition metal catalysis- Reformatsky reaction, Wurtz reaction, Pinacol coupling, Simmons-Smith reaction, Mukaiyama reaction, Heck reaction, Ullmann's coupling.

UNIT-III

Solvent Free Reactions: Solvent free techniques- Reactions on solid mineral supports, Phase Transfer Catalysis- C-alkylation, N-alkylation, S-alkylation, Darzen's reaction, Wittig reaction. Ultrasound assisted green synthesis- Oxidation, Reduction, Hydroboration, Bouveault reaction, Strecker reaction, Microwave assisted green synthesis- Biginelli reaction, Aza-Michael reaction, Suzuki reaction, Stille reaction, Sonogashira reaction.

UNIT-IV

Ionic liquids: Definition- Types of Ionic Liquids-Synthesis of Ionic Liquids- Selection of ionic liquids- physical properties- Application in organic synthesis- alkylation, allylation, oxidation, reduction, polymerization, hydrogenation, hydroformylation, alkoxy-carbonylation, carbon-carbon bond forming reactions, alkene metathesis.

Books suggested:

1. New Trends in Green Chemistry by V.K. Ahluwalia, M. Kidwai.
2. Green Chemistry: Environment Friendly Alternatives by Rashmi Sanghi, M M Srivastava
3. Green Solvents for Organic Synthesis by V.K. Ahluwalia, Rajender S. Varma
4. Green Analytical Chemistry by Mihkel Koel and Mihkel Kaljurand

CHE 306(a): (Open Elective)- SPECTRAL TECHNIQUES

UNIT – I: ULTRAVIOLET AND VISIBLE SPECTROSCOPY **15 Hrs**

Various electronic transitions (185-800nm.), Beer-Lambert Law, effect of solvent on electronic transitions , ultraviolet bands for carbonyl compounds, unsaturated carbonyl compounds, dienes, Fieser-Woodward rules for conjugated dienes and carbonyl compounds

UNIT – II : INFRARED SPECTROSCOPY **15 Hrs**

Instrumentation and sample handling, characteristic vibrational frequencies of alkanes, alkenes, alkynes, aromatic compounds, alcohols, ethers, phenols, amines, ketones, aldehydes, esters, amides, acids and anhydrides. Effect of hydrogen bonding.

UNIT – III: ATOMIC ABSORPTION SPECTROSCOPY: FLAME AAS: **15 Hrs**

Principle, Instrumentation – Sources of radiation (HCL and EDL), Different types of burners, Interferences- Physical, Chemical, spectral and back ground correction, and methods of minimization

GF AAS: Principle and technique –Comparison between Flame AAS and furnace AAS, Applications of AAS, Comparison between Atomic Absorption & Flame Photometry.

UNIT –IV: MASS SPECTROMETRY **15 Hrs**

Principle, instrumentation, different methods of ionization, EI, CI, FD and FAB, Mass spectra-molecular ion, base peak, meta-stable peak, nitrogen rule and Mc Lafferty rearrangement. Mass spectral fragmentation of organic compounds and common functional groups. Normal and branched alkanes, alkenes, cycloalkanes, benzene and its derivatives, alcohols and phenols, ethers, aldehydes and ketones, carboxylic acids and their derivatives , amines and nitro compounds. Examples of mass spectral fragmentation of organic compounds with respect to their structure determination.

Books Suggested:

1. Organic spectroscopy, W.Kemp 5th Ed, ELBS .2.
2. Spectroscopy of organic compounds, RM Silversteen and others 5th Ed, John Wiley 1991
3. Spectroscopy of organic compounds, PS Kalsi, Wiley, 1993
4. NMR in chemistry – A Multi nuclear introduction, William Kemp, Mc Millan 1986
5. Spectroscopic methods in Organic Chemistry, DH Williams & I Flemmi TMH . 2005

CHE 306(B): (OPEN ELECTIVE)-CHROMATOGRAPHIC TECHNIQUES

Unit –I: Introduction - Classification of Chromatographic methods – Column chromatography-Adsorption phenomenon: Nature of adsorbents-Solvent systems-Differential migration-Separation of mixture of o-/p-nitro anilines (A demonstration experiment).

15 Hrs

Unit –II: Thin-Layer Chromatography (TLC)-Coating materials and preparation of TLC plates- Solvents for development-Detection of compounds in TLC- R_f values in TLC- Applications of TLC in chemistry-Preparative TLC – Demonstration experiment in TLC.

Unit –III: High-Performance Liquid Chromatography (HPLC) - Application of HPLC-HPLC instrument-Stationary phases in HPLC-Normal and reversed phase HPLC: A comparison- Normal phase HPLC: Principle-Retention times in Normal and reversed phase HPLC- Reversed phase HPLC: Principle.

Unit –IV: Gas-Liquid Chromatography- Instruments for Gas-Liquid Chromatography- Gas-Chromatographic Columns and the Stationary Phase- Application of Gas-Liquid Chromatography- Gas-Solid Chromatography.

Reference Books:

1. Analytical chemistry: G L David Krupadanam, D.Vijaya prasad, K.Varaprasad Rao, KLN Reddy, C.Sudhakar.
2. . Analytical chemistry: Skoog West Holler.
3. Modern Analytical Chemistry : David Harvey DePauw University.
4. J.G.Dick. Analytical Chemistry,McGraw Hill,New Delhi, (1973).

SEMESTER-III (PHYSICAL CHEMISTRY)**CHE-PC-301 CORE-THEORY PHYSICAL CHEMISTRY III****UNIT-I Applications of Group Theory****15 Hrs**

Construction of reducible and irreducible representations, Determination of Character Co ordinate of C_{2v} point group based on $3N$ Co ordinates. Standard reduction formula, Determination of normal modes of vibrations of SO_2 , NH_3 , $POCl_3$, $PtCl_4^{2-} \cdot H_2O_2$ molecules. Mutual exclusion Principle, Direct Product, Accidental Degeneracy and Fermi resonance Group Theory and Spectroscopy: IR Spectral activity of NH_3 molecule, selection rules, symmetry Criteria for optical activity, symmetry restrictions on dipole moments, symmetry and stereo isomerism. Prediction of IR and Raman Spectral activity of H_2O and CO_2 .

UNIT-II: X-ray Diffraction:**15 Hrs****(D) Solid State Chemistry**

Dislocation of Solids, Schottky and Frenkel defects, insulators, a, d semiconductors, Band theory of solids, solid state reactions.

(E) Bragg conditions-Miller Indices- Laue method, Bragg method, Debye Scherrer method of X-ray structural analysis of crystals. Index reflections, identification of unit cells from systematic absences in diffraction pattern- structure of simple lattices and X-ray intensities- structure factor and its relation to intensity and electron density- Description of procedure for X-ray structure analysis (NaCl and KCl)

(F) Electron Diffraction: Scattering intensity Vs scattering angle, Wierlequation, and its importance. Measurement techniques, Elucidation of structures of simple gas phase molecules, Low energy electron diffraction (LEED) for the study of surfaces.

UNIT-III: SPECTROSCOPY**15 Hrs**

Microwave spectroscopy: classification of molecules, rigid rotator model, effect of isotopic substitution on the transition frequencies, intensities- stark effect.

Infrared spectroscopy: Linear harmonic oscillator, zero point energy, anharmonicity, Mores potential energy diagram, fundamental and overtone transitions, hot bands and combinations bands. Vibration-rotation spectroscopy, PQR branches, selection rules, factors affecting the band positions and intensities for IR region.

Raman spectroscopy: Classical and quantum theories of Raman effect, pure rotational, pure vibrational Raman spectroscopy, selection rules, mutual exclusion principle, resonance Raman spectroscopy and coherent antistokes Raman spectroscopy. Vibrational- rotational Raman spectroscopy.

UNIT-IV: POLYMER SOLUTIONS**15 Hrs**

Thermodynamics of polymer dissolution, effect of molecular weight on solubility, solubility of crystalline and amorphous polymer, heat of dissolution, regular solution theory, Hildebrand solubility parameter, Flory-Huggins theory of polymer solutions, conformational entropy, osmotic pressure and viscosity of polymer solutions. Molecular weight determination by light scattering, ultra centrifugation and sedimentation equilibrium method. Liquid Crystals- synthesis and applications

Books Suggested

8. F.A.Cotton : Introduction to Group theory for chemists.
9. Geroge Davidson Elsevier : Introductory Group Theory for Chemists.
10. Gurdeep Raj , Ajay Bhagi&Vinod Jain : Group Theory and Symmetry in Chemistry
11. Instrumental methods of analysis – M.H.Willard, Meritt Jr. and J.A.Dean
12. Principles of instrumental analysis – Skoog and West
13. F. W. Billmeyer, Jr.: Text Book of Polymer Science. Wiley Interscience.
14. V. R. Gowariker, N. V. Viswanathan, JayadevSreedhar.: polymer Science. New Age international Publishers.

CHE 302: CORE THEORY: ORGANIC SPECTROSCOPY AND APPLICATIONS

UNIT-I: ULTRAVIOLET AND VISIBLE SPECTROSCOPY:

15Hrs

Various electronic transitions (185-800 nm), effect of solvent on electronic transitions, ultraviolet bands for carbonyl compounds, unsaturated carbonyl compounds, dienes, conjugated polyenes. Fisher-Woodward rules for conjugated dienes and carbonyl compounds, ultraviolet spectra of aromatic and heterocyclic compounds. Steric effect in biphenyls.

UNIT – II: INFRARED SPECTROSCOPY

15Hrs

Instrumentation and sample handling. Characteristic vibrational frequencies of alkanes, alkenes, alkynes, aromatic compounds, alcohols, ether, phenols and amines. Detailed study of vibrational frequencies of carbonyl compounds (ketones, aldehydes, esters, amides, acids, anhydrides, lactones, lactams and conjugated carbonyl compounds). Effect of hydrogen bonding and solvent effect on vibrational frequencies, overtones, combination bands and fermi resonance, FT-IR

UNIT –III: ¹H NMR spectroscopy: Magnetic properties of nuclei, Principles of NMR. Instrumentation, CW and pulsed FT instrumentation, equivalent and non equivalent protons, enantiotopic and diastereotopic protons, Chemical shifts, factors affecting the chemical shifts, electronegativity and anisotropy, shielding and deshielding effects, Signal integration, Spin-spin coupling: vicinal, germinal and long range, Coupling constants and factors affecting coupling constants.

Applications of ¹H NMR spectroscopy: Reaction mechanisms (cyclic bromonium ion, electrophilic and nucleophilic substitutions, carbocations and carbanions), E, Z isomers, conformation of cyclohexane and decalins, keto-enol tautomerism, hydrogen bonding, proton exchange processes (alcohols, amines and carboxylic acids), C-N rotation. Stereochemistry, hindered rotation, Karplus curve variation of coupling constant with dihedral angle. Simplification of complex spectra, nuclear magnetic double resonance, contact shift reagents, nuclear Overhauser effect (NOE).

¹³C NMR spectroscopy: General considerations, chemical shift (aliphatic, olefinic, alkyne, aromatic, heteroaromatic and carbonyl carbon), coupling constants. Two dimensional NMR spectroscopy-COSY.

UNIT-IV: MASS SPECTROMETRY

15Hrs

Introduction, ion production, type of ionization, EI, CI, FD, and FAB-factors affecting fragmentation, ion analysis, ion abundance. Mass spectral fragmentation of organic compounds, common functional groups, molecular-ion peak, metastable peak, Mc. Lafferty rearrangement. Nitrogen rule, isotope labeling. High resolution mass spectrometry, Examples of mass spectral fragmentation of organic compounds with respect to their structure determination.

Books suggested:

1Organic spectroscopy, W. Kemp 5th Ed, ELBS

2Spectroscopy of organic compounds, RM Silversteen and others, 5th Ed, John Wiley

3Spectroscopy of organic compounds, P.S. Kalsi, Wiley, 1993.

4NMR in chemistry-A multi nuclear introduction, William Kemp, Mc Millan, 1986.

5Spectroscopic methods in Organic chemistry, DH Williams & I Flemmi,

PHYSICAL CHEMISTRY PRACTICALS

CHE-PC-303: Core-Practical PRACTICAL-I

1. Chemical Kinetics:

- a) Study of the kinetics of halogenations of acetone.
- b) Determination of activation energy of reaction between iodide and Persulphate
- c) Determination rate constant of oxidation of iodide ion by persulphate ion and study the effect of neutral salt (KCl) on this reaction.

2. Flame Photometry:

- a) Determination of Na
- b) Determination of K
- c) Determination of Cu

CHE- PC-304: Core-Practical PRACTICAL-II

3. Conductometry:

- a) Titration of mixture of halides
- b) Titration of mixture of HCl+HOAC
- c) Saponification of an ester

4. Colorimetry:

- a) Estimation of Manganese
- b) Estimation of Iron
- c) Estimation of Phosphate
- d) Titration of copper Vs EDTA

CHE-305 GENERIC ELECTIVE (A) ORGANIC CHEMISTRY III

UNIT I: REAGENTS IN ORGANIC SYNTHESIS

15 Hrs

Use of the following reagents in organic synthesis: Anhydrous AlCl₃, Boran trifluoride, N-Bromosuccinimide, Diazomethane, Dicyclohexylcarbodiimide, Lead tetraacetate, Ziegler-Natta catalysts, DDQ, Dithianes, Merrifield resin.

UNIT-II: ORGANOMETALLIC REAGENTS

15 Hrs

Synthesis and applications of Grignard reagents, Organolithium, Zinc, Copper, Mercury, Palladium and Rhodium compounds in Organic Synthesis, Homogeneous catalytic hydrogenation and hydroformylation reactions

UNIT III: ASYMMETRIC SYNTHESIS

15 Hrs

Topocity - Prochirality- Substrate selectivity - Diastereoselectivity and enantioselectivity-Substrate controlled methods-use of chiral substrates - examples

Auxiliary controlled methods-Use of chiral auxiliaries-Chiral enolates-alkylation of chiral imines – Stereoselective Diels-Alder reaction

Reagent controlled methods-Use of chiral reagents-Asymmetric oxidation-Sharpless epoxidation-Asymmetric reduction-Use of lithium aluminium hydride and borate reagents.

UNIT IV: METHODS OF ORGANIC SYNTHESIS

15 Hrs

- i. **Oxidations:** (a) Alcohols to carbonyls-Chromium (iv) oxidants-Dimethyl sulfoxide oxidation, periodate oxidation, Oppenauer oxidation, oxidation with manganese dioxide, oxidation with silver carbonate (b) Alkenes to epoxides-peroxide induced epoxidations. (c) Alkenes to diols-oxidation with potassium permanaganate, osmium tetroxide, Prevost reaction (d) Ketones to esters-Bayer-Villiger oxidation (e) Oxidative bond cleavage-cleavage of alkenes by transition metals. (f) Oxidation of alkyl or alkenyl fragments-selenium dioxide and chromium trioxide oxidations.
- ii. **Reductions :** Reduction with lithium aluminium hydride, sodium borohydride, alkoxides, bis- methoxy ethoxy aluminium hydride, Boran aluminium hydride and derivatives-catalytic hydrogenation-dissolving metal reductions, Non-Metallic reducing agents including enzymatic and microbial reductions.

Books suggested:

1. Advanced Organic Chemistry-Reactions, Mechanism and Structure, Jerry March, John Wiley.
2. Advanced Organic Chemistry, F.A. Carey and R.J Sundberg, Plenum.
3. A Guide Book to Mechanism in Organic Chemistry, Peter Sykes, Longman.
4. Structure and Mechanism in Organic Chemistry, C.K.Inglod, Cornell University Press.
5. Organic Chemistry, R.T Morrison and R.N. Boyd, Prentice - Hall.
6. Name reactions and reagents in organic synthesis, B.P. Muway and M.G Ellord, John Wiley.
7. Modern Organic Reactions, H.O. House, Benjamin.
8. Principles of Organic Synthesis, R.O.C Norman and J.M Coxon, Blackie Academic & Professional.
9. Reaction Mechanism in Organic Chemistry, P.S. Kalsi, New Age International.
10. Principles of organometallic chemistry, P. Powell, ELBS.
11. Organo transition metal chemistry-Applications to organic synthesis, S.G. Davis, Pergmon.
12. Stereochemistry to Organic Compounds, E.L. Eliel and others, John Wiley.
13. Stereochemistry to Organic Compounds, D. Nasipuri, New Age International.
14. Stereochemistry, P.S.Kalsi, Wiley Eastern.

CHE-305 GENERIC ELECTIVE (B) GENERIC ELECTIVE INORGANIC SPECTROSCOPY & THERMAL METHODS OF ANALYSIS

UNIT –I: THERMAL METHODS OF ANALYSIS 15 Hrs

Thermo gravimetry –Principle, Factors affecting the results, instrumentation. Application with special reference to $\text{CuSO}_4 \cdot 5\text{H}_2\text{O}$, $\text{CaC}_2\text{O}_4 \cdot 2\text{H}_2\text{O}$. Different thermal analysis – principle, instrumentation, difference between TG and DTA, applications with special reference to the clays and minerals.

Different scanning calorimetry –principle, and applications to inorganic materials like chlorates and perchlorates, ammonium nitrate.

UNIT –II: MOSSBAUER SPECTROSCOPY and NQR **15 Hrs**

Mossbauer spectroscopy: Basic principles, Recoil energy, Doppler shift, Chemical shift, Quadrupole effects, Magnetic effects. Instrumentation, spectral parameters and spectrum display.

Application of the technique to the studies of (1) bonding and structures of Fe^{2+} and Fe^{3+} compounds, (2) Sn^{2+} and Sn^{4+} compounds.

NQR spectroscopy: Basic principles of NQR spectroscopy, quadrupole nuclei, quadrupole moments, electric field gradient, coupling constant and applications.

UNIT –III: ELECTRON SPIN RESONANCE SPECTROSCOPY **15 Hrs**

Basic Principles, Hyper fine splitting, Factors affecting the 'g' value. Isotropic and anisotropic hyperfine coupling constants, Hamiltonian and spin densities. Zero field splitting and Kramer's degeneracy, Relaxation process and line widths. Instrumentation and Applications. The EPR spectrum of bis(salicylidimine)-copper(II) complex, study of inorganic free radicals, biological applications of Electron Spin Resonance (Study of free radicals and Iron-sulfur proteins)

UNIT –IV: PHOTO ELECTRON SPECTROSCOPY **15 Hrs**

Photoelectric effect, Koopmans's theorem, ionization energy.

X-ray photoelectron spectroscopy (ESCA): Principle, Binding energies, Chemical shift, Applications of XPS to Qualitative analysis, to surface studies and structural analysis.

Ultraviolet photoelectron spectroscopy- Principle, application of UPES in studying the molecular orbitals of O_2 and N_2 molecules.

Block diagram of photoelectron spectrophotometer. Sources of radiation, detectors.

Auger spectra – Principle, Applications of Auger spectra to surface studies and use of Auger spectra as a finger print tool.

Books Suggested:

1. F.A.Cotton and G.Wilkinson, Advanced In-organic chemistry VI Edition, 1999. John Wiley & sons. Inc., New York.
2. J.E. Huheey, E.A. Keiter and R.L. Keiter: Inorganic Chemistry, Principles of Structure and Reactivity (4th Ed.) (Addison-Wesley)
3. Gary Wulfsberg: Inorganic Chemistry (5th Ed. (Viva Books)
4. J.D. Lee: Concise Inorganic Chemistry (Blackwell)
5. W.L. Jolly: Modern Inorganic Chemistry (McGraw-Hill)
6. R.L. Carlin: Magneto-chemistry (Springer-Verlag)
7. R.L. Dutta and A. Syamal: Elements of Magnetochemistry (Affiliate East-West).
8. K. Hussain Reddy – Text book of Bioinorganic chemistry

CHE-305 GENERIC ELECTIVE (C) GREEN CHEMISTRY**UNIT-I**

Fundamentals and significance of Green Chemistry: Discussion of the current state of chemistry and the environment and the definition of green chemistry. Assessment of the impact of chemistry in the environment and definition of risk hazard. An introduction to the tools of green chemistry and its fundamental principles.

Principles of Green Chemistry: Prevention of waste / by-products, Hazardous products- Designing of safer chemicals- Selection of appropriate solvents and starting materials- Use of protecting groups and catalysis- Designing of biodegradable products.

UNIT-II

Catalysis for Green Chemistry: Use of biocatalysts- Biochemical Oxidation, Biochemical Reduction, Enzyme Catalyzed Hydrolytic Process, Modified biocatalysis- transition metal catalysis- Reformatsky reaction, Wurtz reaction, Pinacol coupling, Simmons-Smith reaction, Mukaiyama reaction, Heck reaction, Ullmann's coupling.

UNIT-III

Solvent Free Reactions: Solvent free techniques- Reactions on solid mineral supports, Phase Transfer Catalysis- C-alkylation, N-alkylation, S-alkylation, Darzen's reaction, Wittig reaction. Ultrasound assisted green synthesis- Oxidation, Reduction, Hydroboration, Bouveault reaction, Strecker reaction, Microwave assisted green synthesis- Biginelli reaction, Aza-Michael reaction, Suzuki reaction, Stille reaction, Sonogashira reaction.

UNIT-IV

Ionic liquids: Definition- Types of Ionic Liquids-Synthesis of Ionic Liquids- Selection of ionic liquids- physical properties- Application in organic synthesis- alkylation, allylation, oxidation, reduction, polymerization, hydrogenation, hydroformylation, alkoxy-carbonylation, carbon-carbon bond forming reactions, alkene metathesis.

Books suggested:

1. New Trends in Green Chemistry by V.K. Ahluwalia, M. Kidwai.
2. Green Chemistry: Environment Friendly Alternatives by Rashmi Sanghi, M M Srivastava
3. Green Solvents for Organic Synthesis by V.K. Ahluwalia, Rajender S. Varma
4. Green Analytical Chemistry by Mihkel Koel and Mihkel Kaljurand

CHE 306(A): (OPEN ELECTIVE) SPECTRAL TECHNIQUES

UNIT – I: ULTRAVIOLET AND VISIBLE SPECTROSCOPY 15 Hrs

Various electronic transitions (185-800nm.), Beer-Lambert Law, effect of solvent on electronic transitions, ultraviolet bands for carbonyl compounds, unsaturated carbonyl compounds, dienes, Fieser-Woodward rules for conjugated dienes and carbonyl compounds

UNIT – II : INFRARED SPECTROSCOPY 15 Hrs

Instrumentation and sample handling, characteristic vibrational frequencies of alkanes, alkenes, alkynes, aromatic compounds, alcohols, ethers, phenols, amines, ketones, aldehydes, esters, amides, acids and anhydrides. Effect of hydrogen bonding.

UNIT – III: ATOMIC ABSORPTION SPECTROSCOPY: FLAME AAS: 15 Hrs

Principle, Instrumentation – Sources of radiation (HCL and EDL), Different types of burners, Interferences- Physical, Chemical, spectral and back ground correction, and methods of minimization

GF AAS: Principle and technique –Comparison between Flame AAS and furnace AAS, Applications of AAS, Comparison between Atomic Absorption & Flame Photometry.

UNIT –IV: MASS SPECTROMETRY 15 Hrs

Principle, instrumentation, different methods of ionization, EI, CI, FD and FAB, Mass spectra-molecular ion, base peak, meta-stable peak, nitrogen rule and Mc Lafferty rearrangement. Mass spectral fragmentation of organic compounds and common functional groups. Normal and branched alkanes, alkenes, cycloalkanes, benzene and its derivatives, alcohols and phenols, ethers, aldehydes and ketones, carboxylic acids and their derivatives, amines and nitro compounds. Examples of mass spectral fragmentation of organic compounds with respect to their structure determination.

Books Suggested:

1. Organic spectroscopy, W.Kemp 5th Ed, ELBS .2.
2. Spectroscopy of organic compounds, RM Silversteen and others 5th Ed, John Wiley 1991
3. Spectroscopy of organic compounds, PS Kalsi, Wiley, 1993
4. NMR in chemistry – A Multi nuclear introduction, William Kemp, Mc Millan 1986
5. Spectroscopic methods in Organic Chemistry, DH Williams & I Flemmi TMH . 2005

CHE 306(B): (OPEN ELECTIVE)CHROMATOGRAPHIC TECHNIQUES

Unit –I: Introduction - Classification of Chromatographic methods – Column chromatography-Adsorption phenomenon: Nature of adsorbents-Solvent systems-Differential migration-Separation of mixture of o-/p-nitro anilines (A demonstration experiment).

Unit –II: Thin-Layer Chromatography (TLC)-Coating materials and preparation of TLC plates- Solvents for development-Detection of compounds in TLC- R_f values in TLC- Applications of TLC in chemistry-Preparative TLC – Demonstration experiment in TLC.

Unit –III: High-Performance Liquid Chromatography (HPLC) - Application of HPLC- HPLC instrument-Stationary phases in HPLC-Normal and reversed phase HPLC: A comparison- Normal phase HPLC: Principle-Retention times in Normal and reversed phase HPLC- Reversed phase HPLC: Principle.

Unit –IV: Gas-Liquid Chromatography- Instruments for Gas-Liquid Chromatography- Gas-Chromatographic Columns and the Stationary Phase- Application of Gas-Liquid Chromatography- Gas-Solid Chromatography.

Reference Books:

1. Analytical chemistry: G L David Krupadanam, D.Vijaya prasad, K.Varaprasad Rao, KLN Reddy, C.Sudhakar.
2. Analytical chemistry: Skoog West Holler.
3. Modern Analytical Chemistry : David Harvey DePauw University.
4. J.G.Dick. Analytical Chemistry,McGraw Hill,New Delhi, (1973).

M. Sc., ORGANIC CHEMISTRY**FOURTH SEMESTER**

(CBCS syllabus for the students admitted from 2016-2017)

CHE OC-401: CORE THEORY: ORGANIC SYNTHESIS-I**UNIT-I: Chemistry of Organo Boron, Phosphorus, Sulfur and Silicon reagents 15Hrs**

Electronic structure and bonding in Boron, Phosphorus, Sulphur and Silicon compounds- Their reactivity and applications in Organic Synthesis.

Boron Reagents-Hydroboration-Organoboranes in the formation of C-C bonds, alcohols, amines, halogen and carbonyl compounds-Free radical reactions of organoboranes.

Phosphorus Reagents- Formation of carbon-carbon double bonds-Functional group transformations – deoxygenation reactions-reactivity as electrophiles- conversion of alcohols to alkyl halides, Wittig reaction and nucleophiles - Corey-Winters reaction, Michaelis-Arbusov reaction-Perkow reaction and Mitsunobu reaction.

Sulphur Reagents- Sulphur ylides, stabilized and non-stabilized – Preparation and reactivity Pummerer reaction – sulphonyl carbanions-Julia reaction

Silicon reagents-Peterson's olefination, influence of trialkyl silyl reagents in electrophilic reactions, aryl silanes, alkenyl silanes, alkynyl silanes, allyl silanes.

UNIT-II: PHOTOCHEMISTRY**15Hr**

Photochemical energy, photochemical excitations, Franck-Condon principle, electronic transitions, Jablonski diagram, singlet and triplet states, energy transfer in photochemical reactions - photosensitization reactions and quantum yield.

Photochemistry of carbonyl compounds - Norrish Type-I and Norrish Type-II reactions, Photo Reduction and Paterno-Buchi reaction. Photochemistry of α,β -unsaturated ketones, enones, dienones and p-benzoquinones.

Photochemistry of unsaturated systems (olefins), cis-trans isomerization and dimerization reactions, Photochemistry of conjugated dienes - 1,3-butadiene, aromatic compounds, Photoaddition (1,2- & 1,4- additions) and Photosubstitution reactions of benzene derivatives. Photo-Fries rearrangement and Barton reaction.

UNIT III: PERICYCLIC REACTIONS**15 Hrs**

Molecular orbital symmetry, Frontier orbitals of ethylene, 1,3 butadiene, 1,3,5-hexatriene and allyl and pentadienyl system. Classification of pericyclic reactions. Woodward-Hoffmann correlation diagrams. FMO and PMO (Möbius Hückel) approach. Electrocyclic reactions-Conrotatory and disrotatory. $4n$, $4n+2$ and allyl systems. Cycloadditions-antarafacial and suprafacial additions, $4n$ and $4n+2$ systems, $2+2$ addition of ketene, $1,3$ dipolar cycloadditions and cheletropic reactions.

Sigmatropic rearrangements - Suprafacial and antarafacial shifts of H, Sigmatropic shifts involving carbon moieties, $3,3$ and $5,5$ Sigmatropic rearrangements. Claisen, Cope and Oxy-Cope rearrangements. Ene reaction

UNIT IV: SYNTHETIC POLYMERS**15 Hrs**

Polymer Reactions-Addition and condensation polymerization processes- Bulk, Solution, Suspension and Emulsion polymerization.

Stereospecific Polymers-Preparation and significance- classification of polymers based on physical properties-Thermoplastics-Thermosetting plastics-Fibers and elastomers- General applications.

Preparation of Polymers-Preparation of Polymers based on different types of monomers Industrial applications-olefin polymers-Diene polymers-nylons-Glyptal resins-Urea-formaldehyde, phenol-formaldehyde and melamine resins- Epoxy resins - Ion exchange resins.

CHE OC-402: CORE THEORY: ORGANIC SYNTHESIS-II**UNIT-I: DESIGNING OF ORGANIC SYNTHESIS****15 Hrs**

Disconnection Approach-Classification of organic reactions. Functionalisation and interconversion of functional groups, formation of carbon-carbon single and double bonds, general strategy, disconnection and synthon approach, retrosynthetic analysis, key intermediates and starting materials in designing a synthesis, linear and convergent synthesis, reconnections. The importance of the order of events in organic synthesis, one group C-X and two group C-X disconnections, chemoselectivity, reversal of polarity, cyclisation reactions, amine synthesis.

Protecting Groups-Principles of protection of alcohol, amine, carbonyl and carboxyl groups.

One Group C-C Disconnections-Alcohols and carbonyl compounds, regioselectivity. Alkene synthesis, use of acetylenic compounds in organic synthesis.

Two Group C-C Disconnections-Diels-Alder reaction, 1,3-difunctionalised compounds, unsaturated carbonyl compounds, control in carbonyl condensations, 1,5-difunctionalised compounds, Michael addition and Robinson annulation.

UNIT II: MULTI STEP SYNTHESIS

15 hrs

Multi step synthesis of some complex naturally occurring compounds involving through retrosynthetic analysis and control of stereochemistry, Longifolene, Taxol, Juvabione, Fediracamyne A.

UNIT III: ANTIMALARIALS AND ANTIBIOTICS

15 hrs

Antimalarials: Synthesis and activity of Quinoline group – Quinine, Plasmoquine and Chloroquine – Acridine group – Quinacrine – Guanidine group – Paludrine.

Antibiotics: Synthesis and activity of Penicillin, Chloramphenicol and Streptomycin – Broad spectrum antibiotics – Tetracyclines, Novobiocin.

Chemotherapy: Structure – activity relationships.

UNIT-IV: BIOMOLECULES

15 Hrs

Peptides and Proteins-Methods of peptide synthesis, sequence determination, structure of oxytocin, proteins-classification, structure, conformation and properties. Nucleic acids-Nucleosides, Nucleotides, DNA and RNA, structure and conformations, replication, translation of genetic material, genetic code, gene expression, gene mutation, protein synthesis.

Book References:

1. Modern Synthetic Reactions, H.O. House, W.A Benjamin.
2. Some Modern Methods of Organic Synthesis, W. Carruthers, Cambridge University Press.
3. Advanced Organic Chemistry, F.A. Carey and R.J Sundberg, Plenum.
4. Advanced Organic Chemistry, Reactions Mechanisms and Structure J. March, John Wiley.
5. Principles of Organic Synthesis, R.O.C. Norman and J.M Coxon, Blackie
6. Academic and Professional.
7. Advanced Organic Chemistry Part A & B, F.A Carey and R. J Sunderg, Plenum Press.
8. Structure and Mechanism in Organic Chemistry C.K.Inglod, Cornell University Press.
9. Reaction Mechanism in Organic Chemistry, P.S. Kalsi, New Age International.
10. Modern Synthetic Reactions, H.O. House, W.A. Benjamin.
11. Chemistry of Organic Natural Products, O.P. Agrawal, Vols., 1 & 2, Goel Pubs.
12. Natural Products Chemistry K.B.G. Torssell, John Wiley, 1983.
13. Principles of biochemistry, A.L.Lehninger worth publishers
14. A Text book of Biochemistry, A.V.S.S. Rama Rao
15. Biochemistry, L. Stryer, Fremann pubs.
16. Biochemistry, Voet and Voet, John Wiley

ORGANIC CHEMISTRY PRACTICALS

CHE 0C 403: PRACTICAL-I

Spectral identification of organic compounds by UV, IR, NMR (^1H & ^{13}C) & Mass spectroscopy.

DEMONSTRATION EXPERIMENTS

- 1 IR – Interpretation of IR spectrum of alcohols, ketones, aldehydes and other standard materials
- 2 AAS: Demonstration of AAS – Determination of Zn, Cd, Pb, Mn, Fe and Ni in effluents using AAS.
- 3 Spectrofluorimetry – estimation of quinine and fluorescein
- 4 Ion selective electrodes – estimation of F^- , S^{2-} and CN^- in effluents using ion selective electrode meter.
- 5 Polarography and Anode stripping voltametry
 - (a) Polarography and Anode stripping voltametry – behavior of Cd, Zn, Pb in a mixture.
 - (b) Determination of Pb and Cd in samples using Anode stripping voltametry
- 6 Gas chromatography- Determination of pesticides
- 7 HPLC- Determination of pesticides
- 8 NMR
 - a) Demonstration of NMR spectrometer and study of hydrogen bonding in a given alcohol or phenol.
 - b) Interpretation of NMR chemical shifts of ethyl benzene, ethyl alcohol
- 9 TGA, DTA, DSC – Demonstration of TG, DTA and DSC and study of decomposition of calcium oxalate, calcium carbonate, copper sulfate, oxalic acid.
- 10 pH metry
 - a) Determination of alkalinity in a colored effluent using pH metric end point.
 - b) Determination of purity of commercial HCl, H_2SO_4 , H_3PO_4 and CH_3COOH using pH metric end point

CHE 0C 404:PRACTIAL II/ PROJECT WORK

CHE OC-405(a) : (GENERIC ELECTIVE): HETEROCYCLES AND NATURAL PRODUCTS

UNIT-I: NOMENCLATURE AND FIVE MEMBERED HETEROCYCLES 15 HRS

Systematic nomenclature (Hantzsch-Widman nomenclature) for fused and bridged heterocycles, Five membered heterocycles with two heteroatoms: Synthesis and reactions of pyrazole, imidazole, isoxazole, oxazole, isothiazole and thiazole

UNIT-II: BENZOFUSED FIVE MEMBERED AND SIX MEMBERED HETEROCYCLES 15 HRS

Benzofused five membered heterocycles: Synthesis and reactions of Benzopyrazoles, Benzimidazoles and Benzoxazoles

Six Membered heterocycles with two or more heteroatoms: Synthesis and reactions of diazines (pyridazine, pyrimidine & pyrazine) and triazines (1,2,3-, 1,2,4- 1,3,5- triazines)

UNIT-III: STEROIDS AND HORMONES 15 HRS

Occurrence, nomenclature, basic skeleton, Diel's hydrocarbon and stereochemistry. Isolation, structure determination and synthesis of Cholesterol (total synthesis not expected), Bile acids, Androsterone, Testosterone, Estrone, Progesterone. Biosynthesis of steroids.

UNIT-IV: FLAVONOIDS AND ISOFLAVONOIDS 15 Hrs

Occurrence, nomenclature and general methods of structure determination. Isolation and synthesis of Apigenin, Luteolin, Kaempferol, Quercetin, Butein, Daidzein, Biosynthesis of

flavonoids and isoflavonoids: Acetate Pathway and Shikimic acid Pathway. Biological importance of flavonoids and isoflavonoids.

1. Heterocyclic chemistry Vol. 1-3, R.R. Gupta, M.Kumar and V. Gupta, Springer Verlag.
2. The Chemistry of Heterocycles, T. Eicher and S. Hauptmann, Thieme.
3. Heterocyclic Chemistry, J.A. Joule, K. Mills and G.F. Smith, Chapman and Hall.
4. Heterocyclic Chemistry, T.L. Gilchrist, Longman Scientific Technical.
5. Contemporary Heterocyclic Chemistry, G.R. Newkome and W.W. Paudler, Wiley-Inter Science.
6. An Introduction to the Heterocyclic Compounds, R.M. Acheson, John Wiley.
7. Comprehensive Heterocyclic Chemistry, A.R. Katritzky and C.W. Rees, eds. Pergamon Press.
8. Organic Chemistry, Vol. 2, I. L. Finar, ELBS.
9. Introduction to Flavonoids TA Geissman

CHE 405 (b): (GENERIC ELECTIVE): BIOINORGANIC, BIOORGANIC, BIOPHYSICAL

UNIT-I: BIO-INORGANIC CHEMISTRY- I

15 Hrs

Metal complexes as oxygen carriers –Heme proteins –Hemoglobin and myoglobin –Non heme proteins –hemerythrin and hemocyanin – model synthetic complexes of iron, cobalt and copper. Co-enzymes Vitamin B₁₂, carboxy peptidase and superoxidedismutase.

Electron Transfer in Biology: Structure and functions of metalloproteins in electron transfer processes –catalase –peroxidase –cytochromes and iron –sulphur proteins –synthetic models.

UNIT – II: BIOINORGANIC CHEMISTRY- II: Metal ion transport and storage in biological systems, Metal ions in Biology, Molecular mechanism of ion transport across membranes: ionophores, photosynthesis.

Hydrolytic metalloenzymes: Carbonic anhydrase, carboxy peptidase, calcium in control processes, calcium and muscle contraction, calcium and secretion, calcium in blood clotting mechanisms. Therapeutic uses of enzymes.

Importance of trace metals in biology: Metal ions as chelating agents in medicine, trace metal ions and metal and non-metal deficiency. Biological nitrogen fixation, in-vivo and in-vitro nitrogen fixation.

UNIT-III: BIOORGANIC CHEMISTRY

Carbohydrates: Structure and biological functions of mucopolysaccharides, glycoproteins, and glycolipids- Role of sugars in biological recognition- Blood group substances

Lipids: Essential fatty acids-structure and function of triglycerols, Glycerophospholipids, cholesterol, bile acids prostaglandins- composition and functioning of lipoproteins

Enzymes: Nomenclature and classification, properties, factors affecting enzyme catalysis, enzyme inhibition- reversible and irreversible inhibition. Uses of enzymes in food drink industry and clinical laboratories.

UNIT-IV: BIOPHYSICAL CHEMISTRY:

Standard free energy change in biochemical reactions, exergonic and endergonic reactions, hydrolysis of ATP, thermodynamics of biopolymer solutions, chain configuration of bio polymers, calculation of average dimensions. Membrane equilibrium, ion transport through cell membrane. dialysis and its function. Structure and functions of proteins, enzymes, DNA and RNA in living systems, forces involved in bio polymer interactions, electrostatic forces, hydrophobic forces, molecular expansion, and dispersion forces.

Books Suggested

- 1.M.N. Hughes, The Inorganic chemistry of Biological Processes, John wiley and Sons, New York 2nd Edition, 1981.
- 2.A Text book of Biochemistry , A.V.S.S.Rama Rao
- 3.Physical chemistry by Atkenes
- 4.Physical chemistry by Albertz.
- 5.Bio physical chemistry by Van Holde
- 6.Bio Physics by Narayanam
- 7.Organic Chemistry, Vol. 2, I. L. Finar, ELBS.
- 8.Chemistry of Natural Products, P.S.Kalsi, Kalyani Publishers.
- 9.Chemistry of Organic Natural Products, O. P. Agarwal, Vols., 1 & 2, Geol Pubs.
- 10.Natural products Chemistry K.B.G. Torrsell, John Wiley, 1983.
- 11.Burger's Medicinal Chemistry, M.E. Wolff, John Wiley
- 12.Medicinal Chemistry, A. Kar, New Age International

CHE 405 (c): (GENERIC ELECTIVE): NANOMATERIALS AND FUNCTIONAL MATERIALS

UNIT-I:Fundamental Principles. Definitions and Classification of functional nanomaterials. Historical development. Size & Scale, Units, Scaling Laws, Atoms, Molecules, & Clusters, Supramolecules. Nanoscale Phenomena, Tunneling, Chemical Bonds (types and strength), Intermolecular Forces, Molecular and Crystalline Structures, Hierarchical Structures and Functionality, Surfaces and Interfaces, Bulk to Surface transition, Self-Assembly and surface reconstruction.

UNIT-II: Properties and characterization of NanoMaterials. Size dependence of properties, Phenomena and Properties at Nanoscale, Brief introduction to calculational approaches, Mechanical / Frictional, Optical, Electrical Transport, Magnetic properties. Electron Microscopy, Scanning Probe Microscopies, Near field microscopy, Micro- and near field Raman spectroscopy, Surface-enhanced Raman spectroscopy, X-ray photoelectron spectroscopy

UNIT-III: Synthesis of Nanomaterials. Fabrication techniques: Self-Assembly, Self-Replication, Sol-Gels, Langmuir-Blodgett thin films, Nanolithography, Bio-inspired syntheses, Microfluidic processes, Chemical Vapor Deposition, Metals Colloidal gold, Silver and other metals clusters, Semiconductors, Cadmium Sulfide, silicon, Fullerenes / Carbon nanotubes, Nano-composites, Nanoporous Materials, Biological Materials. Applications of Nanomaterials. Nanoelectronics, Nanosensors, Environmental Biological, Energy storage and fuel cells

UNIT-IV: Overview of inorganic functional materials, their properties and applications. Introduction to solid state chemistry. Crystal structure and amorphous materials. Defects and non-stoichiometric solid solutions. Band theory and electronic conductivity. Synthesis and processing of inorganic materials. Properties of inorganic materials: superconductivity, magnetic, dielectric and optical properties

Books Suggested:

1. Nanomaterials- Synthesis, Properties and Applications, Edited by A.S. Edelstein and R.C. Cammarata, Institute of Physics Publishing, London, 1998.
2. Handbook of Nanostructured Materials and Nanotechnology, Edited by H.S.

- Nalwa Vols. 1-5, Academic Press (2000).
3. Science of Fullerenes and Nanotubes, by M.S. Dresselhaus, G. Dresselhaus and P.Eklund, Academic Press (1996).
 4. Nanostructured Carbon for Advanced Applications, Edited by G. Benedek et al, Kluwer Academic Publishers (2001).

CHE 406 (a): OPEN ELECTIVE: DRUG CHEMISTRY

UNIT – I: NATURAL PRODUCTS AS LEADS FOR NEW DRUGS

Occurrence, Structure and therapeutic uses of Drugs acting on Central Nervous System
 Morphine alkaloids (morphine, codeine, thebaine, heroin, pethidine)
 Cannabinoids (9-cannabinol, Tetrahydrocannabinol)
 Neuromuscular Blocking Agents (Curare, Decamethonium)
 Vinca Alkaloids (Vincristin and Vinblastin), Taxol and Taxotere, podophyllotoxin,
 Etoposide, Teniposide.

UNIT – II: CARDIOVASCULAR DRUGS

Definition, Classification, Nomenclature, Structure and Synthesis.
 Cardiac glycosides (ex: Digoxin, Digitoxin);
 Antihypertensive drugs (ex: Methyl dopa, Clonidine hydrochloride);
 Antiarrhythmic agents (ex: Quinidine sulfate);
 Antisymphetic drugs (ex: Propranolol hydrochloride, Verapamil hydrochloride);
 Vasopressor drugs (ex: Prenylamine, Buphenine).

UNIT – III: AUTACOIDS

Definition, Occurrence, Isolation, Nomenclature, Classification, Synthesis, Biosynthesis and Stereochemical structures of Prostaglandins. Structural elucidation of PGE₁, PGE₂; Synthesis and biosynthesis of PGE₂, PGF_{2α}.
 Structure and Biosynthesis of Thromboxane A₂ and Prostacyclin (synthesis not expected).

UNIT – IV: ANTI-INFLAMMATORY DRUGS

Definition, Classification, Nomenclature, Structure and Synthesis.
 Paracetamol, Aspirin (Antipyretic), Salol, Cinchophen, Antipyrine, Phenylbutazone.
 Indomethacin, Tolmetin, Ibuprofen, Diclofenac, Naproxen.

Books suggested:

1. Medicinal Chemistry by Ashitosh Kar
2. Medicinal Chemistry by D. Sriram, P. Yogeeswari
3. Medicinal Chemistry by David A. Williams, Thomas L. Lemke
4. Medicinal Chemistry by V. Alagarsamy
5. Biochemistry by U. Satyanarayana
6. Natural Products Chemistry and Applications by Sujata V. Bhat, B.A. Nagasampagi, S. Meenakshi
7. Medicinal Chemistry by V.K. Ahluwalia, Madhu Chopra
8. Medicinal Chemistry by Balkishen Razdar
9. Advanced Practical Medicinal Chemistry by Ashutosh Kar
10. Chemistry of Organic Natural Products by O. P. Agarwal, Vols., 1 & 2, Geol Pubs.
11. Chemistry of Natural Products by S. V. Bhat, B.A. Nagasampagi, M. Sivakumar
12. Natural Products Chemistry by K.B.G. Torrsell, John Wiley, 1983.

CHE 406(b): OPEN ELECTIVE:ELECTRO ANALYTICAL TECHNIQUES

Unit I

Types and Classification of Electro analytical Methods.

i) Potentiometry- Types of electrodes, Hydrogen gas, Calomel, Quin hydrone and glass electrodes. Determination of pH. Potentiometric titrations.

ii) Conductometry – Definition of terms – conductivity, specific conductivity, cell constant. Mobility of ions, Conductometric titrations.

Unit II

D.C Polarography : Dropping mercury electrode- Instrumentation-polarogram. Types of Currents : Residual, Migration, Limiting. Two and Three electrode assemblies. Ilkovic equation

(derivation not necessary) and its consequences. Types of limiting Currents: Adsorption, Diffusion, Kinetic. Applications of polarography in qualitative and quantitative analysis. Analysis of mixtures. Application to inorganic and organic compounds. Determination of stability constants of complexes.

Unit III

(i) A.C.polarography (ii) Square-wave polarography (iii) Pulse polarography (iv) Differential pulse polarography(V) Cyclic Voltammetry: Principle, instrumentation, reversible and irreversible cyclic voltammograms.

Unit IV

Ion selective electrodes

Ion-sensitive electrodes –types of ion sensitive electrodes –metal based cation and anion sensitive electrodes, solid membrane electrodes. Liquid ion-exchange electrodes, gas sensing membrane electrodes.

Books Suggested

1. H.W. Willard, LL.Merrit and J.A.Dean: Instrumental Methods of Analysis. Affiliated East-West).
2. G.H. Jeffery J. Bassett, J. Mendham and R.C. Denny. Vogel's Text Book of Quantitative Chemical Analysis (ELBS).
3. D.A. Skoog and D.M. West: Principles of Instrumental Analysis (Holt, Rinehart and Wilson).
4. J.G. Dick : Analytical Chemistry (Mc Graw Hill).