ST. XAVIER'S COLLEGE (AUTONOMOUS),

PALAYAMKOTTAI-627 002

M.Sc. Chemistry Course pattern

w.e.f. JUNE 2023

Sem	Part	Status	Sub. Code	Title of the Paper	Hrs	Cdt
I	A	Core-1	23PCHC11	Organic Reaction Mechanism-I	6	5
		Core-2	23PCHC12	Structure and Bonding in Inorganic Compounds	6	5
		Core- 3	23PCHC13	Organic Chemistry Practical -I	4	2
		Core- 4	23PCHC14	Organic Chemistry Practical -II	4	2
		EC-1	23PCHE11	Nano and Supramolecular Chemistry	5	3
		EC-2	23PCHE12	Molecular Spectroscopy	5	3
					30	**20**
II	A	Core-5	23PCHC21	Organic reaction mechanism-II	5	5
		Core-6	23PCHC22	Thermodynamics and Chemical Kinetics	5	5
		Core-7	23PCHC23	Inorganic Chemistry Practical -I	4	2
		Core-8	23PCHC24	Inorganic Chemistry Practical-II	4	2
		EC-3	23PCHE21	Bio Inorganic Chemistry	4	3
		EC-4	23PCHE22	Medicinal Chemistry	4	3
	B	SEC-1	23PCHS21	Soft Skill-2 Chemistry in Consumer Products	4	2
					30	**22**
III	A	Core-9	23PCHC31	Organic synthesis and Photochemistry	5	5
		Core-10	23PCHC32	Coordination Chemistry-I	5	5
		Core-11	23PCHC33	Quantum Chemistry and Group Theory	5	5
		Core-12	23PCHC34	Physical Chemistry Practical- I	4	2
		Core – 13	23PCHC35	Analytical Instrumentation technique Practicals	4	2
		EC-5	23PCHE31	Biomolecules and Heterocyclic compounds	4	3
	B	SEC-2	23PCHS31	Mini project and Seminar	3	2
		Internship	23PCHI35	Carried out in summer vacation at the end of Sem II	-	2
					30	**26**
	A	Core-14	23PCHC41	Coordination Chemistry-II	6	5
		Core-15	23PCHC42	Electrochemistry	6	5
		Project	23PCHC43	Project with Viva Voce	10	7
		EC-6	23PCHE41	Physical Chemistry Practical-II	4	3

IV	B	SEC-3	23PCHS41	Training for competitive Examination	4	2
	C	Extension Activities		STAND (Student Training and Action for Neighbourhood Development)	-	1
					30	**23**
	Additional Compulsory Courses					
	I PG	Value - Added	23PCHVA1	Fundamentals in Phytochemistry		**3**
	II PG	Extra Credit Course	23PCHEC1	Industrial Chemistry		**3**
			23PCHEC2	Forensic Chemistry		
			23PCHEC3	Health Chemistry		
			23PCHEC4	Environmental Chemistry		
				Total	**120**	**97**

Abbreviation

C- Core**,** EC- Elective Course**,** SEC- Skill Enhancement Course**,** I- Internship

ORGANIC REACTION MECHANISM – I

23PCHC11

Semester-I **Core-1** **Hours/W: 6** **Credits: 5**

Course Outcomes:

By the end of the course the student will be able to

CO1: recall the basic principles of organic chemistry (K1).

CO2: understand the formation and detection of reaction intermediates of organic reactions (K2).

CO3: apply the principles of kinetic and non-kinetic methods to determine the mechanism of reactions (K3).

CO4: classify the aromatic and non-aromatic compounds using Huckel's & Craig's rule (K4).

CO5: predict the reaction mechanism of organic reactions and stereochemistry of organic compounds (K5).

CO6: design and synthesize new organic compounds by correlating the stereochemistry of organic compounds (K6).

UNIT I: Methods of Determination of Reaction Mechanism (18 Hrs)

Reaction intermediates, The transition state, Reaction coordinate diagrams, Thermodynamic and kinetic requirements of reactions: Hammond postulate. Methods of determining mechanism: non-kinetic methods - product analysis, determination of intermediates-isolation, detection, and trapping. Cross - over experiments, isotopic labelling, isotope effects and stereo chemical evidences. Kinetic methods - relation of rate and mechanism. Effect of structure on reactivity: Hammett and Taft equations. Linear free energy relationship.

UNIT II: Aromatic and Aliphatic Electrophilic Substitution (18 Hrs)

Aromaticity: Aromaticity in benzenoid, non-benzenoid, heterocyclic compounds and annulenes. Aromatic electrophilic substitution: Orientation and reactivity of di- and poly substituted phenol, nitrobenzene and halobenzene. Reactions involving nitrogen electrophiles: nitration, nitrosation and diazonium coupling; Sulphur electrophiles: sulphonation; Halogen electrophiles: chlorination and bromination; Carbon electrophiles: Friedel-Crafts alkylation, acylation and arylation reactions. Aliphatic electrophilic substitution Mechanisms: SE2 and SEi, SE1- Mechanism and evidences.

UNIT III: Aromatic and Aliphatic Nucleophilic Substitution

(18 Hrs)

Aromatic nucleophilic substitution: Mechanisms - S_NAr, S_N1 and Benzyne mechanisms - Evidences - Reactivity, Effect of structure, leaving group and attacking nucleophile. Reactions: Oxygen and Sulphur-nucleophiles, Bucherer and Rosenmund reactions, von Richter, Sommlet- Hauser and Smiles rearrangements. S_N1, ion pair, S_N2 mechanisms and evidences. Aliphatic nucleophilic substitutions at an allylic carbon, aliphatic trigonal carbon and vinyl carbon.S_N1, S_N2, S_Ni, and S_E1 mechanism and evidences, Swain- Scott, Grunwald - Winstein relationship - Ambident nucleophiles

UNIT IV: Stereochemistry-I (18 Hrs)

Introduction to molecular symmetry and chirality – axis, plane, center, alternating axis of symmetry. Optical isomerism due to asymmetric and dissymmetric molecules with C and N based chiral centres. Optical purity, prochirality, enantiotopic and diastereotopic atoms, groups, faces, axial and planar chirality. Racemic modifications: Racemization by epimerization and mutarotation. D, L system, Cram's and Prelog's rules: R, S-notations, proR, proS, side phase and re phase Cahn-Ingold-Prelog rules, absolute and relative configurations. Configurations of allenes, spiranes, biphenyls, binaphthyls. Topicity and pro stereoisomerism, chiral shift reagents and chiral solvating reagents. Asymmetric synthesis. Stereoselective and stereospecific synthesis.

UNIT V: Stereochemistry-II (18 Hrs)

Conformation and reactivity of acyclic systems, intramolecular rearrangements, neighbouring group participation. Stability of five and six-membered rings: mono and disubstituted cyclohexanes, conformation and reactivity in cyclohexane systems. Fused and bridged rings: bicyclic- cis & trans decalins and Brett's rule. Optical rotation and optical rotatory dispersion, conformational asymmetry, CD and ORD curves, octant rule, configuration and conformation, Cotton effect, axial haloketone rule and determination of configuration.

Text Books:

1. J. March and M. Smith, Advanced Organic Chemistry, 5th edition, John-Wiley and Sons.2001.
2. E. S. Gould, Mechanism and Structure in Organic Chemistry, Holt, Rinehart and Winston Inc., 1959.
3. P.S.Kalsi, Stereochemistry of carbon compounds, 8th edition, New Age International Publishers, 2015.
4. P. Y. Bruice, Organic Chemistry, 7th edition, Prentice Hall, 2013.
5. J.Clayden, N. Greeves, S. Warren, Organic Compounds, 2nd edition, Oxford University Press, 2014.

Reference Books:

1. F.A. Carey and R.J. Sundberg, Advanced Organic Chemistry Part-A and B, 5th edition, Kluwer Academic Plenum Publishers, 2007.
2. D. G. Morris, Stereochemistry, RSC Tutorial Chemistry Text 1, 2001.
3. N.S. Isaacs, Physical Organic Chemistry, ELBS, Longman, UK, 1987.
4. E. L. Eliel, Stereochemistry of Carbon Compounds, Tata-McGraw Hill, 2000.
5. I. L. Finar, Organic chemistry, Vol-1 & 2, 6th edition, Pearson Education Asia, 2004.

STRUCTURE AND BONDING IN INORGANIC COMPOUNDS

23PCHC12

Semester-I **Core-2** **Hours / W : 6** **Credits: 5**

Course Outcomes:

By the end of the course the student will be able to

CO1: recall the fundamental knowledge on the structural aspects of ionic crystals (K1).
CO2: summarize the basic concepts, techniques involved and defects found in solid state and outline the structure of main group compounds and clusters (K2).
CO3: determine the geometry and structure of inorganic compounds and its defects (K3).
CO4: compare the structural features of crystal system, and classify the defects, silicates, polyacid and techniques adopted in solid state chemistry (K4).
CO5: evaluate the physical properties of ionic crystals, structure of boranes, crystal growth methods and the effects of defects (K5).
CO6: predict the structure of main group compounds and clusters, point group and the sampling methods used in instrumental techniques (K6).

UNIT I: Structure of main group compounds and clusters

(18 Hrs)

VSEPR Theory and its applications. Effect of lone pair and electronegativity of atoms (Bent's rule) on the geometry of the molecules; Structure of silicates - applications of Paulings rule of electrovalence - isomorphous replacements in silicates – ortho, meta and pyro silicates – one dimensional, two dimensional and three-dimensional silicates. Structural and bonding features of B-N, S-N and P-N compounds; Poly acids – types, examples and structures; Borane cluster: Structural features of closo, nido, arachano and klado; carboranes, hetero and metalloboranes; Wade's rule to predict the structure of borane cluster; main group clusters –zintl ions and Jemmis mno rule.

UNIT II: Solid state chemistry – I (18 Hrs)

Crystal lattice, Unit cell, Symmetry operations in crystals, glide planes and screw axis; point group and space group; Crystal System and Bravais Lattices. Packing of ions in simple, hexagonal and cubic close packing, voids in crystal lattice, Radius ratio. Solid state energetics: Lattice energy – Born-Lande equation - Kapustinski equation, Madelung constant.

UNIT III: Solid state chemistry – II (18 Hrs)

Structural features of the crystal systems: Rock salt, CsCl, Zinc blende & wurtzite, fluorite and anti-fluorite, rutile, cadmium iodide and nickel arsenide; Spinels -normal and inverse types and perovskite structures. Covalent Crystals- diamond, Graphite and fullerene

UNIT IV: Techniques in solid state chemistry (18 Hrs)

X-ray diffraction technique: Bragg's law, Powder diffraction method – Principle and Instrumentation; Interpretation of XRD data – JCPDS files, Phase purity, Scherrer formula, lattice constants calculation; Systematic absence of reflections; Electron diffraction technique – principle, instrumentation and application. Superconductivity-BCS theory- High and low temperature superconductors

UNIT V: Band theory and defects in solids (18 Hrs)

Defects in crystals – point defects (Schottky, Frenkel, metal excess and metal deficient) and their effect on the electrical and optical property. Linear defects and its effects due to dislocations. Band theory – features and its application of conductors, insulators and semi conductors, Intrinsic and extrinsic semi conductors

Text Books:

1. A R West, Solid state Chemistry and its applications, 2nd Edition (Students Edition), John Wiley & Sons Ltd., 2014.
2. L Smart, E Moore, Solid State Chemistry – An Introduction, 4th Edition, CRC Press, 2012.
3. K. F. Purcell and J. C. Kotz, Inorganic Chemistry; W.B. Saunders company: Philadelphia, 1977.
4. J. E. Huheey, E. A. Keiter and R. L. Keiter, Inorganic Chemistry; 4th ed.; Harper and Row: New York, 1983.

Reference Books:

1. D. E. Douglas, D.H. McDaniel and J. J. Alexander, Concepts and Models in Inorganic Chemistry, 3rd Ed, 1994.
2. C N R Rao and J Gopalakrishnan, New Directions in Solid State Chemistry, 2nd Edition, Cambridge University Press, 1991.
3. T. Moeller, Inorganic Chemistry, A Modern Introduction; John Wiley: New York, 1982.
4. D. F. Shriver, P. W. Atkins and C.H. Langford; Inorganic Chemistry; 3rd ed.; Oxford University Press: London, 2001.
5. Mandeep Dalal, A Text Book of Inorganic Chemistry, Volume-I, International edition, Dalal Institute, 2017.

ORGANIC CHEMISTRY PRACTICAL-I

23PCHC13

Semester-I **Core-3** **Hours / W: 4** **Credits: 2**

Course Outcomes:

By the end of the course the student will be able to

CO1: separate the mixture of compounds in microscale (K2).

CO2: experiment the idea into synthesis of organic compounds (K3).

CO3: analyse the organic compounds for functional groups (K4).

CO4: develop the skill in crystallization technique (K6).

UNIT I: Separation and analysis

A. Two component mixtures. B. Three component mixtures.

Unit II Preparation of Organic Compound (Single Stage)

(i) Oxidation of toluene to benzoic acid

ii) Bromination of Acetanilide

(iii) Nitration of phenol

(iv) Glucosazone

(v) Methyl orange dye

(vi) methyl red dye

Text Books:

1. Gnanapragasam. N.S., Ramamurthy. G., Organic Chemistry Lab Manuel, S. Viswanathan Pvt. Ltd.

Reference Books:

1. Furniss, Hannaford, Smith, Tatchell, Vogel's textbook of Practical Organic Chemistry, Pearson education.

ORGANIC CHEMISTRY PRACTICAL-II

23PCHC14

Semester-I **Core-4** **Hours / W: 4** **Credits: 2**

Course Outcomes:

By the end of the course the student will be able to

CO1: recall the principle underlying estimations of organic compounds (K2).

CO2: compute the reactions of estimated organic compounds (K3).

CO3: estimate the organic compounds in the research laboratories and industry(K4).

CO4: design the new separation techniques in future(K6).

UNIT I: Estimations

a) Estimation of Phenol (bromination)

b) Estimation of Aniline (bromination)

c) Estimation of Glucose (redox)

d) Estimation of Ascorbic acid (iodimetry)

e) Estimation of Glycine (acidimetry)

f) Estimation of Formalin (iodimetry)

UNIT II: Two stage preparations

a) p-bromoacetanilide from aniline

b) p-nitroaniline from acetanilide

c) 1,3,5-Tribromobenzene from aniline

d) Acetylsalicyclic acid from methyl salicylate

e) Benzilic acid from benzoin

Text Book:

1. Gnanapragasam. N.S., Ramamurthy. G., Organic Chemistry Lab Manuel, S. Viswanathan Pvt. Ltd.

Reference Book:

1. Furniss, Hannaford, Smith, Tatchell, Vogel's textbook of Practical Organic Chemistry, Pearson education.

NANO AND SUPRAMOLECULAR CHEMISTRY

23PCHE11

Semester-I **EC-1** **Hours / W: 5** **Credits: 3**

Course Outcomes:

By the end of the course the student will be able to

CO1: recognize the methods of fabricating nanostructures and concepts of supramolecular chemistry (K1).

CO2: relate the properties of nanomaterials to reduce dimensionality of the material (K2).

CO3: organize the tools for properties of nanostructures and dendrimers. (K3).

CO4: illustrate the applications of nanomaterials and supramolecules (K4).

CO5: appraise the characters of various nano materials synthesized by new technologies (K5).

CO6: design synthetic routes for new nano materials and supramolecular assemblies (K6).

UNIT-I: Introduction of nanomaterials and nanotechnologies (15 Hrs)

Introduction-role of size, classification-0D, 1D, 2D, 3D. Synthesis - Bottom –Up, Top–Down, consolidation of Nano powders. Features of nanostructures, Background of nanostructures. Techniques of synthesis of nanomaterials, Tools of the nanoscience. Applications of nanomaterials and technologies.

UNIT-II: Synthetic methods and characterization of Nanomaterials (15 Hrs)

Synthesis- Physical and chemical methods - inert gas condensation, arc discharge, laser ablation, sol-gel, solvothermal and hydrothermal-CVD-types, metallo organic, plasma enhanced, and low-pressure CVD. Microwave assisted and electrochemical synthesis. Characterization – SEM, TEM and AFM - principle, instrumentation and applications.

UNIT-III: Thermal and Mechanical Properties of Nanomaterials (15 Hrs)

Mechanical properties of materials, theories relevant to mechanical properties. Techniques to study mechanical properties of nanomaterials, adhesion and friction, thermal properties of nanomaterials Nanoparticles: gold and silver, metal oxides: silica, iron oxide and alumina - synthesis and properties.

Unit IV: Supramolecular Chemistry **(15 Hrs)**

Definition and development of Supramolecular chemistry, Supramolecular chemistry, Host-Guest chemistry, Development of Supramolecular chemistry, concepts of Lock and key interactions, Host-Guest chemistry, and self- assembly, Nature of Supramolecular interactions, Supramolecular chemistry of fullerenes, Fullerene as Host and guest. Role of crown ethers, podands, cryptands, spherands, calixarenes, and siderophores in Supramolecular chemistry

Unit- V: Supramolecular Assemblies and devices **(15 Hrs)**

Molecular self-Assembly-Catenanes, Rotaxanes and pseudo Rotaxanes. Statistical approaches to Catenanes and Rotaxanes. Catenanes from (pi- pi) stacking interactions. Dendrimers - Synthetic methodology – Divergent and convergent methodologies. Dendrimer Host- Guest chemistry, Dendritic photochemical devices, Molecular electronic devices, Molecular wire, Molecular rectifier, Molecular switch-1,2-dithienyl system.

Text Books:

1. S. Mohan and V. Arjunan, Principles of Materials Science, MJP Publishers, 2016.
2. Arumugam, Materials Science, Anuradha Publications,2007.
3. Giacavazzo et. al., Fundamentals of Crystallography, International Union of Crystallography. Oxford Science Publications, 2010.
4. Woolfson, An Introduction to Crystallography, Cambridge University Press, 2012.
5. James F. Shackelford and Madanapalli K. Muralidhara, Introduction to Materials Science for Engineers. 6th edn., Pearson Press, 2007.
6. J.W. Steed, J.L. Atwood, Supramolecular chemistry, 2000, John Willey & sons Ltd. New York.

Reference Books:

1. S.Mohan and V. Arjunan, Principles of Materials Science, MJP Publishers, 2016.
2. Arumugam, Materials Science, Anuradha Publications, 2007.
3. Giacavazzo *et. al*., Fundamentals of Crystallography, International Union of Crystallography. Oxford Science Publications, 2010
4. J. M. Lehn, Supramolecular Chemistry, Concepts and perspectives, VCH; Weinhein, 1995.

MOLECULAR SPECTROSCOPY

23PCHE12

Semester-I **EC-2** **Hours / W: 5** **Credits: 3**

Course Outcomes:

By the end of the course the student will be able to

CO1: recall the basic principles of spectroscopy (K1).

CO2: understand the importance of rotational and Raman spectroscopy (K2).

CO3: apply vibrational spectroscopic techniques for diatomic & polyatomic molecules (K3).

CO4: examine the NMR, ^{13}C NMR, 2D NMR – COSY, NOESY, ^{31}P, ^{19}F NMR and ESR spectroscopic techniques (K4).

CO5: evaluate electronic spectra of simple molecules using electronic spectroscopy (K5).

CO6: develop the knowledge on structural elucidation of simple molecules using Mass Spectrometry, EPR and Mossbauer Spectroscopy techniques (K6).

UNIT-I: Rotational and Raman Spectroscopy (15 Hrs)

Rotation of molecules. Rotational spectra of diatomic and polyatomic molecules. Intensities of rotational spectral lines, effect of isotopic substitution. Non-rigid rotators. Classical theory of the Raman effect, polarizability as a tensor, polarizability ellipsoids, quantum theory of the Raman effect, Pure rotational Raman spectra of linear and asymmetric top molecules, Stokes and anti-Stokes lines. Vibrational Raman spectra, Raman activity of vibrations, rule of mutual exclusion, Polarization of Raman scattered photons.

UNIT-II: Vibrational Spectroscopy (15 Hrs)

Infra-red spectroscopy – review of linear harmonic oscillator – vibrational energies of diatomic molecules – selection rule – Zero point energy, dissociation energy, force constant and bond strength – Anharmonicity, Morse potential energy diagram, vibration-rotation spectroscopy – P,Q,R, branches – Breakdown of Oppenheimer approximation vibration of polyatomic molecules – overtones, hot bands, combination and differences bands – instrumentation – principle of FT-IR.

UNIT-III: Electronic spectroscopy (15 Hrs)

Electronic Spectroscopy: Electronic spectroscopy of diatomic molecules, Frank-Condon principle, dissociation and predissociation spectra. Types of electronic transitions-influence of solvents and H-bonding on lambda max values. Woodward-Fischer Rules to calculate lambda max values of conjugated dienes and alpha beta unsaturated ketones and Scott's rule.

UNIT-IV: NMR spectroscopy (15 Hrs)

Chemical shift, Factors influencing chemical shifts: electronegativity and electrostatic effects; Mechanism of shielding and deshielding. Spin systems: First order and second order coupling of AB systems, Simplification of complex spectra- Lanthanide shift reagents and deuterium exchange. Spin-spin interactions: Homonuclear coupling interactions - AX, AX_2, AB types. Vicinal, germinal and long-range coupling-spin decoupling. Nuclear Over hauser effect (NOE), Factors influencing coupling constants. ^{13}C NMR and structural correlations. Brief introduction to 2D NMR – COSY, NOESY.

UNIT-V: Mass Spectrometry and EPR Spectroscopy (15 Hrs)

Basic principles - Base peak - Molecular ion peak- Metastable peak -Isotopic peak - Nitrogen rule- General rules for fragmentation pattern: McLafferty rearrangement retro Diels-Alder reaction – ortho effect - Fragmentation pattern of simple compounds of amines, acids and phenols. EPR spectra of anisotropic systems - anisotropy in g-value, causes of anisotropy, anisotropy in hyperfine coupling, hyperfine splitting caused by quadrupole nuclei. Zero-field splitting (ZFS) and Kramer's degeneracy.

Text Books:

1. C. N. Banwell and E. M. McCash, Fundamentals of Molecular Spectroscopy, 4th Ed., Tata McGraw Hill, New Delhi, 2000.
2. R. M. Silverstein and F. X. Webster, Spectroscopic Identification of Organic Compounds, 6th Ed., John Wiley & Sons, New York, 2003.
3. W. Kemp, Applications of Spectroscopy, English Language Book Society, 1987.
4. R. S. Drago, Physical Methods in Chemistry; Saunders: Philadelphia, 1992.

Reference Books:

1. P.W. Atkins and J. de Paula, Physical Chemistry, 7th Ed., Oxford University Press, Oxford, 2002.
2. I. N. Levine, Molecular Spectroscopy, John Wiley & Sons, New York, 1974.
3. A. Rahman, Nuclear Magnetic Resonance-Basic Principles, Springer-Verlag, New York,1986.
4. K. Nakamoto, Infrared and Raman Spectra of Inorganic and coordination Compounds, Part-B: 5th ed., John Wiley& Sons Inc., New York, 1997.
5. J. A. Weil, J. R. Bolton and J. E. Wertz, Electron Paramagnetic Resonance; Wiley Interscience, 1994.

ORGANIC REACTION MECHANISM-II
23PCHC21

Semester-II **CORE-5** **Hours/W: 5** **Credits: 5**

Course Outcomes:

By the end of the course the student will be able to

CO1: recall the basic principles of aromaticity of organic and heterocyclic compounds (K1).
CO2: understand the mechanism of various types of organic reactions (K2).
CO3: predict the suitable reagents for the conversion of selective organic compounds (K3).
CO4: correlate the principles of substitution, elimination, and addition reactions (K4).
CO5: Assess the importance of reagents in organic reactions (K5).
CO6: design new routes to synthesis organic compounds (K6).

UNIT-I: Elimination Reactions **(15 Hrs)**

Mechanisms: E2, E1, and E1CB mechanisms. Syn- and anti-eliminations. Orientation of the double bond: Hoffmann and Saytzeff rules- Chugaev reaction, Cope reactions. Reactivity: Effect of substrate, attacking bases, leaving group and medium. Stereochemistry of eliminations in acyclic and cyclic systems, pyrolytic elimination.

Unit-II Synthetic Organic Name Reactions **(15 Hrs)**

Jones Oxidation, Dakin reaction, Bouveault –Blanc eaction, Bamford Stevens reaction, Doebner Miller synthesis, Duff reaction, Elbs Persulfate oxidation, Mukaiyama reaction, Pechmann Condensation, Ritter reaction, Sarett Oxidation, Thorpe reaction, Suzuki and Mitsunobu reaction

UNIT-III: Rearrangements **(15 Hrs)**

Rearrangements to electron deficient carbon: Pinacol-pinacolone and semi-pinacolone rearrangements and applications. Wagner-Meerwein, Demjanov, Baker-Venkataraman, Benzilic acid and Wolff rearrangements. Rearrangements to electron deficient nitrogen: Hofmann, Curtius, Schmidt, Lossen and Beckmann rearrangements. Rearrangements to electron deficient oxygen: Baeyer-Villiger oxidation. Rearrangements to electron rich atom: Favorskii, Stevens, [1,2]-Wittig and [2,3]-Wittig rearrangements. Fries and Photo Fries rearrangement. Intramolecular rearrangements – Claisen, Cope, oxy-Cope rearrangements.

UNIT-IV: Addition to Carbon Multiple Bonds: Mechanisms **(15 Hrs)**

(a) Addition to carbon-carbon multiple bonds- Addition reactions involving electrophiles, nucleophiles, free radicals, carbenes and cyclic mechanisms-Orientation and reactivity, hydrogenation of double and triple bonds, Michael reaction, addition of oxygen and Nitrogen; (b) Addition to carbon-hetero atom multiple bonds: Mannich reaction, acids, esters, nitrites, addition of Grignard reagents, Wittig reaction, Prins reaction. Mechanism of condensation reactions involving enolates –Stobbe reactions. Hydrolysis of esters and amides, ammonolysis of esters.

Unit V Reagents in organic synthesis **(15 Hrs)**

Reagents in Organic Synthesis: SeO_2, $KMnO_4$, OsO_4, HIO_4, DDQ, NBS and m- CPBA, Reduction involving complex metal hydrides DIBAH, Tri – n-butyl tinhydride, Baker yeast. Phase transfer catalysts, crown ether, LDA, $(CH_3)_3SiI$, Aluminium isopropoxide, diazomethane, Organo rhodium compounds. AIBN, Gilman reagent, Merrifield resin, Collin's reagent, 1,3 dithiane and CAN.

Text Books:

1. J. March and M. Smith, Advanced Organic Chemistry, 5th ed., John-Wiley and Sons. 2001.
2. E. S. Gould, Mechanism and Structure in Organic Chemistry, Holt, Rinehart and Winston Inc., 1959.
3. P. S. Kalsi, Stereochemistry of carbon compounds, 8thedn, New Age International Publishers, 2015.
4. P. Y.Bruice, Organic Chemistry, 7thedn.,Prentice Hall, 2013.
5. R. T. Morrison, R. N. Boyd, S. K. Bhattacharjee Organic Chemistry, 7th edn., Pearson Education, 2010.

Reference Books:

1. S. H. Pine, Organic Chemistry, 5thedn, McGraw Hill International Edition, 1987.
2. L. F. Fieser and M. Fieser, Organic Chemistry, Asia Publishing House, Bombay, 2000.
3. E.S. Gould, Mechanism and Structure in Organic Chemistry, Holt, Rinehart and Winston Inc., 1959.
4. T. L. Gilchrist, Heterocyclic Chemistry, Longman Press, 1989.
5. J. A. Joule and K. Mills, Heterocyclic Chemistry, 4thed., John-Wiley, 2010.

THERMODYNAMICS AND CHEMICAL KINETICS

23PCHC22

Semester-II **CORE-6** **Hours / W: 5** **Credits: 5**

Course Outcomes:

By the end of the course the student will be able to

CO1: explain the classical and statistical concepts of thermodynamics (K1).

CO2: discuss the various thermodynamic and kinetic determination (K2).

CO3: compute the theories of reactions rates and fast reactions (K3).

CO4: correlate the thermodynamic concepts to study the kinetics of chemical reactions (K4).

CO5: evaluate the thermodynamic methods for real gases ad mixtures (K5).

CO6: integrate the classical and statistical thermodynamics (K6).

UNIT-I: Classical Thermodynamics **(15 Hrs)**

Partial molar properties-Chemical potential, Gibb's- Duhem equation-binary and ternary systems. Determination of partial molar quantities. Thermodynamics of real gases - Fugacity- determination of fugacity by graphical and equation of state methods-dependence of temperature, pressure and composition. Thermodynamics of ideal and non-ideal binary mixtures, Duhem - Margulis equation applications of ideal and non-ideal mixtures. Activity and activity coefficients-standard states.

UNIT-II: Statistical thermodynamics **(15 Hrs)**

Introduction of statistical thermodynamics concepts of thermodynamic and mathematical probabilities-distribution of distinguishable and non-distinguishable particles. Assemblies, ensembles, canonical particles. Maxwell - Boltzmann, Fermi Dirac & Bose-Einstein Statistics- comparison and applications. Partition functions-evaluation of translational, vibrational and rotational partition functions for monoatomic, diatomic and polyatomic ideal gases. Thermodynamic functions in terms of partition functions-calculation of equilibrium constants. Statistical approach to Thermodynamic properties: pressure, internal energy, entropy, enthalpy, Gibb's function, Helmholtz function, equilibrium constants and equipartition principle. Heat capacity of solids-Einstein and Debye models.

UNIT-III: Irreversible Thermodynamics **(15 Hrs)**

Theories of conservation of mass and energy entropy production in open systems by heat, matter and current flow, force and flux concepts. Onsager theory-validity and verification- Onsager reciprocal relationships. Electro kinetic and thermomechanical effects-Application of irreversible thermodynamics to biological systems.

UNIT-IV: Kinetics of Reactions **(15 Hrs)**

Theories of reactions-effect of temperature on reaction rates, collision theory of reaction rates, Unimolecular reactions -Lindeman and Christiansen hypothesis- molecular beams, collision cross sections, effectiveness of collisions, Potential energy surfaces. Transition state theory-evaluation of thermodynamic parameters of activation-applications of ARRT to reactions between atoms and molecules, Factors determine the reaction rates in solution - primary salt effect and secondary salt effect, Homogeneous catalysis- acid- base

catalysis-mechanism of acid base catalysed reactions-Bronsted catalysis law, enzyme catalysis-Michaelis-Menton catalysis.

UNIT-V: Kinetics of complex and fast reactions (15 Hrs)

Kinetics of complex reactions, reversible reactions, consecutive reactions, parallel reactions, chain reactions. Chain reactions-chain length, kinetics of $H_2 - Cl_2$ & $H_2 - Br_2$ reactions (Thermal and Photochemical reactions) - Rice Herzfeld mechanism(Pyrolysis of acetaldehyde). Study of fast reactions-relaxation methods- temperature and pressure jump methods electric and magnetic field jump methods -stopped flow flash photolysis methods and pulse radiolysis.

Text Books:

J. Rajaram and J.C. Kuriacose, Thermodynamics for Students of Chemistry, 2nd edition,S.L.N.Chand and Co., Jalandhar, 1986.

2. I.M. Klotz and R.M. Rosenberg, Chemical thermodynamics, 6th edition, W.A. BenjaminPublishers, California, 1972.
3. M.C. Gupta, Statistical Thermodynamics, New Age International, Pvt. Ltd., New Delhi, 1995.
4. K.J. Laidler, Chemical Kinetics, 3rd edition, Pearson, Reprint - 2013.

Reference Books:

1. D.A. Mcqurrie and J.D. Simon, Physical Chemistry - A Molecular Approach, Viva Books Pvt. Ltd., New Delhi, 1999.
2. R.P. Rastogi and R.R. Misra, Classical Thermodynamics, Vikas Publishing, Pvt. Ltd., New Delhi, 1990.
3. S.H. Maron and J.B. Lando, Fundamentals of Physical Chemistry, Macmillan Publishers, New York, 1974
4. K.B. Ytsiimiriski, "Kinetic Methods of Analysis", Pergamom Press,1996.

INORGANIC CHEMISTRY PRACTICAL-I

23PCHC23

Semester-II **CORE-7** **Hours/W: 4** **Credits: 2**

Course Outcomes:

By the end of the course the student will be able to

CO1: classify the cations into various groups (K2).

CO2: determine the concentration of metal ions by complexometric methods (K3).

CO3: compare the different methods of quantitative analysis using EDTA titrations (K4).

CO4: integrate the qualitative ideas into the field of industry (K6).

UNIT-I: Analysis of mixture of cations

Analysis of a mixture of four cations containing two common cations and two rare cations. Cations to be tested.

Group-I : W, Tl and Pb.
Group-IA : Se and Te
Group-II : Mo, Cu, Bi and Cd.
Group-III : Tl, Ce, Th, Zr, V, Cr, Fe, Ti and U.
Group-IV : Zn, Ni, Co and Mn.
Group-V : Ba, Ca and Sr.
Group-VI : Li and Mg.

UNIT-II: Complexometric Titration

1. Estimation of zinc, nickel, magnesium, and calcium.
2. Estimation of mixture of metal ions-pH control, masking and demasking agents.

Text Books:

1. V. V. Ramanujam, Inorganic Semimicro Qualitative Analysis; 3rdedn., The National Publishing Company, Chennai, 1974.
2. G. Svehla, Vogel's Text book of Macro and Semimicro Qualitative Inorganic Analysis, 5thedn., Longman, London and Newyork.
3. G.H. Jeffery, J. Bassett, J. Mendham, R.C. Denney, "Vogel's Text book of Inorganic Quantitative Analysis", 5thed., Longman Scientific & Technical, New York.

Reference books:

1. G. Pass, and H. Sutcliffe, Practical Inorganic Chemistry; Chapman Hall, 1965.
2. W. G. Palmer, Experimental Inorganic Chemistry; Cambridge University Press, 1954.

INORGANIC CHEMISTRY PRACTICAL - II

23PCHC24

Semester-II **CORE-8** **Hours / W: 4** **Credits: 2**

Course Outcomes:

By the end of the course the student will be able to

CO1: recall the principle, theory and applications of gravimetric analysis (K2).

CO2: demonstrate the synthesis of various inorganic coordination complexes (K3).

CO3: categorize the complex preparation based on the conditions (K4).

CO4: interpret the separation of ions in the inorganic mixture (K5).

UNIT-I: Quantitative Analysis

Separation and estimation of the following mixtures by gravimetric and volumetric methods.

1. Nickel (G) and Copper (V)
2. Calcium (G) and Copper (V)
3. Barium (G) and Calcium (V)
4. Nickel (G) and Iron (V)
5. Zinc (G) and Copper (V)
6. Copper (G) and Calcium (V)

UNIT-II: Preparation of metal complexes

Preparation of Inorganic complexes:

a. Preparation of tristhioureacopper(I)sulphate
b. Preparation of potassium trioxalatochromate(III)
c. Preparation of tetramminecopper (II) sulphate
d. Preparation of hexathioureacopper(I) chloridedihydrate
e Preparation of sodium trioxalatoferrate(III)
f. Preparation of hexathiourea lead(II) nitrate

Text Books

1. Vogel's Text book of Inorganic Quantitative Analysis, 4th ed., ELBS, London.
2. G.H. Jeffery, J. Bassett, J. Mendham, R.C. Denney, "Vogel's Text book of Inorganic Quantitative Analysis", 5th ed., Longman Scientific & Technical, New York.

Reference books

1. G. Pass, and H. Sutcliffe, Practical Inorganic Chemistry; Chapman Hall, 1965.
2. W. G. Palmer, Experimental Inorganic Chemistry; Cambridge University Press, 1954

BIOINORGANIC CHEMISTRY

23PCHE21

Semester-II **EC-3** **Hours/W: 4** **Credits: 3**

Course Outcomes:

By the end of the course the student will be able to

CO1: recall the biological importance of trace elements (K1).

CO2: express role of the redox couples in biological systems (K2).

CO3: develop the knowledge on significance and toxicity of metals in medicine (K3).

CO4: comment the enzymic action of metals in living systems (K4).

CO5: criticize the role of metals in nitrogen fixation and photo synthetic transport(K5).

CO6: predict the biological importance, toxicity and enzymic action of metals (K6).

UNIT-I: Essential trace elements **(12 Hrs)**

Selective transport and storage of metal ions: Ferritin, Transferrin and siderophores; Sodium and potassium transport. Metalloenzymes: Zinc enzymes–carboxypeptidase and carbonic anhydrase. Iron enzymes–catalase, peroxidase. Copper enzymes – superoxide dismutase, Plastocyanin, Ceruloplasmin, Tyrosinase. Coenzymes - Vitamin-B_{12} coenzymes.

UNIT-II: Transport Proteins **(12 Hrs)**

Oxygen carriers -Hemoglobin and myoglobin - Structure and oxygenation Bohr Effect. Binding of CO, NO, CN^- to Myoglobin and Hemoglobin. Biological redox system: Cytochromes-Classification, cytochrome a, b and c. Cytochrome P-450. Non-heme oxygen carriers-Hemerythrin and hemocyanin. Iron-sulphur proteins- Rubredoxin and Ferredoxin- Structure and classification.

UNIT-III: Nitrogen fixation **(12 Hrs)**

Introduction, types of nitrogen fixing microorganisms. Nitrogenase enzyme - Metal clusters in nitrogenase- redox property - Dinitrogen complexes transition metal complexes of dinitrogen - nitrogen fixation via nitride formation and reduction of dinitrogen to ammonia. Photosynthesis: photosystem-I and photosystem-II-chlorophylls structure and function.

UNIT-IV: Metals in medicine **(12 Hrs)**

Metal Toxicity of Hg, Cd, Zn, Pb, As, Sb. Therapeutic Compounds: Vanadium-Based Diabetes Drugs; Platinum-Containing Anticancer Agents. Chelation therapy; Cancer treatment. Diagnostic Agents: Technetium Imaging Agents; Gadolinium MRI Imaging Agents. Gold-anti-arthritis drug, Lithium-mental disorder drug.

Unit- V: Biochemistry of metals and non-metals **(12 Hrs)**

Biochemistry of Calcium, Bio minerals of calcium- calcite, Apatite and Fluorapatite, Storage of calcium, Calcium signalling proteins, Transport of calcium- calmodulin, Role of calcium in muscle contraction, Role of calcium in blood clotting, Biological importance of nitric oxide- relaxation of smooth muscles, muscle contraction, transmission of signals in brain cells and cytotoxic function in macrophages.

Text Books:

1. Williams, D.R. –Introduction to Bioinorganic chemistry.
2. F.M. Fiabre and D.R. Williams– The Principles of Bioinorganic Chemistry, Royal Society of Chemistry, Monograph for Teachers-31
3. K. F. Purcell and J. C. Kotz, Inorganic Chemistry; W.B. Saunders company: Philadelphia, 1977.
4. J. E. Huheey, E. A. Keiter and R. L. Keiter, Inorganic Chemistry; 4th ed.; Harper and Row: New York, 1983.
5. G.N. Mugherjea and Arabinda Das, Elements of Bioinorganic Chemistry - 1993.
6. R. Gopalan, V. Ramalingam, Concise Coordination Chemistry, S. Chand, 2001.

Reference Books:

1. M.Satake and Y.Mido, Bioinorganic Chemistry- Discovery Publishing House, New Delhi (1996)
2. M.N. Hughes, 1982, The Inorganic Chemistry of Biological processes, II Edition, Wiley London.
3. R. W. Hay, Bio Inorganic Chemistry, Ellis Horwood, 1987.
4. R. M. Roat-Malone, Bio Inorganic Chemistry, John Wiley, 2002.
5. T. M. Loehr, Iron carriers and Iron proteins, VCH, 1989.

MEDICINAL CHEMISTRY

23PCHE22

Semester-II **EC-4** **Hours/W: 4** **Credits: 3**

Course Outcomes:

By the end of the course the student will be able to

CO1: describe the factors that affect its absorption, distribution, metabolism, and excretion, and hence the considerations to be made in drug design (K1).

CO2: explain the relationship between drug's chemical structure and its therapeutic properties. (K2).

CO3: identify different targets for the development of new drugs for the treatment of infectious and GIT (K3).

CO4: examine the different theories of drug actions at molecular level. (K4).

CO5: justify the importance of antibiotics in living systems (K5).

CO6: Predict the drug properties based on its structure (K6).

UNIT-I: Introduction to receptors **(12 Hrs)**

Introduction, targets, Agonist, antagonist, partial agonist. Receptors, Receptor types, Theories of Drug – receptor interaction, Drug synergism, Drug resistance, physicochemical factors influencing drug action.

UNIT-II: Antibiotics **(12 Hrs)**

Introduction, Targets of antibiotics action, classification of antibiotics, enzyme-based mechanism of action, SAR of penicillin and tetracycline, clinical application of penicillin, cephalosporin. Current trends in antibiotic therapy.

UNIT-III: Antihypertensive agents and diuretics **(12 Hrs)**

Classification of cardiovascular agents, introduction to hypertension, etiology, types, classification of antihypertensive agents, classification and mechanism of action of diuretics, Furosemide, Hydrochlorothiazide, Amiloride.

UNIT-IV: Bio-Regulatory Drugs **(12 Hrs)**

Cardiac glycosides-anti-arrhythmic drugs, Hypoglycemic drugs. Anti-neoplastic drugs, antimetabolites. Medicinal Chemistry of Antidiabetic Agents Introduction, Types of diabetics, Drugs used for the treatment, chemical classification, Mechanism of action, Treatment of diabetic mellitus. Chemistry of insulin, sulfonyl urea.

UNIT-V: Analgesics, Antipyretics and Anti-inflammatory Drugs **(12 Hrs)**

Introduction, Mechanism of inflammation, classification and mechanism of action. paracetamol, Ibuprofen, Diclofenac, naproxen, indomethacin, phenylbutazone and meperidine.

Text Books:

1. Wilson and Gisvold's textbook of organic medicinal and pharmaceutical chemistry,
2. Wilson, Charles Owens: Beale, John Marlowe; Block, John H, Lipincott William, 12th edition, 2011.
3. Graham L. Patrick, An Introduction to Medicinal Chemistry, 5th edition, Oxford University Press, 2013.
4. Jayashree Ghosh, A text book of Pharmaceutical Chemistry, S. Chand and Co. Ltd, 1999,1999 edn.
5. O. LeRoy, Natural and synthetic organic medicinal compounds, Ealemi, 1976.
6. S. Ashutosh Kar, Medicinal Chemistry, Wiley Eastern Limited, New Delhi, 1993

Reference Books:

1. Foye's Princles of Medicinal Chemistry, Lipincott Williams, Seventh Edition, 2012
2. Burger's Medicinal Chemistry, Drug Discovery and Development, Donald J. Abraham, David P. Rotella, Alfred Burger, Academic press, 2010.
3. Wilson and Gisvold's Textbook of Organic Medicinal and Pharmaceutical Chemistry, John M. Beale Jr and John M. Block, Wolters Kluwer, 2011, 12th edn.
4. P. Parimoo, A Textbook of Medical Chemistry, New Delhi: CBS Publishers.1995.
5. S. Ramakrishnan, K. G. Prasannan and R. Rajan, Textbook of Medical Biochemistry,Hyderabad: Orient Longman. 3rd edition, 2001.

CHEMISTRY IN CONSUMER PRODUCTS
23PCHS21

Semester-II **SEC-1** **Hours/W: 4** **Credits: 2**

Course Outcomes:

By the end of the course the student will be able to

CO1: learn about basic knowledge in chemical consumer Products (K1).
CO2: understand the chemical composition and their applications of consumer products (K2).
CO3: make use of applications of milk and milk products(K3).
CO4: classify the soaps, detergents, pigments, perfumes and milk products (K4).
CO5: criticize the bio role and side effects of drugs (K5).
CO6: makeup the day to day life articles(K6).

UNIT-I: SOAPS AND DETERGENTS (12 Hrs)

Soap — definition and types — manufacture of different types of soaps (toilet soaps, transparent soaps and liquid soaps) and their uses — cleansing action of soaps. Detergents — classification of detergents (cationic, anionic and non-ionic) — comparison of soaps and detergents. Dry cleaning and its effect on the environment.

UNIT- II: PIGMENTS AND PERFUMES (12 Hrs)

Pigments — Definition — Examples — colours imparted by the pigments and their uses (lithopone, titanium dioxide, ultramarine blue, Red lead, chrome green). Perfumes — Ingredients of perfumes- Isolation of essential oils — Artificial flavours — apple, grape, banana, pineapple, jackfruit (Naming of a few compounds only structure not needed)

UNIT -III: DRUGS CHEMISTRY (12 Hrs)

Drugs- Definition — Importance of some common drugs with examples — mouth washes — antacids — analgesics — antipyretics — sedatives and hypnotics. Anaesthetics — Basic requirements of anaesthetics — Classification with examples — distinction between antiseptics and disinfectants.

UNIT-IV: CHEMISTRY OF FIREWORKS (12 Hrs)

Gun powder-process of making Cobra eggs magic serpent, manufacture of toy caps (paper caps). Common fireworks – Chinese crackers, maroon, crackers (atom bomb), palm leaf cracker, flower pot or fountains, rockets. Fancy fireworks-parachute, 7 or 9 or 12 or 14 sounds or mines or salute.

UNIT- V: MILK PRODUCTS (12 Hrs)

Composition of milk and milk products. Types of milk - Special milks - sterilized milk -flavoured milk - irradiated / vitaminized milk - toned milk-condensed milk. Fermented milks - Cultured butter milk - Acidophilus milk - Yoghurt (Firm-bodied milk). Milk products: Preparation of khoa - gulabjamun - rasagulla and ice cream.

Text Books:

1. Jayashree Ghosh, Fundamental concepts of Applied chemistry, 2006, S. Chand & Company Ltd. New Delhi.
2. P.C. Jain and Monika Jain, Engineering chemistry, Dhanpat Rai & Sons, New Delhi.

Reference Books:

1. B. K. Sharma, Industrial Chemistry Goel Publishing House, 2003, Meerut.
2. Jayashree Ghosh, Text Book of pharmaceutical chemistry 2003 S. Chand and company, New Delhi

ORGANIC SYNTHESIS AND PHOTOCHEMISTRY

23PCHC31

Semester-III **Core-09** **Hours/W: 5** **Credits: 5**

Course Outcomes:

By the end of the course the student will be able to

CO1: recall the basic principles of organic chemistry and to understand the various reactions of organic compounds with reaction mechanisms (K1).

CO2: understand the versatility of various special reagents and to correlate their reactivity with various reaction conditions (K2).

CO3: identify the synthetic strategies in the preparation of various organic compounds (K3).

CO4: predict the suitability of reaction conditions in the preparation of tailor-made organic compounds (K4).

CO5: evaluate the disconnection approach and identifying suitable synthons to effect successful organic synthesis (K5).

CO6: design and synthesize novel organic compounds with the methodologies learnt during the course (K6).

UNIT-I: Planning an Organic Synthesis and Control elements (15 Hrs)

Preliminary Planning –retrosynthetic analysis, alternate synthetic routes, available starting materials and resulting yield of alternative methods. Examples on retrosynthetic approach, calculation of yield. Retrosynthesis in stereochemistry. Planning of synthesis – Rules for Disconnection approach, Synthons and synthetic equivalents, Synthon Approach-Nucleophiles and electrophiles. Introduction of functional groups. Functional group addition

UNIT-II: Organic Synthetic Methodology: (15 Hrs)

Retrosynthetic analysis; Alternate synthetic routes. Synthesis of organic mono and bifunctional compounds via disconnection approach. One group disconnection- alcohol, olefins, ketones and acids. Two group disconnection: 1,2-, 1,3- and 1,4- difucntional compounds. Linear Vs convergent synthesis. Convergent and divergent synthesis. advantages of convergent synthesis, Synthesis based on umpolung concepts of Seebach. Use of protective groups, activating groups-Protection and deprotection of hydroxyl, carboxyl, carbonyl, thiol and amino groups. Functional group interconversion.

UNIT-III: Pericyclic Reactions (15 Hrs)

Pericyclic reactions - Molecular orbital symmetry; frontier orbitals of ethylene,1,3-butadiene,1,3,5- hexatriene and allyl system. Classification of pericyclic reactions Woodward-Hoffmann correlation diagrams. FMO and transition state aromaticity approach-selection rules.Electrocyclic reactions- conrotatory and disrotatory motions; 4n and 4n+2 system. Cycloaddition reactions: suprafacial and antara facial additions; 4n and 4n+2 system. Sigmatropic reactions - Woodward-Hofmann rule and FMO method - Suprafacial and antara facial shifts of Hydrogen - Sigmatropic shifts inoving carbon moieties. 1,3-,1,5- and 3,3-sigmatopic rearrangements. Correlation diagram approach to simple systems. Dis and

conrotatory ring closure of 1,3-butadiene, 1,3,5-hexatriene and $\pi^{2s}+\pi^{2s}$and $\pi^{4s}+ \pi^{2s}$ cycloaddition reactions.

UNIT-IV: Organic Photochemistry-I (15 Hrs)

Organic photochemistry - Basic principle-Beer-Lambert's law-Stark Einstein law-Grothus Draper's law-Quantum yield-Classifications of reactions based on quantum yield electronic transitions; Reactions of electronically excited ketones; $\pi \rightarrow \pi^*$ triplets; Norrish type-I and type-II cleavage reactions; photo reductions of ketones; Paterno-Buchi reactions.

UNIT-V: Organic Photochemistry-II (15 Hrs)

Photochemistry of α,β-unsaturated ketones; cis-trans isomerisation. Photon energy transfer reactions, Photo addition- photo addition of alkene to carbonyl compounds. Photochemistry of aromatic compounds; photochemical rearrangements-Photo Fries rearrangement; Reaction of conjugated cyclohexadienone to 3,4-diphenyl phenols; Barton's reactions.; di-π-methane rearrangement;

Text Books:

1. F. A. Carey and Sundberg, Advanced Organic Chemistry, 5th edn, Tata McGraw-Hill, New York, 2003.
2. J. March and M. Smith, Advanced Organic Chemistry, 5th ed., John-Wiley and sons, 2007.
3. R. E. Ireland, Organic synthesis, Prentice Hall India, Goel publishing house, 1990.
4. Clayden, Greeves, Warren, Organic Chemistry, Oxford University Press, Second Edition, 2016.
5. M. B. Smith, Organic Synthesis 3rd edn, McGraw Hill International Edition, 2011.

Reference Books:

1. Gill and Wills, Pericyclic Reactions, Chapman Hall, London, 1974.
2. Stuart Warren and Paul Wyatt, Organic Synthesis-The Disconnection Approach, Wiley, 2nd edn.,
3. J.A. Joule, G.F. Smith, Heterocyclic Chemistry, Garden City Press, Great Britain, 2004.
4. W. Caruthers, Some Modern Methods of Organic Synthesis 4thedn, Cambridge University Press, Cambridge, 2007.
5. H. O. House. Modern Synthetic reactions, W.A. Benjamin Inc, 1972.

COORDINATION CHEMISTRY – I

23PCHC32

Semester-III **Core-10** **Hours/W: 5** **Credits: 5**

Course Outcomes:

By the end of the course the student will be able to

CO1: recall the various theories of coordination compounds. (K1).

CO2: Understand the spectroscopic and magnetic properties of coordination complexes (K2).

CO3: develop the knowledge on the stability of complexes and various experimental methods to determine the stability of complexes (K3).

CO4: Comprehend the kinetics and mechanism of substitution reactions in octahedral and square planar complexes (K4).

CO5: evaluate the stability and reaction mechanism of coordination compounds (K5).

CO6: Predict the electronic transitions in a complex based on correlation diagrams and UV-visible spectral details (K6).

UNIT I: Modern theories of coordination compounds **(15 Hrs)**

Crystal field theory - splitting of d orbitals in octahedral, tetrahedral and square planar symmetries - measurement of 10Dq - factors affecting 10Dq - spectrochemical series - crystal field stabilization energy for high spin and low spin complexes- evidences for crystal field splitting - site selections in spinels and anti-spinels - Jahn Teller distortions and its consequences. Molecular Orbital Theory and energy level diagrams concept of Weak and strong fields, Sigma and pi bonding in octahedral, square planar and tetrahedral complexes.

UNIT-II: Spectral characteristics of complexes **(15 Hrs)**

Term states for d ions - characteristics of d-d transitions - charge transfer spectra - selection rules for electronic spectra - Orgel correlation diagrams - Sugano-Tanabe energy level diagrams - nephelauxetic series - Racah parameter and calculation of inter-electronic repulsion parameter.

UNIT-III: Stability and Magnetic property of the complexes **(15 Hrs)**

Stability of complexes: Factors affecting stability of complexes, Thermodynamic aspects of complex formation, Stepwise and overall formation constants, Stability correlations, statistical factors and chelate effect, Determination of stability constant and composition of the complexes: Formation curves and Bjerrum's half method, Potentiometric method, Spectrophotometric method, Ion exchange method, Polarographic method and Continuous variation method (Job's method) Magnetic property of complexes: Spin-orbit coupling, effect of spin-orbit coupling on magnetic moments, quenching of orbital magnetic moments.

UNIT-IV: Kinetics and mechanisms of substitution reactions of octahedral and square planar complexes **(15 Hrs)**

Inert and Labile complexes; Associative, Dissociative and SN^1CB mechanistic pathways for substitution reactions; acid and base hydrolysis of octahedral complexes; Classification of metal ions based on the rate of water replacement reaction and

their correlation to Crystal Field Activation Energy; Substitution reactions in square planar complexes: Trans effect, theories of trans effect and applications of trans effect in synthesis of square planar compounds; Kurnakov test.

UNIT-V: Electron Transfer reactions in octahedral complexes (15 Hrs)

Outer sphere electron transfer reactions and Marcus-Hush theory; inner sphere electron transfer reactions; nature of the bridging ligand in inner sphere electron transfer reactions. Photo-redox, photo-substitution and photo-isomerisation reactions in complexes and their applications. Complementary and non-complementary reactions.

Text Books:

1. J E Huheey, EA Keiter, RL Keiter and OK Medhi, Inorganic Chemistry – Principles of structure and reactivity, 4th Edition, Pearson Education Inc., 2006
2. G L Meissler and D ATarr, Inorganic Chemistry, 3rd Edition, Pearson Education Inc., 2008
3. D. Bannerjea, Co-ordination Chemistry, TATA Mcgraw Hill, 1993.
4. B. N. Figgis, Introduction to Ligand Fields, Wiley Eastern Ltd, 1976.

F. A. Cotton, G. Wilkinson.; C. A. Murillo; M. Bochmann, Advanced Inorganic Chemistry, 6th ed.; Wiley Inter-science: New York, 1988

Reference Books:

1. Keith F. Purcell and John C. Kotz, Inorganic Chemistry, Saunders Publications, USA, 1977.
2. Peter Atkins and Tina Overton, Shriver and Atkins' Inorganic Chemistry, 5th Edition, Oxford University Press, 2010.
3. Basic Inorganic Chemistry, F. A. Cotton, G. Wilkinson, P. L. Gauss, John Wiley, 2002, 3rd edn.
4. Concepts and Models of Inorganic Chemistry, B. Douglas, D. McDaniel, J. Alexander, John Wiley, 1994, 3rd edn.
5. Inorganic Chemistry, D. F. Shriver, P. W. Atkins, W. H. Freeman and Co, London, 2010.

QUANTUM CHEMISTRY AND GROUP THEORY

23PCHC33

Semester-III **Core-11** **Hours/W: 5** **Credits: 5**

Course Outcomes:

By the end of the course the student will be able to

CO1: know the importance of quantum mechanical models of particle in a box, rigid rotor and harmonic oscillator (K1).

CO2: understand the essential characteristics of wave functions and need for the quantum mechanics (K2).

CO3: apply the quantum mechanics to hydrogen and polyelectronic systems (K3).

CO4: familiarize the symmetry in molecules and predict the point groups (K4).

CO5: justify the characteristics of wave functions and symmetry functions (K5).

CO6: predict the vibrational modes, hybridization using he concepts of group theory (K6).

UNIT-I: Quantum Chemistry **(15 Hrs)**

Introduction to quantum mechanics, Black - body radiation and photoelectric effect. Wave function – eigenfunctions and eigenvalues – orthogonality and normalization. Schrodinger time independent wave equation, Postulates of quantum mechanics -- different types of functions – different types of operators. Quantum mechanical operators – position operator, linear momentum operator, angular momentum operator, kinetic energy operator and Hamiltonian operator – their nature and Hermitian operator – commutation relationship among L_x, L_y, L_z and L^2 operators. Setting up Schrodinger equation, solution & interpretation with regard to particle in a 1 –D box and 3 – D box. Schrodinger equation for electron in a ring, rigid rotor and simple harmonic oscillator.

UNIT-II: Applications of Quantum Chemistry-I **(15 Hrs)**

Setting up Schrodinger equation for H – atom, separation into three equations (without derivation), quantum numbers and their importance . Approximation methods – Need for approximation, Perturbation theory – Time independent Perturbation (First order only), Application of perturbation theory to particle in one dimensional box and anharmonic oscillator. Principle of variation method and its proof. Variation methods and its applications to hydrogen atom and helium atom.

UNIT-III: Applications of Quantum Chemistry-II **(15 Hrs)**

Hatrefock Self consistent method, Hohenberg-Kohn theorem and Kohn-Sham equation. Pauli's exclusion principle and Slater determination. The Born – Oppenheimer approximation, MO & VB theories as applied to hydrogen molecular ion (H_2^+) and hydrogen molecule, Coulomb integral exchange integral and overlap integral, Construction of sp, sp^2 and sp^3 hybrid orbitals, Huckel molecular orbital theory – principles, applications and calculations of pi electron energies to ethylene and butadiene.

UNIT-IV: Group theory **(15 Hrs)**

Groups, sub groups, symmetry elements, operations, classification-axial and non-axial. Dihedral point groups- C_n, C_{nh}, D_n, D_{nh}, D_{nd}, Td and Oh. Matrix representation and classes of symmetry operations, reducible irreducible and direct product representation. The Great orthogonality theorem – irreducible representation and reduction formula, construction of character table for C_{2v}, C_{2h}, C_{3v} and D_{2h} point groups.

UNIT-V: Applications of group theory **(15 Hrs)**

Standard reduction formula, Group Theory (GT) applied to determine hybridization scheme in CH_4 and BF_3. Application of GT to normal mode analysis of $[PtCl_4]^{2-}$, H_2O, NH_3 and BF_3 and CO_2 Symmetry properties of integrals and symmetry – based selection rule for vibrational spectra – Identification of IR and Raman active fundamentals. Selection rule for electronic transition – prediction of electronic transitions in formaldehyde. – Application of GT to trans – 1, 3 – butadiene and benzene- calculations and delocalization energy in trans – 1, 3 – butadiene and benzene.

Text Books:

1. R.K. Prasad, Quantum Chemistry, New Age International Publishers, New Delhi, 2010, 4th revised edition.
2. F. A. Cotton, Chemical Applications of Group Theory, John Wiley & Sons, 2003, 2nd edition.
3. A. Vincent, Molecular Symmetry and Group Theory. A Programmed Introduction to Chemical Applications, John and Willy & Sons Ltd., 2013, 2nd Edition.
4. T. Engel & Philip Reid, Quantum Chemistry and Spectroscopy, Pearson, New Delhi, 2018, 4th edition.
5. G. K. Vemulapalli, Physical Chemistry, Prentice Hall of India Pvt. Ltd. 2001.
6. D.A. McQuarrie, Quantum Chemistry, Viva Books PW. Ltd, 2013, 2nd edition.

Reference Books:

1. N. Levine, Quantum Chemistry, Allyn& Bacon Inc, 1983, 4th edition.
2. D.A. McQuarrie and J. D. Simon, Physical Chemistry, A Molecular Approach, Viva Books Pvt. Ltd, New Delhi, 2012.
3. R. P. Rastogi & V. K. Srivastava, An Introduction to Quantum Mechanics of Chemical Systems, Oxford & IBH Publishing Co., New Delhi, 1999.
4. R.L. Flurry. Jr, Symmetry Group Theory and Chemical applications, Prentice Hall. Inc, 1980
5. J. M. Hollas, Symmetry in Molecules, Chapman and Hall, London, 2011, Reprint

PHYSICAL CHEMISTRY PRACTICAL-I
23PCHC34

Semester-III **Core-12** **Hours/W: 5** **Credits: 2**

Course Outcomes:

By the end of the course the student will be able to

CO1: summarize the principles of conductometry, thermochemistry and potentiometry (K2)

CO2: perform the conductometric titrations between acids and salt mixtures against bases and apply the electrochemical methods for determining its concentration. (K3)

CO3: determine the pKa and Ka values of the weak acid by titrating against a strong base using a quinhydrone electrode. (K4)record and interpret the experimental data and construct acid- base graph(K4)

CO4: Prepare different buffer solutions and can determine the pH values of buffer solutions and solubility products by using quinhydrone electrode and glass electrode. (K5)

CO5: justify the validity of Debye-Huckel Onsager theory (K5)

UNIT-I: Conductivity Experiments

1.Determination of equivalent conductance of a strong electrolyte & the verification of DHO equation.
2. Verification of Ostwald's Dilution Law & Determination of pKa of a weak acid.
3. Verification of Kohlrausch's Law for weak electrolytes.
4. Determination of solubility of a sparingly soluble salt.
5. Acid-base titration (strong acid and weak acid vs NaOH).
6. Precipitation titrations (mixture of halides only).
7. Determination of strength of sodium acetate and acetic acid in an acetic buffer

UNIT-II: Potentiometric Experiments

1. Acid-Base titrations (SA and WA vs NaOH)
2. Dissociation constant of acetic acid in dioxane and water by titrating with KOH
3. Solubility product of AgX
4. Estimation of halides in water samples by potentiometry

Text Books:

1. B. Viswanathan and P.S.Raghavan, Practical Physical Chemistry, Viva Books, New Delhi, 2009.
2. Sundaram, Krishnan, Raghavan, Practical Chemistry (Part II), S. Viswanathan Co. Pvt., 1996.
3. V.D. Athawale and Parul Mathur, Experimental Physical Chemistry, New Age International (P) Ltd., New Delhi, 2008.
4. E.G. Lewers, Computational Chemistry: Introduction to the Theory and Applications of Molecular and Quantum Mechanics, 2nd Ed., Springer, New York, 2011.

References:

1. J. B. Yadav, Advanced Practical Physical Chemistry, Goel Publishing House, 2001.
2. G.W. Garland, J.W. Nibler, D.P. Shoemaker, Experiments in Physical Chemistry, 8th edition, McGraw Hill, 2009.
3. J. N. Gurthu and R. Kapoor, Advanced Experimental Chemistry, S. Chand and Co., 1987.
4. Shailendra K Sinha, Physical Chemistry: A laboratory Manual, Narosa Publishing House Pvt, Ltd., New Delhi, 2014.
5. F. Jensen, Introduction to Computational Chemistry, 3rd Ed., Wiley-Blackwell.

ANALYTICAL INSTRUMENTATION TECHNIQUES PRACTICALS
23PCHC35

Semester-IV CORE-13 Hours/W: 4 Credits: 2

Course Outcomes:

By the end of the course the student will be able to

CO1: understand the principles associated with various inorganic organic and physical chemistry experiments (K2).

CO2: analyse different constituents through instrumental methods of analysis (K4).

CO3: evaluate different contaminants in materials using turbidimetry and conductivity measurements (K5).

CO4: design chromatographic methods for identification of species (K6).

UNIT I Chromatographic Analysis and Water Analysis

1. Paper Chromatography-
   a) Separation ink dyes
   b) Separation of mixture of metal ions
2. Thin Layer Chromatography-
   a) Separation of mixture of Azo dyes
   b) Purity check of p-nitroacetanilide
   c) TLC check of Analgesic drugs.
3. Column Chromatography
   a) Separation of $KMnO_4$ and $K_2Cr_2O_7$
   b) column analysis of Spinach extract.
4. Determination of caffeine in soft drinks by HPLC
5. Analysis of water quality through COD, DO, BOD measurements.

UNIT II: Interpretation and identification of the given spectra of various organic compounds arrived at from the following instruments

1.UV-Visible
2.IR
3.Raman
4.NMR
5.ESR
6.Mass

Text Books:

1. Vogel's Text book of Practical Organic Chemistry, 5th Ed, ELBS/Longman, England, 2003.
2. G. H. Jeffery, J. Bassett, J. Mendham and R. C. Denney, Vogel's Textbook of Quantitative Chemical Analysis; 6th ed., ELBS, 1989.
3. J. D. Woollins, Inorganic Experiments; VCH: Weinheim,1995.
4. B. Viswanathan and P.S.Raghavan, Practical Physical Chemistry, Viva Books, New Delhi, 2009.

5. Sundaram, Krishnan, Raghavan, Practical Chemistry (Part II), S.Viswanathan Co. Pvt., 1996.

Reference Books:

1. N. S. Gnanapragasam and G. Ramamurthy, Organic Chemistry – Lab manual, S. Viswanathan Co. Pvt. Ltd, 2009.
2. J. N. Gurtu and R. Kapoor, Advanced Experimental Chemistry, S. Chand and Co., 2011.
3. J. B. Yadav, Advanced Practical Physical Chemistry, Goel Publishing House, 2001.
4. G.W. Garland, J.W. Nibler, D.P. Shoemaker, Experiments in Physical Chemistry, 8th edition, McGraw Hill, 2009.
5. J. N. Gurthu and R. Kapoor, Advanced Experimental Chemistry, S. Chand and Co., 1987.

BIOMOLECULES AND HETEROCYCLIC COMPOUNDS

23PCHE31

Semester-III EC-5 Hours / W: 4 Credits: 3

Course Outcomes:

By the end of the course the student will be able to

CO1: learn the basic concepts and biological importance of biomolecules and natural products (K1).

CO2: explain various of functions of carbohydrates, proteins, nucleic acids, steroids and hormones (K2).

CO3: integrate and assess the different methods of preparation of structurally different biomolecules and natural products (K3).

CO4: illustrate the applications of biomolecules and their functions in the metabolism of living organisms (K4).

CO5: analyse and rationalise the structure and synthesis of heterocyclic compounds (K5).

CO6: develop the structure of biologically important heterocyclic compounds by different methods (K6).

UNIT I: Chemistry and metabolism of carbohydrates (12 Hrs)

Definition, classification and biological role of carbohydrates. monosaccharides: Linear and ring structures (Haworth formula) of ribose, glucose, fructose and mannose (structure determination not required), Disaccharides: Ring structures (Haworth formula) of Polysaccharides: Starch, glycogen and cellulose (structure only)..

UNIT II: Steroids and Hormones (12 Hrs)

Steroids-Introduction, occurrence, nomenclature, configuration of substituents. Diels' hydrocarbon, stereochemistry, classification, biological importance of cholesterol. Hormones-Introduction, classification, functions of sex hormones- androgens and estrogens, adrenocortical hormones-cortisone and cortisol structure and functions of non-steroidal hormones-adrenaline and thyroxin.

UNIT III: Proteins and nucleic acids (12 Hrs)

Separation and purification of proteins – dialysis, gel filtration and electrophoresis. Catabolism of amino acids – transamination, oxidative deamination and decarboxylation. Structure, methods for the synthesis of nucleosides – direct combination, conversion of nucleoside to nucleotides. Primary and secondary structure of RNA and DNA, Watson-Crick model.

UNIT-IV: Amino acids and Vitamins (12 Hrs)

Introduction, classification, stereochemistry of amino acids, separation. Vitamins-Definition, classification, structure, synthesis and functions of Vitamins A, D, E, K, C and B (Structural elucidation is not required)

UNIT-V: Fused Ring Heterocyclic Compounds (12 Hrs)

Benzo fused five membered rings: Indole, isoindole and benzofuran. Preparation and properties. Benzo fused six membered rings: Quinoline and isoquinoline: Preparation by ring closure reactions, Reactions: Electrophilic and nucleophilic substitutions, oxidation and reduction reactions. (Mechanism not required).

Text Books:

1. T. K Lindhorst, Essentials of Carbohydrate Chemistry and Biochemistry, Wiley VCH, North America,2007.
2. I. L. Finar, Organic Chemistry Vol-2, 5th edition, Pearson Education Asia, 1975.
3. V. K. Ahluwalia and M. Goyal, Textbook of Heterocyclic compounds, Narosa Publishing, New Delhi,2000.
4. M. K. Jain and S. C. Sharma, Modern Organic Chemistry, Vishal Publishing Co., Jalandhar, Delhi, 2014.
5. V. K. Ahluwalia, Steroids and Hormones, Ane books pub., New Delhi,2009.

Reference Books:

1. I. L. Finar, Organic Chemistry Vol-1, 6thedition, Pearson Education Asia, 2004.
2. Pelletier, Chemistry of Alkaloids, Van Nostrand Reinhold Co,2000.
3. Shoppe, Chemistry of the steroids, Butterworthes,1994.
4. I. A. Khan, and A. Khanum. Role of Biotechnology in medicinal & aromatic plants, Vol 1 and Vol 10, Ukkaz Publications, Hyderabad,2004.
5. M. P. Singh. and H. Panda, Medicinal Herbs with their formulations, Daya Publishing House, Delhi,2005.

MINI PROJECT & SEMINAR PRESENTATION

23PCHS31

Semester-III **SEC-2** **Hours/W: 3** **Credits: 2**

MINI PROJECT: Literature Review and Seminar Presentation

INTERNSHIP

23PCHI35

Semester-III **Internship** **Hours/W: -** **Credits: 2**

- All PG students will undergo internship during the summer holidays of the first year after completing II semester.
- Two credits will be given for internship.
- Minimum Days: 30
- Minimum working time per day: 3 Hrs. & Maximum working Time: 5 Hrs.
- The places of internship can be government offices, Panchayats, MP, MLA offices, private institutions, companies, production units etc.
- The HoD of the departments will give a letter of introduction to each student.
- The students will identify the company / institution for internship.
- The students will be divided equally based on the number of professors available in the departments. Each professor will serve as a guide to the assigned students.
- The students will finalize the institutions / companies for the internship in consultation with the guides.
- The students shall maintain a work diary which will be countersigned by the managers / authorities of the company in which the students do the internship on daily basis.
- The work diary, Work completion certificate obtained from the company and a comprehensive report on the learning outcomes will be submitted to the guides at the end of the internship.
- Viva will be conducted based on the experience of the internship in the month of August. The guide will be the internal examiner and another faculty from the same department will serve as the external examiner.

COORDINATION CHEMISTRY-II

23PCHC41

Semester-IV **CORE-14** **Hours /W : 6** **Credits: 5**

Course Outcomes:

By the end of the course the student will be able to

CO1: recognize the fundamental concepts and structural aspects of organometallic compounds (K1).

CO2: Understand the structure and bonding in olefin, allyl, cyclopentadienyl and carbonyl containing organometallic compounds (K2).

CO3: apply 18 and 16 electron rule for organometallic compounds (K3).

CO4: analyse the structure and bonding in coordination complexes (K4).

CO5: evaluate the spectral characteristics of selected complexes (K5).

CO6: predict the structure of coordination complexes using spectroscopic tools such as IR, NMR, ESR, Mossbauer and optical rotatory dispersion studies to interpret the structure of molecules by various spectral techniques (K6).

UNIT I: Chemistry of organometallic compounds **(15 Hrs)**

Classification of organometallic compounds based on M-C bond – 18 and 16 electron rule; Bonding in metal – olefin complexes (example: Zeise's salt), metal-acetylene and metal-allyl complexes; Metal-cyclopentadienyl complexes – Examples and MO approach to bonding in ferrocene. fluxional isomerism. Metal – carbonyl complexes: MO diagram of CO; Structure and bonding – bonding modes, MO approach of M-CO bonding, π-acceptor nature of carbonyl group, synergistic effect (stabilization of lower oxidation states of metals); Carbonyl clusters: Low and high nuclearity carbonyl clusters – Structures based on polyhedral skeleton electron pair theory or Wade's rule.

UNIT II: Reactions and catalysis of organometallic compounds **(15 Hrs)**

Reactions of organometallic compounds: Oxidative addition, reductive elimination (α and β eliminations), migratory insertion reaction and metathesis reaction. Organo-metallic catalysis: Hydrogenation of olefins (Wilkinson's catalyst), hydroformylation of olefins using cobalt or rhodium catalysts (oxo process), oxidation of olefin (Wacker process), olefin isomerisation, water gas shift reaction, cyclo-oligomerisation of acetylenes using Reppe's catalysts, Monsanto process. Ziegler-Natta Catalyst-polymerisation of olefins.

UNIT III: Inorganic spectroscopy -I **(15 Hrs)**

IR spectroscopy: Effect of coordination on the stretching frequency-sulphato, carbonato, sulphito, aqua, nitro, thiocyanato, cyano, thiourea, DMSO complexes; IR spectroscopy of carbonyl compounds. NMR spectroscopy- Introduction, applications of ^{15}N, ^{19}F, ^{31}P, ^{11}B-NMR spectroscopy in structural identification of inorganic complexes, fluxional molecules, quadrupolar nuclei- effect in

NMR spectroscopy. NQR Spectroscopy- introduction, interpretation of e^2Qq data- structural information from NQR spectra- interpretation of NQ coupling constants.

UNIT IV: Inorganic spectroscopy-II (15 Hrs)

Introductory terminologies: g and A parameters-definition, explanation and factors affecting g and A; Applications of ESR to coordination compounds with one and more than one unpaired electrons – hyperfine and secondary hyperfine splitting and Kramer's doublets; ESR spectra of V(II), Mn(II), Fe(II), Co(II), Ni(II), Cu(II) complexes, bis(salicylaldimine)copper(II) and $[(NH_3)_5Co\text{-}O_2\text{-}Co(NH_3)_5]^{5+}$. Mossbauer spectroscopy – Mossbauer effect, Recoil energy, Mossbauer active nuclei, Doppler shift, Isomer shift, quadrupole splitting and magnetic interactions. Applications of Mössbauer spectra to Fe and Sn compounds.

UNIT V: Photo Electron Spectroscopy (15 Hrs)

Theory, Types, origin of fine structures - shapes of vibrational fine structures – adiabatic and vertical transitions, PES of homonuclear diatomic molecules (N_2, O_2) and heteronuclear diatomic molecules (CO, HCl) and polyatomic molecules (H_2O, CO_2, CH_4, NH_3) – evaluation of vibrational constants of the above molecules. Koopman's theorem- applications and limitations. Surface techniques-XPES and ESCA- Applications- NaN3, Auger Electron Spectroscopy.

Text Books:

1. J E Huheey, EA Keiter, RL Keiter and OK Medhi, Inorganic Chemistry – Principles of structure and reactivity, 5th Edition, Pearson Education Inc., 2006
2. G L Meissler and D A Tarr, Inorganic Chemistry, 3rd Edition, Pearson Education Inc., 2008
3. D. Banerjee, Co-ordination Chemistry, TATA Mcgraw Hill, 1993.
4. B D Gupta and A K Elias, Basic Organometallic Chemistry: Concepts, Syntheses and Applications, University Press, 2013.
5. F. A. Cotton, G. Wilkinson.; C. A. Murillo; M. Bochmann, Advanced Inorganic Chemistry, 6th ed.; Wiley Inter-science: New York, 1988.

Reference Books:

1. Crabtree, Robert H. The Organometallic Chemistry of the Transition Metals. 3rd ed. New York, NY: John Wiley, 2000.
2. P Gütlich, E Bill, A X Trautwein, Mossbauer Spectroscopy and Transition Metal Chemistry: Fundamentals and Applications, 1st edition, Springer-Verlag Berlin Heidelberg, 2011.
3. Concepts and Models of Inorganic Chemistry, B. Douglas, D. McDaniel, J. Alexander, John Wiley, 1994, 3rd edn.
4. K. F. Purcell, J. C. Kotz, Inorganic Chemistry; Saunders: Philadelphia, 1976.
5. R. S. Drago, Physical Methods in Chemistry; Saunders: Philadelphia, 1977.

ELECTROCHEMISTRY
23PCHC42

Semester-IV **Core-15** **Hours/W: 6** **Credits: 3**

Course Outcomes:

By the end of the course the student will be able to

CO1: knowledge on storage devices and electrochemical reaction mechanism (K1).
CO2: understand the behaviour of electrolytes in solution and compare the structures of electrical double layer of different models (K2).
CO3: highlight the different types of over voltages and its applications in electroanalytical techniques (K3).
CO4: discuss the theories of electrolytes, electrical double layer, electrodics and activity coefficient of electrolytes (K4).
CO5: discuss the mechanism of electrochemical reaction and different thermodynamic mechanism of corrosion (K5).
CO6: predict the kinetics of electrode reactions applying Butler-Volmer and Tafel equations. (K6).

UNIT-I: Ionics **(15 Hrs)**

Arrhenius theory -limitations, van't Hoff factor and its relation to colligative properties. Deviation from ideal behavior. Ionic activity, mean ionic activity and mean ionic activity coefficient-concept of ionic strength, Debye Huckel theory of strong electrolytes, activity coefficient of strong electrolytes Determination of activity coefficient ion solvent and ion-ion interactions. Born equation. Debye-Huckel Bjerrum model. Derivation of Debye-Huckel limiting law at appreciable concentration of electrolytes modifications and applications. Electrolytic conduction-Debye-Huckel Onsager treatment of strong electrolyte-qualitative and quantitative verification and limitations. Evidence for ionic atmosphere. Ion association and triple ion formations.

UNIT II: Electrode- electrolyte interface **(15 Hrs)**

Interfacial phenomena -Evidences for electrical double layer, polarizable and non-polarizable interfaces, Electrocapillary phenomena - Lippmann equation electro capillary curves. Electro-kinetic phenomena electro-osmosis, electrophoresis, streaming and sedimentation potentials, colloidal and poly electrolytes. Structure of double layer: Helmholtz -Perrin, Guoy- Chapman and Stern models of electrical double layer. Zeta potential and potential at zero charge. Applications and limitations.

UNIT-III: Electrodics of Elementary Electrode Reactions **(15 Hrs)**

Behaviour of electrodes: Standard electrodes and electrodes at equilibrium. Anodic and Cathodic currents, condition for the discharge of ions. Nernst equation, polarizable and non-polarizable electrodes. Model of three electrode system, over potential. Rate of electro chemical reactions: Rates of simple elementary reactions. Butler-Volmer equation-significance of exchange current density, net current density and symmetry factor. Low and high field approximations. symmetry factor and transfer coefficient Tafel equations and Tafel plots.

UNIT-IV: Electrodics of Multistep Multi Electron System (15 Hrs)

Rates of multi-step electrode reactions, Butler - Volmer equation for a multi-step reaction. Rate determining step, electrode polarization and depolarization. Transfer coefficients, its significance and determination, Stoichiometric number. Electro-chemical reaction mechanisms-rate expressions, order, and surface coverage. Reduction of I^{3-}, Fe^{2+}, and dissolution of Fe to Fe^{2+}. Overvoltage - Chemical and electro chemical, Phase, activation and concentration over potentials. Evolution of oxygen and hydrogen at different pH.

UNIT-V: Concentration Polarization, Batteries and Fuel cells (15 Hrs)

Modes of Transport of electro active species - Diffusion, migration and hydrodynamic modes. Role of supporting electrolytes. Polarography-principle and applications. Principle of square wave polarography. Cyclic voltammetry- anodic and cathodic stripping voltammetry and differential pulse voltammetry. Sodium and lithium-ion batteries and redox flow batteries. Mechanism of charge storage: conversion and alloying. Capacitors- mechanism of energy storage, charging at constant current and constant voltage. Energy production systems: Fuel Cells: classification, alkaline fuel cells, phosphoric acid fuel cells, high temperature fuel cells.

Text Books:

1. D. R. Crow, Principles and applications of electrochemistry, 4thedition, Chapman & Hall/CRC, 2014.
2. J. Rajaram and J.C. Kuriakose, Kinetics and Mechanism of chemical transformations Macmillan India Ltd., New Delhi, 2011.
3. S. Glasstone, Electro chemistry, Affiliated East-West Press, Pvt., Ltd., New Delhi, 2008.

Reference Books:

1. J.O.M. Bockris and A.K.N. Reddy, Modern Electro chemistry, vol.1 and 2B, Springer, Plenum Press, New York, 2008.
2. J.O.M. Bockris, A.K.N. Reddy and M.G. Aldeco Morden Electro chemistry, vol. 2A, Springer, Plenum Press, New York, 2008.
3. Philip H. Rieger, Electrochemistry, 2nd edition, Springer, New York, 2010.
4. L.I. Antropov, Theoretical electrochemistry, Mir Publishers, 1977.
5. K.L. Kapoor, A Text book of Physical chemistry, volume-3, Macmillan, 2001.

PROJECT WITH VIVAVOCE
(23PCHC43)

Semester-IV **Core-16** **Hours/W: 10** **Credits: 7**

Structure of the Project Report

1. Cover Page
2. Certificate
3. Declaration
4. Acknowledgement
5. Chapter-I Introduction
6. Chapter-II
7. Chapter-III
8. Chapter-IV
9. Chapter-V Conclusion and Scope for further research

Assessment

Internal : 100 Marks
External : 100 Marks

PHYSICAL CHEMISTRY PRACTICAL-II

23PCHE41

Semester-IV **EC-6** **Hours/W: 4** **Credits: 3**

Course Outcomes:

By the end of the course the student will be able to

CO1: determine the kinetics of adsorption of oxalic acid on charcoal (K3).

CO2: evaluate the order of the reaction, temperature coefficient, and activation energy of the reaction by following pseudo first order kinetics. (K5).

CO3: construct the phase diagram of two component system forming congruent melting solid and find its eutectic temperatures and compositions. (K6).

CO4: develop the potential energy diagram of hydrogen ion, charge density distribution and Maxwell's speed distribution by computational calculation (K6).

UNIT-I: Kinetics

1. Study the kinetics of acid hydrolysis of an ester, determine the temperature coefficient and also the activation energy of the reaction.
2. Study the kinetics of the reaction between acetone and iodine in acidic medium by half-life method and determine the order with respect to iodine and acetone.
3. Determination of Association factor, distribution constant, association constant and mass of benzoic acid distributed between carbon tetrachloride and water.
4. Determination of rate constant of the redox reaction between KI and K2S2O8. Verification of Bronsted Bjerrum Equation

UNIT-II: Phase diagram

Construction of phase diagram for a simple systems

1. Chloroform- Acetic acid-Water
2. Naphthalene-phenanthrene
3. Benzophenone- diphenyl amine

Unit-III: Adsorption Studies

Adsorption of oxalic acid on charcoal & determination of surface area (Freundlich isotherm only).

Text Books:

1. B. Viswanathan and P.S. Raghavan, Practical Physical Chemistry, Viva Books, New Delhi, 2009.

2. Sundaram, Krishnan, Raghavan, Practical Chemistry (Part II), S. Viswanathan Co. Pvt., 1996.
3. V.D. Athawale and Parul Mathur, Experimental Physical Chemistry, New Age International (P) Ltd., New Delhi, 2008.
4. E.G. Lewers, Computational Chemistry: Introduction to the Theory and Applications of Molecular and Quantum Mechanics, 2nd Ed., Springer, New York, 2011.
5. K. Karunakaran, Laboratory Manuel for Physical Chemistry Practicals.

References:

1. J. B. Yadav, Advanced Practical Physical Chemistry, Goel Publishing House, 2001.
2. G.W. Garland, J.W. Nibler, D.P. Shoemaker, Experiments in Physical Chemistry, 8th edition, McGraw Hill, 2009.
3. J. N. Gurthu and R. Kapoor, Advanced Experimental Chemistry, S. Chand and Co., 1987.
4. Shailendra K Sinha, Physical Chemistry: A laboratory Manual, Narosa Publishing House Pvt, Ltd., New Delhi, 2014.
5. F. Jensen, Introduction to Computational Chemistry, 3rd Ed., Wiley-Blackwell.

TRAINING FOR COMPETITIVE EXAMINATION

23PCHS41

Semester-IV SEC-4 Hours/W: 4 Credits: 2

1. Chemistry for UGC-CSIR NET / SET/TRB (2 hours)
2. General studies for UPSC/TNPSC/ other competitive examinations (2 hours)

STAND

Semester-IV Ext. Activities Hours/W: 0 Credit:1

This is an compulsory extension activity for the students.

EXTRA CREDIT COURSES
INDUSTRIAL CHEMISTRY
Subject code: 23PCHEC1

Semester-I **ECC-1** **Hours/W: 0** **Credits:3**

Course Outcomes:

By the end of the Course the student will be able to

CO1: Understand the ethical, historic, philosophical, and environmental dimensions of problems and issues facing industrial chemists (K2)

CO2: Know about fuels, composition, carbonization of coal, gasification, liquefaction, and coal tar-based chemicals and layout for key processes in oil refining. (K1)

CO3. Summarizes the raw materials and manufacturing of glass and cement industry(K3)

CO4. Gain sound knowledge of inorganic materials like silicates, ceramics and cement (K1)

CO5. Conclude the role of petroleum and petrochemical industry, composition, applications, process-cracking. Increasing demand of non-petroleum fuels, synthetic fuels. Petrochemical.(K5)

CO6. Develop skills to estimate various components of fertilizers (K6)

UNIT- I: Cement and Ceramics

Cement -Composition-Types. Portland cement - Composition- Types- Manufacture (Wet and Dry process)-Uses,Setting of cement,Ceramics, Composition- Classification-Manufacture-Properties-uses

UNIT- II: Glass and Matches

Glass- Composition-Types-Formation operations -Melting-Blowing-Pressing-Annealing and finishing-Matches -Composition-Types-Manufacture -Safety matches

UNIT -III: Pigments, Dyes and Paints

Pigments-Classification-Manufacture-Uses, Dyes-Classification- Preparation-Dyeing processes, Paints- Composition-Types-Manufacture-Testing of Paints

UNIT – IV: Plastics and Fibres

Fibres- Natural- Synthetic fibres-Artificial silk-Rayon-Nylon-Trylene.Plastics-Composition-Classification-Manufacture-Properties -Uses

UNIT – V: Fertilizers and Fuels

Fertilizers- Organic fertilizers- Inorganic fertilizers -Preparation –Uses Fuels-Energy resources Industrial gases-Water gas- Producer gas-Oil gas, Natural gas-Coal gas-Gobar gas-Indane gas-Petroleum products and coal products.

Reference Books:

1. B.K. Sharma, Industrial Chemistry, Goel Publishing house Meerut.
2. R.K. Das, Industrial Chemistry.
3. C.N. Sawyer, P.L. McCarty and G.S. Parkin, Chemistry for environmental engineering and science.
4. F. W. Bilmayer, Text Book of Polymer Science, John Wiley & Sons, 1994.
5. A. Rudin, The Elements of Polymer Science and Engineering.
6. P. Ghosh, Polymer Science and Technology of Plastics and Rubbers.

FORENSIC CHEMISTRY

Subject code: 23PCHEC2

Semester: II **ECC-2** **Hours/W: 0** **Credits: 3**

Course Outcome:

By the end of the course the student will be able to

CO1: Examine the crime detection through analytical instruments (K1).

CO2: Understand the crime scene (K2).

CO3: Apply the techniques for forensic analysis(K3).

CO4: Classify the poisons in the living and the dead organisms (K4).

CO5: Evaluate the white-collar crimes(K5).

CO6: Develop the awareness on Aids - causes and prevention (K6).

UNIT I: Introduction to Forensic Science

Definition – history – facilities offered by various divisions of forensic laboratory expert– relevancy of expert opinion – value of expert evidence.

UNIT II: Scene of occurrence with Physical Evidence

Locard's principle of Exchange – preservation and recording of crime scene - search of evidence. Physical evidence – definition - sources and types of physical evidence – control sample - handling pacing , labelling, sealing, forwarding of physical evidence, Chain of evidence – special instruction for special types of exhibits.

UNIT-III: Forensic methods of Analysis

Simple organic analysis – chromatographic techniques – microscopy (comparison of stereoscopic, polarizing and scanning electron microscopy – x-ray diffraction – spectrophotometer. Demonstration: Paper chromatography & amp; TLC to analyse the ink.

UNIT - IV : Alcohol, Narcotics and Poisons

Alcohol and their effects on the body, collection of samples – drunken driving – determination of alcohol – Drug addiction – identification of drug addict – characteristics of drugs (Depressants, stimulants, Hallucinogens) – Toxicology - classification of poison – action of poison on body.

UNIT -V : White Collar Crimes

Characteristic of white collar crimes – classification and forensic investigation of white collar crimes – Cyber-crimes – mode and manner of committing cybercrime.

Reference Books:

1. Nabar B S, Forensic Science, SVP national police academy, Hyderabad.
2. Eckert G. William – Introduction to Forensic Sciences, CRC Press, Second Edition
3. Nanda and Tewari – Forensic Science in India A Vision for the 21st Century, Select Publisher,2001.
4. Saferstein Richard, Criminalistics – An Introduction to forensic science, Prentice Hall , Fifth Edition.

Health Chemistry
Subject code: 23PCHEC3

Semester: III **ECC-3** **Hours/W: 0** **Credits: 3**

Course Outcomes:

By the end of the course the student will be able to

CO1: Recall the basic biological and pharmacological interactions by using both natural products and total synthesis of bioactive molecules (K1).

CO2: demonstrate basic first aid skills needed to control bleeding, ill or injured person and immobilize injuries (K2).

CO3: develop skills to provide one- and two- person cardiopulmonary resuscitation to infants, children and adults (K3).

CO4: Compare the digestion and absorption of carbohydrates, processes involved in their metabolism and regulation of blood sugar (K4).

CO5: deduce the different types of blood lipid, discuss the metabolism of fatty acids and analyze the factors influencing the absorption of cholesterol (K5).

CO6: compile the function and properties of blood, bile pigments and bile acids (K6).

UNIT- I: Health

Definition: Food, Food Pyramid - Health-Hygiene- mal-, under- and overnutrition, their causes and remedies, sanitation, Carbohydrates -Protein- Classification and its Biological functions. Vitamins – Classification and its Biological functions.

UNIT- II: Drugs

Drugs-Types of drugs, Depressant, Anticonvulsant, Narcotics, Antipyretics, Antibiotics, Antiseptics, Analgesics, Muscle Relaxants, Cardiovascular, Vasodepressants, Steroids

UNIT- III: Body fluids

Blood Volume, Blood groups, Coagulation, Blood Pressure, Anemia, Blood Sugar, Hemoglobin- Chemistry Of Respiration-Urine-Electrolyte Balance.

UNIT IV: Enzymes, Hormones, Digestion

Types of enzymes, Enzyme Action, Characters of Hormones- Action, Examples of Essential Hormones-Digestion on Mouth- Stomach-Intestine-Pancreas, Mineral Metabolism

UNIT -V: First Aid for Accidents and Indian Medicinal Plants and Trees

Rules of first aid, Cuts, Abrasions and bruises, bleeding, fractures, burns, fainting, poisonous bites, First aid box, Antidotes for poisoning, Uses of Plant extracts for medicinal purposes - *Azadirachita indica*, *Adathoda Vasica*, *Hibiscus Rosasinensis*, *Cynodondactylon* and *Tinospora cordifoli.*

Reference Books:

1. Deb A C, Fundamentals of Biochemistry, New Central Book Agency, Calcutta, (1994).
2. Satake M and Mido Y, Chemistry for Health Science, Discovery Publishing House, New Delhi, (2003).
3. Jayashree Ghosh, A Text book of Pharmaceutical Chemistry, S. Chand and Co. Ltd, (1999).
4. Ashutosh Kar, Medicinal Chemistry, Wiley Eastern Limited, New Delhi, (1993).
5. Alex V Ramani, Food Chemistry, MJP Publishers, Chennai, (2009).

ENVIRONMENTAL CHEMISTRY

Subject code: 23PCHEC4

Semester: IV ECC-4 Hours/W: 0 Credits: 3

COURSE OUTCOMES:

By the end of the course the student will be able to

CO1: describe the effect of toxic elements on environmental and biological systems (K1).

CO2: demonstrate the knowledge of chemical and biochemical principles of fundamental environmental processes in air, water, and soil (K2).

CO3: Identify the different types of toxic substances & responses and analyse toxicological information(K3).

CO4: analyse the chemical processes involved in different environmental problems (air, water & soil) (K4).

CO5: appraise experimental methods for analysis of water and soil analysis and pollution awareness to society (K5).

CO6: predict the pollutions from diffract industry, pesticides and microorganism (K6).

UNIT – I: Environmental Chemistry

Concept and scope of Environmental Chemistry-Acid base reactions -pH and pOH- Ionic product of water- Common ion effect - Buffer solutions - Solubility and solubility product-Oxidation and reduction -Chemistry of Environmental Trace Elements: Pb, As, Hg and Cd

UNIT – II: Atmospheric Chemistry

Chemical composition of the atmosphere, Chemical and photochemical reactions in the atmosphere, Formation of smog, PAN, Acid rain, Oxygen and ozone chemistry, Catalytic decomposition process of ozone Concept of atmospheric aerosol Chemistry, Greenhouse gases

UNIT – III: Water Chemistry

Physical and chemical properties of terrestrial, Marine water and their environmental significance, Water quality parameters- Physical, chemical and biological, Distribution of chemical species in water; Gases, organic matter and humus matter in water.

UNIT – IV: Soil Chemistry

Chemical & mineralogical composition of soil, Physical properties of soil, Texture-Bulk density-Permeability, Chemical properties -Cation exchange capacity-pH, Macro and micro nutrients

UNIT -V: Chemistry of Organic compounds

Soap, Detergents, Bleaching agents, Chemistry of colloids, Hydrocarbons- PAH-PCBs, Phenols, Chlorofluorocarbons, Pesticides, chemical fertilizers.

Reference Books:

1. A. K. De, Environmental Chemistry.
2. B.K. Sharma, and H. Kaur, Environmental Chemistry.
3. S. E. Manahan, Environmental Chemistry.
4. J. W. Moore and E. A. Moore, Environmental Chemistry.
5. G. W. Vantoon & S. J. Duffy, Environmental Chemistry - A global perspective, Oxford university Press
6. H. Koren, Handbook of Environmental Health and Safety – Principle and practices, Vol. II, Lewis Publishers

Value Added Course

FUNDAMENTALS IN PHYTOCHEMISTRY

Subject code: 23PCHVA1

Semester: II **VA-1** **Hours/W: 0** **Credits: 3**

Course outcome

By the end of the course the student will be able to

CO1: Grasp the basic principles of Extraction methods (K1).

CO2: understand the separation methods and purification strategies involved in isolation of plant materials. (K2).

CO3: analyze the principles key concepts of phytochemistry and able to relate with other fields like agriculture and pharmacology (K3).

CO4: Detect the phytoconstituents using spectroscopic techniques. (K5).

CO5: Create a method to isolate of selected phytoconstituents from the plant source (K6).

Unit 1: Methods of Extraction: (6 Hrs)

Maceration, Percolation, Hot extraction. Continuous Soxhlet extraction and Super critical fluid extractions - its advantage and disadvantages. Special extraction methods - Microwave assisted extraction and Ultra sound extraction.

Unit 2: Methods of separation and isolation: (6 Hrs)

General introduction to separation techniques- liquid-liquid partition technique, solid-liquid partition methods. Chromatographic techniques – Paper – ascending and descending chromatography, Thin layer chromatography - radial chromatography and HPTLC, Column chromatography - Flash chromatography, HPLC and UPLC.

Unit 3: Identification and Characterisation of isolated compounds: (6 Hrs)

Methods of identifications- UV spectroscopy- chlorophyll, Cytochromes, anthocyanin and betacyanin and carotenoids. IR spectroscopy- stretching frequency of alkenes, aromatics, carbonyl groups, amines, cyanides and carboxylic acids. Mass spectroscopy- fragmentation peak and molecular ion peak and NMR spectroscopy chemical shifts and factors depends on chemical shifts of aromatics, hydroxyl groups and implication of NMR spectra.

Unit 4: Important Phytoconstituents: (6 Hrs)

Steroids, Terpenoids- isoprene units, Monoterpenes, sesquiterpenes diterpenes, triterpenes and tetraterpenes and its any two importance in drug discovery. Alkaloids- introduction, classification and its therapeutic and toxicological properties. Introduction to Flavonoids, Tannins, saponin, Essential oil, resin and glycosides.

Unit 5: Modern trends in Phytochemistry and Isolation: (6 Hrs)

Ethnopharmacology and drug design from Indian traditional medicinal plants. Relationship of phytochemistry with agriculture, pharmacology and ecology. Extraction of oil of cloves, Isolation of flavonoids (Rutin, Quercetin and kaempferol) and Tannin(gallic acid).

TEXT BOOKS AND REFERENCES

1. Ahmad, A. & Aqil, F., Phytochemistry: Fundamentals, Modern Techniques, and Applications
2. Harborne, J.B., Phytochemical methods, A Guide to Modern Techniques of Plant Analysis, 2nd edition, Chapman and Hall, London, New York, 1984.
3. Online databases like Kew's Medicinal Plant Database for practical exercises.