JAYARAJ ANNAPACKIAM COLLEGE FOR WOMEN (AUTONOMOUS)

A Unit of the Sisters of St. Anne of Tiruchirappalli

Accredited with 'A' Grade (3rd Cycle) by NAAC

DST - FIST Supported College Since 2015

(Affiliated to Mother Teresa Women's University, Kodaikanal)

PERIYAKULAM – 625 601, THENI DT.
TAMIL NADU.

M.SC. CHEMISTRY
2017 - 2020

DEPARTMENT OF CHEMISTRY

PROGRAMME OUTCOMES - P.G.

PO. NO.	UPON COMPLETION OF THIS PROGRAMME THE STUDENTS WILL BE ABLE TO
1.	Endow with in-depth knowledge, analyze and apply the understanding of their discipline for the betterment of self and society.
2.	Synthesize ideas from various disciplines, enhance the interdisciplinary knowledge and extend it for research.
3.	Gain confidence and skills to communicate orally/ verbally in research platforms and state a clear research finding.
4.	Develop problem solving and computational skills and gain confidence to appear the competitive examination.
5.	Enhance knowledge regarding research by accumulating practical knowledge in specific areas of research.
6.	Achieve idealistic goals and enrich the values to tackle the societal challenges.

PROGRAMME SPECIFIC OUTCOMES - P.G

PSO. NO.	UPON COMPLETION OF THIS PROGRAMME THE STUDENTS WILL BE ABLE TO	PO MAPPED
1	Apply the in depth knowledge about the chemical reactions, mechanisms, theories and to appreciate their applications in organic, inorganic and physical chemistry.	PO - 1
2	Utilize research skills for career in various sectors, academic or industry.	PO - 6
3	Apply problem solving skills and analytical skills and analyse the spectro photometric, analytical, electrometric and chromatographic measurements of compounds.	PO - 1 PO - 2 PO - 4
4	Assess the characteristics of organic and inorganic compounds by qualitative and quantitative skills.	PO - 1 PO - 3
5	Demonstrate small project works by applying their scientific knowledge and formulate the procedure for manuscript and dissertation writing.	PO - 3 PO - 5

PG COURSE PATTERN (2017 - 2020)

Sem.	Code	Title of the paper	Hours	Credits
I	17PCH1C01	Organic Chemistry-I	6	6
	17PCH1C02	Physical Chemistry-I	6	5
	17PCH1C03	Inorganic Chemistry-I	6	6
	17PCH1P01	Practical: Organic Analysis and Estimation	6	3
	17PCH1E1A/ 17PCH1E1B	Computers in Chemistry/ Nano Chemistry	6	4
Total			**30**	**24**
II	17PCH2C04	Organic Chemistry -II	6	5
	17PCH2C05	Physical Chemistry-II	6	6
	17PCH2P02	Practical: Inorganic Analysis and Estimation	6	3
	17PCH2E2A/ 17PCH2E2B	Inorganic Chemistry II / Engineering Chemistry	6	4
	17PCH2I01	Spectroscopy and Chromatography	4	3
	17PGS2S01	Soft Skills	2	1
Total			**30**	**22**
III	17PCH3C06	Organic Chemistry-III	6	5
	17PCH3C07	Physical Chemistry-III	6	5
	17PCH3C08	Inorganic Chemistry-III	6	6
	17PCH3P03	Practical: Physical Chemistry Experiments	6	3
	17PCH3E3A/ 17PCH3E3B	Analytical Chemistry/ Pharmaceutical Chemistry	6	4
Total			**30**	**23**
IV	17PCH4C09	Organic Chemistry -IV	6	5
	17PCH4C10	Physical Chemistry-IV	6	5
	17PCH4C11	Inorganic Chemistry- IV	6	5
	17PCH4R01	Project	12	6
	17PCH4A01	Comprehensive Examination	-	2*
Total			**30**	**21**
Total for all semesters			**120**	**90+2***

*Extra Credit

ORGANIC CHEMISTRY - I

Semester: I **Hours: 6**

Code : 17PCH1C01 **Credits: 6**

COURSE OUTCOMES:

- Interpret the reaction mechanisms based on the principles of bonding, linear free energy relationship, kinetic and thermodynamic aspects of organic reactions.
- Illustrate the concept of aromaticity using Huckel's rule.
- Acquire knowledge on reaction mechanism.
- Apply the knowledge on named reactions and rearrangements to solve the problems in competitive exams.
- Explain the preparation and properties of heterocyclic compounds.

UNIT I

THEORETICAL CONCEPTS OF BONDING AND REACTIVITY:

Types of bonding (ionic, covalent) - orbital theory - shapes - overlap of orbitals - formation of compounds - hybridization -factors influencing reactivity - inductive, electromeric, resonance, mesomeric, hyperconjugative and steric effect - hydrogen bonding - breaking and making of bonds - reaction intermediates (carbocation, carbanion, carbene and nitrene) - energetics of reactions (exergonic and endergonic reactions) energy profile diagram - rate of reactions - difference between transition state and intermediate, methods of determining reaction mechanism (kinetic and non kinetic methods) - Linear free energy relationships - Hammet equation - physical significance of σ , ρ - Taft equation **(18 Hours)**

UNIT II

a. AROMATICITY:

The concept of Aromaticity - aromatic, anti-aromatic and non aromatic compounds- Huckel's rule: Annulene, heterocyclic compounds, ions and polycyclic compounds

b. HETEROCYCLICS:

Preparation and properties of pyrimidine - antipyrine - pyrazole - thiazole - imidazole - isoxazole **(18 Hours)**

UNIT III

REACTION MECHANISM:

SUBSTITUTION REACTIONS: Electrophilic substitution in aromatic system - arenium ion mechanism - mechanisms of nitration, sulphonation, halogenation and Friedel craft alkylation reaction- Nucleophilic substitution in aliphatic system : S_N1, S_N2 , S_N^i, neighbouring group participation (halogen , oxygen, carbon - carbon double bond as neighbouring group) and SET mechanism, Aromatic nucleophilic substitution : Benzyne mechanism **(18 Hours)**

UNIT IV

a. REAGENTS IN ORGANIC SYNTHESIS:

Anhydrous $AlCl_3$, Aluminium isopropoxide, N-Bromo succinimide - Dicyclohexyl carbodiimide - DDQ - Phase transfer catalysts - Lithium diisopropylamide - OsO_4, Baker's yeast - SeO_2 - Lead tetra acetate - Per benzoic acid - Raney Nickel - Sodamide - Lithium Aluminium Hydride - Sodium borohydride -Wilkinson catalyst

b. NAMED REACTIONS:

Acyloin condensation -Birch reduction - Dieckmann - Elbs reaction -Ene reaction - Hofmann elimination - Mannich - Michael- Oppennauer oxidation - Stork enamine reaction - Woodward Prevost hydroxylation reaction - Wittig reaction - Clemmensen reduction **(18 Hours)**

UNIT V

REARRANGEMENTS:

Orton - Lossen - Beckmann, Fries, Favorskii - Curtius - pinacol-pinacalone- Benzillic acid - Baeyer-Villiger oxidation- Cope, Wagner-Meerwein - Claisen - Wolff - Neber - Schimidt-Stevens-Wittig rearrangement **(18 Hours)**

BOOKS FOR REFERENCE:

1. V. K. Ahulvalia, Organic Reaction Mechanisms, Narosa publishing House Pvt. Ltd, 4th edition, 2007 **Unit - I, II, III**
2. Peter Sykes, A guide book to mechanism in Organic chemistry, Pearson Education, 6th edition, 2007 **Unit - I, II**
3. Jerry March, Advanced Organic Chemistry, Reaction mechanism and structure, Wiley Inter science Publications, 6th edition, 2013 **Unit - I, II**
4. L. Finar, Organic chemistry, Vol - II, Pearson Education Ltd., 5th edition, 2012, **Unit - V**

5. S. Renuga, Name Reactionns and Reagents in Organic Synthesis, Vishal Publishing Co., 2016 **Unit - III & IV**

PHYSICAL CHEMISTRY - I

Semester: I **Hours: 6**

Code : 17PCH1C02 **Credits: 5**

COURSE OUTCOMES:

- Explain the fundamentals of molecular spectroscopy.
- Outline the physical aspects of microwave, FT - IR, UV-visible, NMR, ESR, Mossbauer and Raman spectroscopy.
- Apply the FT-IR, Uv-Visible and NMR spectral techniques in research project.
- Evaluate the applications of NMR spectroscopy in determining the structure and in medicine.
- Gain knowledge on the principles and techniques involved in photochemistry and radiation chemistry and formulate the physical processes of electronically excited molecules.

UNIT I: ROTATIONAL SPECTROSCOPY:

Basic aspects of spectroscopy - characterization of electromagnetic radiation - quantization of energy - regions of the spectrum - signal to noise ratio - the width and intensity of spectral lines - Fourier transform - stimulated emission - lasers - Microwave spectroscopy: rotation of molecules - selection rule - diatomic molecules - rigid and non - rigid rotator - the effect of isotopic substitution - linear polyatomic, symmetric top and asymmetric top molecules - microwave oven.

(18 Hours)

UNIT II: VIBRATIONAL SPECTROSCOPY:

Vibration of diatomic molecules - harmonic and anharmonic oscillators - zero point energy - force constant - fundamental absorption and overtones - Fermi resonance - vibration and rotation spectrum of carbon monoxide- vibrations of polyatomic molecules-fundamental vibrations and their symmetry-overtone and combination frequencies-influence of rotation on the spectra of polyatomic molecules - carbon dioxide - analysis by infra-red techniques

RAMAN SPECTROSCOPY:

Raman and Rayleigh scattering - Quantum and classical theories of Raman effect - polarization of light and the Raman effect -mutual exclusion rule - techniques and instrumentation **(18 Hours)**

UNIT III: ELECTRONIC SPECTROSCOPY:

Electronic spectra- electronic spectra of diatomic molecules - Born-Oppenheimer approximation - Franck - Condon principle - dissociation energy

ESR SPECTROSCOPY:

Introduction - instrumentation- ESR spectrum of an unpaired electron - g factor - hyperfine structure of ESR absorption - double resonance in ESR - applications to hydrogen, methyl, benzoquinone free radicals, anthracene and bis-salicylaldimine Cu (II) complex

MOSSBAUER SPECTROSCOPY:

Principles - instrumentation - the chemical shift - quadrupole effect - effect of a magnetic field-applications of iron and tin complexes **(18 Hours)**

UNIT IV

NMR:

Instrumentation-spin and applied field-nature of spinning particles-interaction between spin and a magnetic field-population of energy levels-Larmor precession-relaxation times-Fourier transform in NMR-spin-spin relaxation-spin-lattice relaxation-Hydrogen nuclei-chemical shift-coupling constant-coupling between several nuclei-chemical analysis by NMR technique-exchange phenomena-Nuclei other than Hydrogen-nuclei with spin½ -C^{13} NMR spectroscopy-nuclei with spin greater than ½-quadrapole effects- applications of NMR in medicine-MRI **(18 Hours)**

UNIT V

PHOTOCHEMISTRY AND RADIATION CHEMISTRY:

Physical properties of the electronically excited molecule: excited state dipole moments-excited state pKa, excited state redox potential - Jablonski diagram - Radiative and non radiative decays - Fluorescence, Phosporescence - photosensitisation and chemiluminescence-factors affecting quantum yield-fluorescence quenching-Stern Volmer equation-Experimental techniques in photochemistry - Flash photolysis technique. Radiation chemistry - interaction of radiation with matter, primary effects due to charged particles, linear energy transfer-radiolysis of water-the hydrated electron and its reactions (**18 Hours)**

BOOKS FOR REFERENCE:

1. N. Colin Banwell and M. Elaine McCash Fundamentals of Molecular spectroscopy TATA McGraw Hill Co., 4th edition, 2007 **Unit I-IV**
2. K.K. Rohatgi-Mukherjee, Fundamentals of Photochemistry, Wiely Eastern Ltd., **Unit V**
3. B.R. Puri, L.R. Sharma and S.Pathania, Principles of Physical Chemistry, Vishal Publishing Co., 46th edition, 2012 **Unit I -V**

4. R.S.Drago, Physical Methods in Inorganic Chemistry, W.B.Saunders Company, 1992

INORGANIC CHEMISTRY - I

Semester: I **Hours: 6**

Code : 17PCH1C03 **Credits: 6**

COURSE OUTCOMES:

- Use the periodic table to rationalize similarities and differences of elements, including physical and chemical properties and reactivity
- Explain the concept of the chemistry of lanthanides and actinides
- Describe the nature of bonding in different systems and Manipulate the octet rule and VSEPR theory
- Identify the structure of solid state, and Predict the structure of simple inorganic compound
- Explain the different types of semiconductors and super conductors

UNIT I

a. MODERN PERIODIC TABLE: Periodic law - extended long form of periodic table - groups and periods : general characteristics - classification of elements on the basis of electronic configuration

b. ATOMIC PROPERTIES: Periodicity of properties - size of atoms and ions - atomic radii and ionic radii - periodic trends in atomic radii and ionic radii - ionization energy - factors influencing ionization energy - electron affinity - periodic trends in electron affinity, electro negativity - factors influencing electro negativity

c. GENERAL CHARACTERISTICS OF S AND P- BLOCK ELEMENTS:

Metallic character - polarizing power - melting point and boiling point-oxidizing and reducing properties - electrode potential - oxidation state-diagonal relationship **(18 Hours)**

UNIT II

a.GENERAL CHARACTERISTICS OF D- BLOCK ELEMENTS:

Metallic character - polarizing power-melting point and boiling point - oxidizing and reducing properties - electrode potential - oxidation state - diagonal relationship - colored compounds - unusual magnetic behaviour -catalytic properties - formation of co-ordination compounds

b. GENERAL CHARACTERISTICS OF F- BLOCK ELEMENTS:

Lanthanides - occurrence - electronic configuration - oxidation states-ionic radii - colour and absorption spectra - magnetic properties - oxidation potential-basic character - solubility - double salts - chemical reactivity-complexes - uses.

Actinides - occurrence - electronic configuration - oxidation states - ionic radii - colour - complexes - comparison between lanthanides and actinides - extraction and separation of lanthanides and actinides **(18 Hours)**

UNIT III

IONIC BOND:

Nature of ionic bond - formation of ionic bond: NaCl- factors influencing ionic bonding - classification of Ionic structures: type AX (ZnS, NaCl, CsCl), AX_2 (CaF_2, TiO_2, SiO_2) - radius ratio rules - calculation of radius ratio: coordination number 3 (Planar triangle), 4 (tetrahedral), 6 (Octahedral) - decreasing energy in ionic bond- properties: physical state - electrical conductivity - melting and boiling points - solubility - stability - crystal structure - highly brittle - density - ionic reactions - isomorphism - polarization of ions and Fajans's rule- percentage of ionic character in a polar covalent bond - Hanny Smyth equation **(18 hours)**

UNIT IV

COVALENT BOND:

Lewis theory- Octet Rule (Shape of the Polyatomic molecule) - VSEPR theory- BF_3, NH_3, H_2O, PCl_3, ClF_3, SF_4, I^{3-}, SF_6 - hybridisation - isoelectronic molecules - covalent radii - MO approach to covalent bonding (hetero nuclear) diatomic CO, NO, HF - bond length, bond order and bond energy - bonding in (hetero nuclear) triatomic and polyatomic systems - CO_2 and NH_3, BeH_2 **(18 Hours)**

UNIT V

SOLID STATE CHEMISTRY:

Space lattices - unit cells - crystal system - Bravais lattices-space group-translational symmetry - relationship between molecular and crystallographic symmetry-X-ray diffraction - Bragg's method -rotating crystal method and powder method of X-ray diffraction - indexing of crystal planes - structure of graphite and diamond - spinels - normal and inverse types. Crystal defects - point, line and plane defects in solids - stoichiometric and non stoichiometric defects - Frenkel and Schotky defects

METALLIC BONDING - band theory-conductors-insulators-semiconductors-intrinsic and extrinsic-superconductivity **(18 Hours)**

BOOKS FOR REFERENCE:

1. James E. Huheey Inorganic Chemistry, Dorling Kindersley Pvt. Ltd., 4th edition, 2012 **Units I to V**
2. B.R. Puri, L.R. Sharma and K.C. Kalia, Principles of Inorganic chemistry, Milestone publishers and Distributor, Delhi, 31st edition, 2010 **Units I to V**
3. A.Abdul Jameel, Applications of physical methods to inorganic Compounds, 2007 **Unit V**
4. R.D. Madan, Modern Inorganic Chemistry, S. Chand and Company Ltd., 2nd edition, 2002 **Units I to V**
5. J.D. Lee, concise Inorganic Chemistry, Blackwell publishing, 5th edition, 1996 **Units III, IV**
6. Bodie Douglas, Darl McDaniel, John Alexander, Concepts and Models of Inorganic Chemistry, Wiley- India publishing, 3rd edition,2006 **Units III, IV**

PRACTICAL: ORGANIC ANALYSIS AND ESTIMATION

(Examination at the end of the I semester)

Semester: I **Hours: 6**

Code : 17PCH1P01 **Credits: 3**

COURSE OUTCOMES:

- Identify the organic compounds based on their characteristic qualities
- Apply the knowledge of separation of organic mixture using different solvents
- Demonstrate the quantitative estimation of organic compounds
- Enumerate the empirical skills
- Apply the methods for finding the quality of an organic compound

1. Separation of Organic Mixtures
2. Organic Analysis:

   Reporting aliphatic or aromatic, saturated or unsaturated, detection of elements, identification of functional groups, preparation of derivatives
3. Organic Estimation
   (a) Estimation of Phenol
   (b) Estimation of Aniline
   (c) Estimation of Ethyl Methyl Ketone

BOOKS FOR REFERENCE:

1. N.S.Gnanapragasam and G.Ramamurthy, Organic Chemistry Lab Manual S. Viswanathan Printers and Publishers Pvt.Ltd., 2007
2. Material prepared by the chemistry department

COMPUTERS IN CHEMISTRY

Semester: I **Hours: 6**

Code : 17PCH1E1A **Credits: 4**

COURSE OUTCOMES:

- Recognize microsoft related softwares and various computational methods
- Practice the skills in office automation programs
- Describe the basics of 'C' programming
- Apply 'C' programming to solve problems in chemistry
- Evaluate computer based application in analysis of experimental data

UNIT I

MS Word:

Starting Word - File menu - Edit menu - View menu - Insert menu - Format menu - Tools menu - Table menu

MS Excel:

Starting Excel - Formatting Worksheets - Editing cells Functions - Data management - Creating Charts **(18 Hours)**

UNIT II

MS POWERPOINT:

Starting Powerpoint - Powerpoint presentation - Transition Effects - Animation Effects

INTERNET:

Computer Networks - Internet - Common Internet Services **(18 Hours)**

UNIT III

INTRODUCTION :

Importance of C, Basic structure of C program, character set, key words and identifiers, variables and data types, declaration of variables, assigning values to variables, defining symbolic constants- operators, expressions, type conversions in expression, hierarchy of operations, Input and Output operations **(18 Hours)**

UNIT IV

CONTROL STATEMENTS:

if statement, calculation of pH of a solution, "if…else" statement-finding the largest of 3 numbers, Calculation of number of vibrational modes of linear and

non-linear molecules - switch statement- calculation of RMS, average and most probable velocity, conversion of centigrade to Fahrenheit and vice versa -"goto" statement - finding the sum of squares of 'n' numbers - while statement, do statement **(18 Hours)**

UNIT V

ARRAYS:

One dimensional-two dimensional - declaration and initialization of string variables - reading strings from terminal - writing strings to screen-string handling functions

STRUCTURES AND UNIONS:

Definition of structure-declaration of structure variable-union-definition-difference between structure and union

POINTERS (ELEMENTARY IDEA):

Understanding pointers, accessing the address of a variable **(18 Hours)**

BOOKS FOR REFERENCE:

1. K. V. Raman, Computers in Chemistry, Tata Mcgrew Hill **Unit V**
2. E. Balagurusamy, Programming in ANCI C 2nd edition Tata Mcgrew Hill **Unit III - V**
3. Sr. Helen Chandra, Fundamentals of computers and Office and Automation Acca Publishers, Periyakulam **Unit I - II**.

NANO CHEMISTRY

Semester: I **Hours: 6**

Code : 17PCH1E1B **Credits: 4**

COURSE OUTCOMES:

- Acquire fundamentals of nanomaterials.
- Explain preparation and modification of nanoparticles.
- Discuss the applications of nanochemistry and their advantages with respect to classical materials and device setups.
- Apply special risks pertaining to nanochemistry and provide perspectives on future nanochemistry developments and realize the destructive applications of nanomaterials in war.
- Work in interdisciplinary research groups.

UNIT I

Definition of Nano materials and Nano technology-size dependent properties of nano materials. alternate approaches for the preparation of nano materials-synthetic strategies-gas-phase evaporation method- matrix-isolation technique-sol-gel processing - properties of nano materials -formation of dangling bonds-atom like behavior of nano particles-physiochemical and optical properties

(18 Hours)

UNIT II

Nano medicines- introduction-diagnosis-fluorescent NP for biosensors and biolabelling quantum dots, devices based on nanotechnology for diagnosis-nano materials as therapeutic agents-drug delivery-dendrimers-carbon nano tubes and fullerenes- gene therapy-antimicrobial activity and wound healing-tissue engineering- artificial implants-cosmetics **(18 Hours)**

UNIT III

Nano technology in electronic communication and informatics-Semiconductor lasers, light emitting diode materials- wireless communication-lithography-solar cells(photovoltics) Nano materials for hydrogen production and conversion-fuel cells -rechargeble batteries **(18 Hours)**

UNIT IV

Nano materials for pollution abatement-sensors-green nano technology-purification through smart particles-nanoscale biopolymers-nano materials as catalysts in green manufacturing-protective measures against chemical and biological warfare agents-decontamination through nano materials-nano materials for next generation energy-storage and conversion devices **(18 Hours)**

UNIT V

Advanced nano materials-introduction to silicon and its applications-replace of silicon based components-substitutes to silicon-differences between silicon and carbon in nano field-new plastic resins-applications of nano materials in acid, base, photo and bio-catalysis **(18 Hours)**

COURSE BOOK:

Nano materials, B.Viswanathan, Narosa publishing house, New Delhi, 2013.

ORGANIC CHEMISTRY-II

Semester: II **Hours: 6**

Code : 17PCH2C04 **Credits: 5**

COURSE OUTCOMES:

- Recognize the concepts of Stereoisomerism.
- Acquire knowledge on Conformational Analysis.
- Interpret the uses of UV and IR Spectroscopic techniques.
- Analyze organic compounds using NMR Spectroscopy.
- Apply the principles of spectroscopy to solve the problems in competitive exams.

UNIT I: STEREOISOMERISM:

Chirality-stereoisomerism - axial chirality - planar chirality and helicity - stereochemistry of molecules with axial chirality - atropisomerism - biphenyls, allenes, spiranes and analogues - stereo specific and stereo selective synthesis - topocity and prostereo isomerism - topocity of ligands and faces - enantiotropic ligands and faces - diastereotopic ligands and faces-asymmetric synthesis-asymmetric induction **(18 Hours)**

UNIT II: CONFORMATIONAL ANALYSIS:

Conformations of ethane, n-butane, mono and disubstituted cyclohexanes - conformation and reactivity in acyclic systems - addition reactions - elimination reactions - anti elimination - syn elimination reactions. Conformation and reactivity in cyclic systems nucleophilic substitution reaction at ring carbon - addition reactions to double bonds - electrophilic addition and nucleophilic addition - elimination reactions -conformations of decalins mono and disubstituted decalins - conformations of perhydrophenanthrenes and perhydroanthracenes **(18 Hours)**

UNIT III

IR SPECTROSCOPY:

Molecular vibration, modes of vibration - factors influencing vibrational frequency - applications of IR - identity by finger printing - identification of functional groups

UV SPECTROSCOPY:

Theory of electronic spectroscopy - application to conjugated dienes, trienes, polyenes, α,β - unsaturated carbonyls and benzene and its substituted derivatives, heterocyclic system **(18 Hours)**

UNIT IV

^{1}H NMR SPECTROSCOPY:

Larmor precession - relaxation process - interaction between spin and magnetic field - Chemical shift - factors influencing Chemical shift - spin- spin splitting - coupling constant - vicinal and geminal coupling - NMR shift reagents - Nuclear Over Hauser effect - FT NMR

C^{13} NMR:

Introduction - chemical classes and chemical shifts: aliphatic, olefinic, alkyne, aromatic and carbonyl compounds - coupling constant - structural applications to C^{13} NMR **(18 Hours)**

UNIT V

MASS SPECTROSCOPY

Basic principles - theory - the molecular ion - determination of molecular formula - Mclafferty rearrangement - meta stable ions - nitrogen rule - fragmentation associated with functional groups Applications of IR, UV, NMR and Mass spectral techniques in structural elucidation of organic compounds **(18 Hours)**

BOOKS FOR REFERENCE :

1. D. N. Nasipuri, Stereochemistry of organic compounds, New Age International, 2nd edition, 2008 **Unit II, III.**
2. P. S. Kalsi Stereochemistry, conformation and mechanism, New Age International, 6th edition, 2011 **Unit I.**
3. Alex V Ramani, Leo A. Stanley, C. Mani, Stereochemistry MJP Publishers, 2012 **Unit I, II.**
4. Jag Mohan, Organic Spectroscopy Principles and Applications, Narosa Publishing House 2nd edition, 2012 **Unit IV, V.**
5. Robert M. Silverstein, Francis X. Webster - Wiley India, 6th edition, 2007 **Unit IV, V**

PHYSICAL CHEMISTRY - II

Semester: II **Hours: 6**
Code : 17PCH2C05 **Credits: 6**

COURSE OUTCOMES:

- Compile the various types of electrochemical reactions and their interactions.
- Explain the various features of molar conductance in electrochemistry.
- Apply the principles of electrochemistry to the kinetics of electrode process.
- Analyse the symmetry elements and symmetry operations of molecules.
- Create character table for point groups using G.O.T and apply group theory in hybridization, selection rule for electronic spectroscopy and vibrational spectra.

UNIT I: ELECTROCHEMISTRY - I

The nature of electrolytes - ion activity - ion-ion and ion-solvent interactions - Debye Huckel theory: evidences of ionic atmosphere, asymmetric effect, electrophoretic effect, Debye Huckel equation: derivation and verification of the equation - Debye Huckel Limiting law derivation, applications of Debye Huckel equation - ion association Falkenhagen effect, Wein effect **(18 Hours)**

UNIT II: ELECTROCHEMISTRY - II

Molar conduction, variation of molar conductivity with concentration, conductivity and ionic speeds, Relationship between molar conductivity and concentration: strong completely dissociated electrolytes, weak incompletely dissociated electrolytes, electrolyte systems showing ion paring- electrical migration and transport numbers: Hittorf's method, moving boundary method. Electrode - electrolyte interfaces, Significance of interaction between conducting phases, Electrical double layer: Helmholtz, Gouy chapman, Stern models **(18 Hours)**

UNIT III: ELECTROCHEMISTRY - III

Effect of electrolyte concentrations: Nernst equation, standard electrode potentials, emf of galvanic cells and feasible cell reactions - electrocapilllarity - kinetics of electrode process: Butler-Volmer equation, dependence of current density on over voltage: The Tafel equation, polarized and non-polarized electrodes - fuel cells - electronically conducting polymers **(18 Hours)**

UNIT IV: PRINCIPLES OF GROUP THEORY:

Symmetry elements - symmetry operations - properties of a group - Abelian, non - Abelian and cyclic groups - multiplication table C_{2v} - subgroups - class - products of symmetry operations-point groups - matrices for symmetry operations -

reducible and irreducible representations - statement of orthogonality theorem - properties of irreducible representation - construction of character table (C_{2v}, C_3 and C_{3v}) **(18 Hours)**

UNIT V: APPLICATIONS OF GROUP THEORY:

The relationship between reducible and irreducible representations-hybridization of atomic orbitals in molecules of different geometry - AB_4 tetrahedral, AB_3 triangular, AB linear molecules-symmetries of vibrational modes in non-linear molecules (H_2O, NH_3 and BF_3) - symmetries of vibrational modes in linear molecules (HCN, CO_2) - selection rules for vibrational transitions-pyramidal AB_3(excluding G and F matrices) - trans N_2F_2,CH_4 and SF_6-Mutual exclusion rule for molecules with centre of symmetry-use of group theory in determining the selection rules for the n-π* and π-π* transitions in formaldehyde **(18 Hours)**

BOOKS FOR REFERENCE:

1. D.R.Crow, Principles and applications of Electrochemistry, Chapman and Hall, London, 2nd edition, 1984 **Unit I-II**
2. Atkins, Physical Chemistry, Oxford University Press, 7th edition, 2006 **Unit II**
3. Raman, K.V. Group theory and its applications to Chemistry, TATA McGraw Hill Co, 4th edition, 2007 **Unit IV-V**.
4. F.Albert Cotton, Chemical applications of Group theory, Wiley Eastern Ltd, 3rd edition, 2004 **Unit V**.
5. B.R. Puri, L.R. Sharma S. Pathania, Principles of Physical Chemistry, Vishal Publishing Co. New Delhi 46th edition, 2012 **Unit I-V**

PRACTICAL: INORGANIC ANALYSIS AND ESTIMATION

(Examination at the end of semester II)

Semester: II **Hours: 6**

Code : 17PCH2P02 **Credits: 3**

COURSE OUTCOMES:

- Identify the common and less common metal ions present in the given mixture
- Acquire knowledge on EDTA titrations
- Estimate the hardness of the given sample of water
- Apply Beer-Lamberts' law in colorimetric estimation of metal ions
- Analyze the sample of water collected from different area

Analysis of mixture of cations including less familiar cations like Lithium, Thallium, Molybdenum, Thorium, Selenium, Tellurium, Uranium, Vanadium, Cerium, Zirconium

1. EDTA Titration: Estimation of magnesium, zinc, copper and nickel
2. Estimation of Hardness of water

COURSE BOOKS:

1. V. Venkateswaran, R. Veeraswamy and A. R. Kulandaivelu , Basic principles of Practical chemistry Sultan Chand and sons, 2nd edition, 2012
2. V.V. Ramanujam, Inorganic Semimicro Qualitative Analysis, The National Publishing Co., 3rd edition, 2012

INORGANIC CHEMISTRY - II

Semester: II **Hours: 6**

Code : 17PCH2E2A **Credits: 4**

COURSE OUTCOMES:

- Explain the concepts of acids, bases and non-aqueous solvents.
- Recognize the inorganic polymers, phosphates, related structure with bis chelating agents.
- Describe the concept of boranes and silicates
- Associate the chemistry of P-N and S-N heterocycles with inorganic chains, rings, cages and clusters.
- Recognize supra molecular chemistry and Discuss nuclear energy and its applications.

UNIT I: ACIDS AND BASES:

Introduction - Concepts of acids and bases - Arrhenius concept- Lowry-Bronsted - relative strengths of acids and bases and Lewis concepts - effect of solvent on acid strength and base strength - leveling effect on the basis of solvent system concept - hard and soft acids and bases - pearson concept - HSAB principles and applications

NON-AQUEOUS SOLVENTS:

Classification of solvents - protonic solvents - liquid ammonia and anhydrous hydrogen fluoride - chemical reactions - aprotic solvents - liquid sulphur dioxide and liquid dinitrogen tetroxide - chemical reactions **(18 Hours)**

UNIT II: INORGANIC POLYMERS:

General properties of Inorganic polymers - classification - homoatomic - heteroatomic condensation - addition polymers - coordination polymers - glass transition temperature - phosphorus based polymers - polydiethoxy phosphazines - polyphosphoryl chlorides - polyphosphates - metaphosphates - polyphosphates cross linked phosphates - ultraphosphate glasses - borophosphate glasses - uses of phosphorus polymers - polymeric sulphur nitride - chalogenide glasses - coordination polymers - chain polymers - two dimensional polymers - synthetic coordination polymers - polymers having phthalocyanine and related structure - polymers with bis chelating agents **(18 Hours)**

UNIT III: INORGANIC CHAINS, RINGS AND CAGES:

BORANES AND SILICATES: Borates - types of borates - structure of diborane - boranes - styx numbers - boranes and carboranes - Wades rule - boron nitride - borazines - silicates -types - beryl, talc, mica, zeolites, feldspar, ultramarine - preparation, properties and uses of silicones

P - N HETEROCYCLES: Synthesis of P-N skeleton - reactions of halo phosphazenes - hydrolysis - aminolysis - metathetical reactions - reactions with organo metallic reagents

S - N HETEROCYCLES: S - N heteroatom system-synthesis, properties and structure of sulphur nitrides **(18 Hours)**

UNIT IV: METAL CLUSTERS AND SUPRA MOLECULAR CHEMISTRY:

Introduction - carbonyl clusters - low and high nuclearity carbonyl clusters- electron counting scheme for HNCCs - halide type clusters - di, tri, tetra and hexa nuclear halide clusters - poly atomic zintil anions and cations - cherel phases - introduction - host - guest interaction - molecular and supra molecular self assembly - molecular recognition and complexation - supramolecular structures formed through coordination chemistry - the directional bonding approach - advantages and limitations - dinuclear macrcycles - molecular triangles, rectangles and molecular cages (Pd, Pt based) **(18 Hours)**

UNIT V: NUCLEAR CHEMISTRY:

General characteristics of radioactive decay, decay kinetics - nuclear model - nuclear shell model- nuclear liquid drop model - nuclear fusion-nuclear fission-neutron evaporation and spallation- nuclear reactors- thermal reactors - breeder reactor- reprocessing of spent fuels-recovery of uranium and plutonium-nuclear waste mangement- radio isotopes in analytical applications- direct isotope dilution analysis- nuetron activation analysis- radiation energy for chemical synthesis **(18 Hours)**

BOOKS FOR REFERENCE:

1. B.R. Puri, L.R. Sharma and K.C. Kalia, Principles of Inorganic Chemistry, Milestone publishers and Distributor, Delhi, 31st edition, 2010 **Units I -V**
2. James E. Huheey Inorganic Chemistry, Dorling Kindersley Pvt.Ltd., 4th edition, 2012. **Units I, II and IV**
3. R.D. Madan, Modern Inorganic Chemistry, S. Chand and Company Ltd, 2nd edition, 2002
4. H. R. Allcock, Phosphorous and Nitrogen compounds **Unit III**
5. E. Douglas, H.Mc Daniel, J. Alexander, Concepts and Models of Inorganic chemistry, 3rd edition, 2006 **Units I, IV and V**
6. Bradley, J.Hollidy, Chad. A. Mirkin. Supra molecular coordination chemistry - review - Strategies for the Construction of Supra molecular compounds through coordination chemistry, Angew. Chem. Int.ed.2001, 14, 2022 to 2043. **Unit IV**

7. H. J. Arnikar Essentials of Nuclear Chemistry, New Age international, 4th edition, 2007 **Unit V**
8. R.L. Madan, G.D. Tuli, Inorganic Chemistry, S.Chand's puplishing 1999

ENGINEERING CHEMISTRY

Semester: II **Hours: 6**

Code : 17PCH2E2B **Credits: 4**

COURSE OUTCOMES:

- Associate the engineering aspects of chemistry
- Develop skills in water treatment
- Recognize the chemistry of explosives and propellants
- Describe the characteristics of refractories and abrasives
- Explain the various classes of lubricants and abrasives

UNIT I: WATER TREATMENT:

Effect of water on rocks and minerals - hard and soft water - units of hardness - scale and sludge formation in boilers - disadvantages of scale formation - prevention of scale formation - caustic embrittlement - boiler corrosion - priming and foaming - chemical coagulants used in drinking water - desalination of brackish water **(18 Hours)**

UNIT II: CORROSION:

Corrosion of metals - disadvantages - various forms of corrosion: Underground or soil corrosion, pitting corrosion, waterline corrosion, stress corrosion, microbiological corrosion, erosion corrosion - factors influencing corrosion - metal cladding, metal spraying and cementation - chemical conversion coatings **(18 Hours)**

UNIT III: EXPLOSIVES AND PROPELLANTS:

Explosives - characteristics - classification of explosives - example and properties of the various classes :primary explosives, low explosives, high explosives, plastic explosives - uses of explosives - precautions during storage of explosives, blasting fuses - safety fuse and detonating fuse - rocket propellants - characteristics of a good propellant - classification of propellants - biopropellants **(18 Hours)**

UNIT IV: REFRACTORIES:

Introduction - characteristics - classification of refractories - properties of refractories - manufacture of refractories - conditions leading to failure of a refractory material - common refractory bricks - classification, example and properties - insulating refractories - cermets **(18 Hours)**

UNIT V: LUBRICANTS AND ABRASIVES:

Introduction - function of a lubricant - mechanism of lubrication - classification of lubricants - synthetic lubricants - cutting fluids abrasives - natural and artificial abrasives **(18 Hours)**

BOOKS FOR REFERENCE:

1. P. C. Jain and Monica Jain, Engineering Chemistry, Dhanpat Rai Publishing Company, 12th edition, 1998 **Units I - V**
2. R. Gopalan, D. Vengappayya, S. Nagarajan, Engineering Chemistry, Vikas Publishing House Pvt. Ltd., 1999

SPECTROSCOPY AND CHROMATOGRAPHY

Semester: II **Hours: 4**

Code : 17PCH2I01 **Credits: 3**

COURSE OUTCOMES:

- Gain knowledge on basic principles of spectroscopy.
- Explain the theory of transitions in ultra violet spectroscopy and fundamentals of vibrational spectroscopy.
- Describe the basic concepts in NMR with focus on chemical shift, shielding and deshielding and spin-spin splitting.
- Comprehend the basics of mass spectroscopy and its applications and Apply spectral techniques in elucidation of structure.
- Analyze the physical properties and the structural features of compounds and demonstrate and classify chromatographic techniques.

UNIT I: INTRODUCTION:

Introduction - Electromagnetic radiations - units - Electromagnetic spectrum - absorption and emission spectra - atomic and molecular spectra - Types of molecular spectroscopy

INFRARED SPECTROSCOPY:

Introduction - principle of Infra-red spectroscopy - Theory- Molecular vibrations - vibrational frequency - number of fundamental vibration - selection rules - factors influencing vibrational frequencies - identification of functional groups - finger print region - applications of IR spectroscopy: distinction between two types of hydrogen bonding - study of keto-enol tautomerism and conformational analysis

(12 Hours)

UNIT II: UV - VISIBLE SPECTROSCOPY:

Introduction - the absorption laws - theory of transitions - the chromophore concept - auxochrome - types of absorption bands - effect of conjugation - woodward fishers rules for calculating absorption maximum (λ_{max}) in dienes and α,β unsaturated carbonyl compounds - applications of UV spectroscopy

(12 Hours)

UNIT III: H^1 NMR SPECTROSCOPY:

Introduction - Larmor precision - relaxation, process - Interaction between - spin and magnetic field - chemical shift - factors influencing chemical shift - spin-spin splitting - NMR shift reagent - applications of NMR spectroscopy - simple problems of nuclear magnetic resonance **(12 Hours)**

UNIT IV: MASS SPECTROSCOPY:

Basic principles - theory - molecular ion - determination of molecular formula - Mclafferty rearrangement - metal stable ions - nitrogen rule - general fragmentation modes - simple problems in mass spectroscopy.

Applications of IR, UV, NMR and Mass spectral techniques in structural elucidation of simple organic compounds **(12 Hours)**

UNIT V: CHROMATOGRAPHY:

Introduction - classification - thin layer chromatography - paper chromatography - column chromatography- High Performance Liquid Chromatography - Gas chromatography - Gas Chromatography mass spectrometry : Introduction and Instrumentation **(12 Hours)**

BOOKS FOR REFERENCE:

1. Y.R Sharma, Elementary Organic Spectroscopy, Reprint, Sultan Chand and Sons, 1st Edition, 2011 **Unit I - IV**
2. V.K.Srivastava, K.K.Srivastava, Introduction to Chromatography, S.Chand and Company Ltd., 3rd Edition, 1985 **Unit V**

SOFT SKILLS

Semester: II **Hours: 2**

Code : 17PGS2S01 **Credit: 1**

COURSE OUTCOMES:

- Develop their social, interpersonal, cognitive, ethical, professional, reading and communication skills.
- Increase their self-esteem and confidence.
- Achieve their short and long term goals.
- Prepare and formulate their resumes wisely.
- Face the mock group discussions and interviews with a challenge and choose their right career.

UNIT I: SOFT SKILLS

Introduction - Soft skills - Importance of soft skills - Selling your soft skills - Attributes regarded as soft skills - Soft skills - Social - Soft skills - Thinking - Soft skills - Negotiating - Exhibiting your soft skills - Identifying your soft skills - Improving your soft skills - will formal training enhance your soft skills - Soft Skills training - Train yourself - Top 60 soft skills - Practicing soft skills - Measuring attitude. **(6 Hours)**

UNIT II: CAREER PLANNING

Benefits of career planning - Guidelines for choosing a career - Myths about choosing a career - Tips for successful career planning - Developing career goals - Final thoughts on career planning - Things one should know while starting career and during his/her career. **(6 Hours)**

UNIT III: ART OF LISTENING AND SPEAKING

Two ears, one mouth - Active listening - Kinds of Listening, Common - poor listening habits - Advantages of listening - Listening Tips. Special features of Communication - Process - Channels of Communication - Net Work - Barriers - Tips for effective communication and Powerful presentation - Art of public speaking - Public Speaking tips - Over coming fear of public speaking. **(6 Hours)**

UNIT IV: ART OF READING AND WRITING

Good readers - Benefits - Types - Tips - The SQ3R Technique - Different stages of reading - Rates of Reading - Determining a student's reading rate - Increasing reading rate - Problems with reading - Effective reader - Importance of writing - Creative writing - Writing tips - Drawbacks of written communication. **(6 Hours)**

UNIT V: PREPARING CV / RESUME

Meaning - Difference among Bio-data, CV and Resume - The terms - The purpose of CV writing - Types of resumes - Interesting facts about resume - CV writing tips - CV/Resume preparation - the dos - CV/Resume preparation - the don'ts - Resume check up - Design of a CV - Entry level resume - The content of the resume - Electronic resume tips - References - Power words - Common resume blunders - Key skills that can be mentioned in the resume - Cover letters - Cover letter tips. **(6 Hours)**

COURSE BOOK:

Dr. K. Alex, Soft Skills, Chand & Company Pvt. Ltd., New Delhi.

REFERENCE BOOK:

1. Dr. T. Jeya Sudha & Mr. M.R. Wajida Begum : Soft Skills/Communication Skills, New Century Book House (P) Ltd., Chennai.
2. S. Hariharen, N. Sundararajan & S.P. Shanmuga Priya : Soft Skills, MJP Publishers, Chennai.

SOFT SKILLS

Semester: II **Hours: 2**

Code : 17PGS2S01 **Credit: 1**

QUESTION PATTERN

Part - A	3 Questions to be answered out of 5	Each Carries 4 marks	12 Marks
Part - B	2 Questions to be answered out of 4	Each Carries 9 marks	18 Marks

The Components of Internal Assessment for Soft Skill are as follows

Components	Marks
Test - I	30

Test - II	30
Mock Interview	30
Communication Skill	10
Total	**100**

ORGANIC CHEMISTRY - III

Semester: III **Hours: 6**

Code : 17PCH3C06 **Credits: 5**

COURSE OUTCOMES:

- Acquire knowledge on photochemistry vision and photo dynamic therapy.
- Illustrate the concept of pericyclic reaction in organic synthesis.
- Gain knowledge about the mechanistic pathways of sigmatropic and electrocyclic reactions.
- Apply the knowledge on photochemistry and pericyclic reactions to solve the problems in competitive exams.
- Discuss about the importance of Bioorganic Chemistry.

UNIT I: PHOTOCHEMISTRY I

Introduction - energy of molecule - thermal and photochemical energy - electronic transitions - electronic excitation and molecular orbital view of excitation - Jablonski diagram - organic photosensitisers - quenchers - photochemical reactions of carbonyl compounds: Norrish type I, Norrish type II reactions - α and β cleavage of acyclic and cyclic compounds - intramolecular hydrogen abstraction - intermolecular photo reduction - photo cycloaddition of ketones with unsaturated compounds (Paterno-Buchi reaction) - photo dimerisation of α, β - unsaturated ketones. **(18 Hours)**

UNIT II: PHOTOCHEMISTRY II

Photo rearrangement of enones, dienones, epoxy - ketone - photo Fries rearrangement - di -π methane rearrangement of 1,4 - pentadienes, 3- phenyl alkenes - oxa-di - π methane rearrangement - photo reduction of naphthalene - photo oxidation of butene - cis - trans isomerisation of alkenes (Trans-stilbene) - sensitized cis-trans isomerisation - dimerisation of alkenes (norborane-1, 5-dienes) - photoisomerisation of aromatic compounds (benzene, o-xylene) - Barton reaction - Hofmann - Loeffler - Freytag reaction - photochemistry of vision - photo dynamic therapy. **(18 Hours)**

UNIT III: PERICYCLIC REACTIONS I

Introduction - molecular orbitals of conjugated polyenes, ions and radicals - theory of pericyclic reactions (Frontier molecular orbital method) - stereochemistry (con - dis rotatory motion) - electrocyclic reactions of 4nπ (1, 3 - butadiene) and (4n + 2) π {1, 3, 5 - hexatriene} systems - correlation diagram - Woodward - Hoffmann rule - Huckel-Mobius method. **(18 Hours)**

UNIT IV: PERICYCLIC REACTIONS II

Cycloaddition - theory (FMO method) - (2+2), (4+2) cycloadditions (thermal and Photo induced) - selection rule - Diels-Alder reactions - correlation diagram - Woodward -Hoffmann rule - Huckel-Mobius method - cyclo reversion - 1,3 - dipolar cycloadditions - (4+2) cycloadditions of cations and anions - sigmatropic rearrangement: [1,3], [3,3] - mechanism - selection rule - Cope rearrangement - Claisen rearrangement. **(18 Hours)**

UNIT V: BIOORGANIC CHEMISTRY

Biomimetic chemistry - crown ethers - molecular recognition between crown ethers and specific cations - cyclodextrins - hosts as enzyme mimics - supramolecular chemistry - molecular recognition - molecular self assembly - supramolecular devices - function of insulin - enzymes - general nature of enzymes - nomenclature and classification - cofactors - specificity of enzyme action. **(18 Hours)**

BOOKS FOR REFERENCE:

1. Jagdamba Singh and Jaya Singh, Photochemistry and Pericyclic reactions, New age International Pvt. Ltd, 2nd edition, 2008. **(Unit I - IV)**
2. P. S. Kalsi and J. P. Kalsi, Bioorganic and Supramolecular Chemistry, New Age international, 4thedition, 2008. **(Unit V)**
3. I.L. Finar, Organic Chemistry, volume II, Dorling Kindersley, 5th edition, 2008. **(Unit V)**

PHYSICAL CHEMISTRY - III

Semester: III **Hours: 6**

Code : 17PCH3C07 **Credits: 5**

COURSE OUTCOMES:

- Recognize the concepts of quantum chemistry.
- List the postulates of quantum mechanics and explain their importance.
- Apply quantum mechanical treatment to solve Schrodinger equation for multi electron atom.
- Classify the types of polymers and polymerization and explain the kinetics of polymerization.
- Explain microstructure of polymers and apply various polymer processing technique in the field of Industry.

UNIT I: QUANTUM CHEMISTRY- I

Introduction - wave and particle nature of radiation - de Broglie equation - wave equation - Heisenberg's principle of uncertainty - Schrodinger wave equation derivation - wave function - properties of ψ - conditions of normalization and orthogonality - orthonormal set - Eigen function and Eigen values - operators: addition, subtraction, multiplication, commutator, linear operator, vector operator, Laplacian operator, Hermitian operator and Hamiltonian operator. **(18 Hours)**

UNIT II: QUANTUM CHEMISTRY- II

Schrodinger equation for solving a particle in a 1D box and 3D box - normalization and orthogonality - characteristics of wave function- one dimensional harmonic oscillator - rigid rotor - hydrogen atom - hydrogen atomic orbital - energy of the hydrogen atom and the iso electronic ions. **(18 Hours)**

UNIT III: QUANTUM CHEMISTRY- III

Postulates of quantum mechanics - theorems relating to basic postulates - approximation methods for solving the Schrodinger equation for multi electron atoms : time independent perturbation theory - first order perturbation theory to helium atom - variation theorem - application of variation method to helium atom - Hartree and Hartree - Fock self consistent field method. **(18 Hours)**

UNIT IV: POLYMER CHEMISTRY I

Introduction, chain polymerization, free radical polymerization, ionic polymerization, co-ordination polymerization - Ziegler - Natta catalyst - step condensation - poly condensation, poly addition, kinetics of polymerization: free radical chain polymerization, equation for kinetic chain length, degree of polymerization, cationic polymerization, anionic polymerization - micro structures based on chemical structure and geometrical structure. **(18 Hours)**

UNIT V: POLYMER CHEMISTRY II

Definition of number average and weight average molecular weight - molecular weight determination: cryoscopy - ebulliometry - end group analysis - viscometry - sedimentation velocity method - molecular weight distribution curve - glass transition temperature - transition and associated properties - factors influencing glass transition temperature - crystallinity in polymers - degree of crystallinity - structural regularity and crystallisability - polymer degradation: types, thermal and mechanical degradation - elastomeric materials - fibre forming materials - polymer processing: calendaring - casting(die casting, rotational casting) - injection moulding. **(18 Hours)**

BOOKS FOR REFERENCE:

1. A.K. Chandra, Introductory Quantum Chemistry, TATA McGraw Hill Publishing Company Ltd., New Delhi, 4th edition, 1997. **(Unit I - III)**
2. V.R. Gowarikar, N.V. Viswanathan and Jayadev Sreedhar, Polymer Science, New Age International, reprint 2005. **(Unit IV and V)**

FOR FURTHER REFERENCE:

1. N. Levine, Quantum Chemistry, Prentice Hall of India, Pvt Ltd., 4th edition, 1994. **(Unit I - III)**
2. D.A. McQuarrie, Quantum Chemistry, Viva Books Pvt. Ltd., 2007. **(Unit I - III)**
3. G. S. Misra, Introductory Polymer Chemistry, Wiley Eastern Ltd., 1993. **(Unit IV - V)**
4. B.R. Puri, L.R. Sharma and Madan S. Pathania, Principles of Physical Chemistry, Vishal Publishing Co, 47th edition, 2016. (**Unit I - V)**

INORGANIC CHEMISTRY - III

Semester: III **Hours: 6**

Code : 17PCH3C08 **Credits: 6**

COURSE OUTCOMES:

- Apply theories of bonding and magnetic properties to co-ordination compounds
- Describe the reactions, kinetics and mechanisms of co-ordination compounds
- Explain the different types of magnetic behaviour and their measurement
- Gain knowledge about the spectral properties and application of co-ordination compounds
- Explain the physical methods to inorganic Compounds

UNIT I: CO-ORDINATION COMPOUNDS -I

Co-ordination numbers - co-ordination geometries - isomerism - chelate effect - bonding in co-ordination compounds - crystal field theory - crystal field effect on O_h, T_d and Square planar - factors affecting the magnitude of Δ - spectrochemical series - applications of crystal field theory - Nephelauxetic series - Jahn - Teller effect -ligand field theory - molecular orbital theory - sigma bonding - Pi bonding. **(18 Hours)**

UNIT II: CO-ORDINATION COMPOUNDS - II

Reactions, kinetics and mechanisms: Rate of reaction - rate law - inert and labile complexes - thermodynamic and kinetic stability - mechanism of substitution reactions in octahedral complexes - anation - aquation - acid and base hydrolysis - substitution reactions in square planar complexes - the trans effect -mechanism of redox reactions - outer sphere mechanism -inner sphere mechanism. **(18 Hours)**

UNIT III: CO-ORDINATION COMPOUNDS - III

Electronic spectroscopy: Electronic configuration - term symbols - effect of distortion and spin orbit coupling on electronic spectra - spin multiplicity - derivation of term symbols - term symbols for p^2 and d^2 systems - calculation of

microstates - electronic spectra of transition metal complexes - selection rules - splitting of orbitals in O_h field - ground states of free ions for d^n system and energy level diagrams - Orgel diagram - Tanabe - Sugano diagram - difference between orgel and Tanabe Sugano diagram- calculation of B and 10 Dq - Charge transfer spectra. **(18 Hours)**

UNIT IV: MAGNETO CHEMISTRY OF TRANSITION METAL COMPEXES

Introduction - orbital magnetic moment - spin magnetic moment - diamagnetism - paramagnetism - measurement of magnetic susceptibility: Guoy's method - Faraday's method - ferromagnetism and antiferromagnetism - magnetic behavior of transition metal complexes - paramagnetic properties of metal ions - valance bond approach to magnetic behavior - limitations - crystal field approach to magnetic behavior - quenching of orbital angular momentum. **(18 Hours)**

UNIT V: PHYSICAL METHODS TO INORGANIC COMPOUNDS

IR and Raman spectroscopy: Introduction-selection rules (combination and hot bands) - mutual exclusion principle - difference between Raman and IR spectroscopy - application in structural elucidation of simple molecules: N_2F_2, NO_3^- - vibrational spectra of metal carbonyl complexes - geometry and number of stretching vibrations.

EPR Spectroscopy: g - value - Zero - field splitting - Krammer's degeneracy - applications to VO (II), Co (II), Ni (II) and Cu (II) complexes. **(18 Hours)**

BOOKS FOR REFERENCE:

1. E. Huheey James, Inorganic Chemistry, Principles of structure and reactivity, Dorling Kindersley India Pvt. Ltd., 4th edition, 2007. **(Unit I - III)**
2. B.R. Puri, L.R. Sharma and K.C. Kalia, Principles of Inorganic Chemistry, Milestone publishers and Distributor, Delhi, 32nd edition, 2015. **(Unit III and IV)**
3. A. Abdul Jameel, Applications of physical methods to inorganic compounds, 2007. **(Unit III and V)**

PRACTICAL: PHYSICAL CHEMISTRY EXPERIMENTS

(Examination at the end of III Semester)

Semester: III **Hours: 6**

Code : 17PCH3P03 **Credits: 3**

COURSE OUTCOMES:

- Develop the ability to apply the knowledge and skills in conductometric and potentiometric titrations and equivalent conductance studies
- Evaluate heat of solution, adsorption characteristics and Arrehenius parameters for kinetic study
- Check the validity of Ostwald's dilution law and Debye Huckel Bronsted equation
- Recognize the link between theory and practical
- Undertake hands on lab work which develop problem solving skills in project and for their successful career

1. Conductometric Titration (Mixture of acids Vs Strong base)
2. Verification of Ostwald's dilution law and determination of dissociation constant of weak acid
3. Determination of equivalent conductance of a strong electrolyte at infinite dilution
4. Potentiometry - Precipitation titrations
5. Kinetics of Iodination of acetone
6. Adsorption characteristics of oxalic acid on charcoal
7. Determination of Arrhenius Parameters - Hydrolysis of methyl acetate by acid
8. Verification of Huckel-Bronsted equation
9. Enthalpy of solution by Thermometric method

BOOKS FOR REFERENCE:

1. V. Venkateswaran, R. Veeraswamy and A. R. Kulandaivelu, Basic principles of Practical chemistry, Sultan Chand and Sons, 2nd edition, 1997.
2. B. Viswanathan, P.S. Raghavan, Practical Physical Chemistry, Viva Books Private limited, Ist edition, 2014.

ANALYTICAL CHEMISTRY

Semester: III **Hours: 6**
Code : 17PCH3E3A **Credits: 4**

COURSE OUTCOMES:

- Recognize the progress and development in analytical field
- Gain knowledge about the analytical techniques
- Utilize the various electro analytical techniques for separation
- Analyze the modern methods of separation and estimation
- Apply the thermo analytical methods to gravimetric analysis

UNIT I: COLORIMETRY AND SPECTROPHOTOMETRY

Theory of spectrophotometry and colorimetry - determinations with UV - Visible spectrophotometers - colorimetry - photoelectric colorimeter - colorimetric determination of iron and nickel - spectrophotometry - description of apparatus - spectrophotometric titration - atomoic absorption spectroscopy - elementary theory - instrumentation. **(18 Hours)**

UNIT II: SEPARATION TECHNIQUES

Ion - exchange process: introduction - action of ion exchange resins - ion exchange chromatography - chelating ion exchange resins - applications in analytical chemistry: separation of zinc and magnesium on an anion exchanger, determination of fluoride by cation exchanger- Gas chromatography: principles and applications - High Performance Liquid Chromatography(HPLC): principle, instrumentation, modes, procedure and applications. **(18 Hours)**

UNIT III: THERMAL ANALYSIS

Thermo analytical methods: Thermo Gravimetric Analysis (TGA) - apparatus - factors affecting thermogram - applications of TGA - Differential Thermal Analysis (DTA) - apparatus - applications - comparison of TGA and DTA - principles of thermometric titrations - apparatus - applications -Differential Scanning Colorimetry (DSC). **(18 Hours)**

UNIT IV: ELECTRO ANALYTICAL TECHNIQUES

Voltammetry: principles - linear sweap voltammetry, cyclic voltammetry, differential pulse voltammetry - applications - electrodes and electrolytes -

polarography: basic principles, direct current polarography, commercial polarographs, determination of lead and copper in steel. **(18 Hours)**

UNIT V: DATA ANALYSIS

Limitation of analytical methods - classification of errors - accuracy - precision - how to reduce systematic errors - significant figures - mean and standard deviation - distribution of random errors - reliability of results - confidence interval - comparison of results - t - test -f- test. **(18 Hours)**

BOOKS FOR REFERENCE:

1. G.H. Jeffery, J. Bassett, J. Mendham and R.C. Denney, A Text book of Quantitative Inorganic Analysis including elementary instrumental analysis, ELBS publishers, 4th edition, 1978. **(Unit I - V)**
2. Williard D. Merit, Instrumental methods of Analysis, CBS publishers, 7th edition, 2007. **(Unit IV)**
3. J. Mendham, R.C. Denny, J.D. Barnes M J K Thomas, Vogel's textbook of quantitative chemical analysis, 6th edition, 2005. (**Unit V)**

FOR FURTHER REFERENCE:

1. P. C. Jain & Monica Jain, Engineering Chemistry, Dhanpat Rai Publishing Company, 17th edition, 2008. (**Unit I - V)**
2. Chatwal Anand, Instrumental methods of Chemical Analysis, Himalaya Publishing House, 2nd edition, 1984. **(Unit I - V)**

PHARMACEUTICAL CHEMISTRY

Semester: III **Hours: 6**

Code : 17PCH3E3B **Credits: 4**

COURSE OUTCOMES:

- Associate the knowledge on drug action with metabolism
- Describe the various aspects of pharmaceutical chemistry
- Discuss the importance, classification and characteristics of drugs
- Gain knowledge about stereo chemical nomenclature
- Recognize the importance of chemotherapy for treating diseases

UNIT I: SYNTHETIC DRUGS

Introduction: characteristics of drugs - development of synthetic drugs - nature and sources of drugs - some important terminology: pharmacy, pharmacology, medicinal chemistry, pharmacodynamics, pharmacokinetics, molecular pharmacology, pharmacophore, antimetabolites, actinomycetes, bacteria, virus, fungi, mutation, chemotherapy, pharmacopocia, pharmacopocia, pharmacognosy, toxicology, pharmacotherapcutics. **(18 Hours)**

UNIT II: BIOLOGICAL CLASSIFICATION OF DRUGS

Biological classification - drugs acting on central nervous system and peripheral nervous system - chemotherapeutic drugs - pharmaco dynamic agents - metabolic disease and endocrine function - chemical classification of drugs.

STEREOCHEMICAL NOMENCLATURE

D and L system - R-S system - Z-E isomerism. **(18 Hours)**

UNIT III: DRUG ACTION:

Mechanism of action: extracellular site - cellular sites - drug receptors and biological responses - drug receptor binding-metabolism of drugs - phase I and phase II - biotransformation on the pharmacological activity - absorption of drugs - routes of administration - factors affecting absorption. **(18 Hours)**

UNIT IV: ORGANIC PHARMACEUTICAL AIDS:

Preservatives - antioxidants - emulsifying agents: colouring, flavouring and sweetening agents, stabilizing and suspending agents - ointment bases and related agents - solvents. **(18 Hours)**

UNIT V: THERAPEUTIC AGENTS:

Anti - cancer agents: Types of tumours - some common causes of cancer - spread of cancer - treatment of cancer-structure, uses and adverse effects of chlorambucil and methotrexat.

Sulpha drugs: Preparation, properties and therapeutic uses of sulphanilamide, sulphadiazine and sulphapyridine.

Antibiotics: Classification of antibiotics - chloroamphenicol: properties and therapeutic uses - penicillin - types - therapeutic uses - tetracyclines - types - therapeutic uses. **(18 Hours)**

BOOKS FOR REFERENCE:

1. O.D Tyagi M. Yadav, A Text book of synthetic drugs, Anmol publications, 1st edtion, 1990. **(Unit II and V)**
2. Jeyashree Ghosh, Text book of Pharmaceutical Chemistry, S. Chand Company Ltd., 1st edition, 1997. **(Unit I, III and IV)**

ORGANIC CHEMISTRY - IV

Semester: IV **Hours: 6**

Code : 17PCH4C09 **Credits: 5**

COURSE OUTCOMES:

- Apply the knowledge on retro synthesis and disconnection approach to solve the problems in competitive exams.
- Elucidate the structure of alkaloids and terpenoids.
- List out the importance of hormones.
- Discuss about the structure and functions of steroids.
- Classify vitamins, flavones and carotenoids.

UNIT I: ORGANIC SYNTHESIS

Synthons and synthetic equivalents - nucleophilic and electrophilic synthons - Umplong reactions - routine functional group transformations and interconversions of simple functionalities - retro synthesis - disconnection approach - formation of C-C, C-O and C-N bonds - organo magnesium and organo boron compounds - Robinson annulation reaction - linear and convergent synthesis - protection and deprotection - chemo and regioselectivities.

(18 Hours)

UNIT II: TERPENOIDS

Physiological and bio-synthesis of citral and geraniol - structural elucidation of myrcene and α - pinene.

ALKALOIDS

Physiological and bio - synthesis of nicotine, atropine, papavarine, morphine- structural elucidation of cocaine and papavarine. **(18 Hours)**

UNIT III: STEROIDS AND HORMONES

Steroids - Introduction - function of steroids and sterols - isolation and biological function of bile acids - source, properties and colour reactions of cholesterol. Hormones - introduction - differences between hormones and vitamins - classification of hormones - sex hormones - oestrogens - gestrogens, progesterone and testosterone - structure and functions (no structural elucidation)

- adrenocortical hormones - relationship to physiological activity - non - steroid hormones - adrenaline, thyroxine - biosynthesis of oestrogens. **(18 Hours)**

UNIT IV: VITAMINS

Introduction - Discovery - Classification and nomenclature of vitamins - Isolation, biological functions and avitaminoses of Vitamin A,B, B_2, B_6, B_{12}, C, D, E, H and K - constitution of vitamin A, C and K_2 - provitamins. **(18 Hours)**

UNIT V: FLAVONES AND FLAVONOLS

Introduction - occurrence - isolation, general properties and basic unit in flavones and flavonols - general methods for determination of the structure offlavones taking flavone as an example - constitution of quercetin - structural relationship between flavonols (queretin), anthocyanidins (cyaniding chloride) and catechins - biogenetic relationship between flavonols, anthocyanidins and catechins.

CAROTENOIDS

Introduction - classification - isolation and separation - characteristics of carotenoids - principal methods in elucidating the constitution of carotenoids - functions of carotenoids - constitution of γ - carotene and Xanthophyll. **(18 Hours)**

BOOKS FOR REFERENCE:

1. Stuart Warren, Organic Synthesis: The Disconnection Approach, Wiley India Pvt. Ltd., Reprint, 2016. **(Unit I)**
2. Francis A. Carey and Richard J. Sundberg Advanced Organic Chemistry Part B: Reactions and Synthesis, Springer Science, 5th edition, 2007. **(Unit I)**
3. W. Carruthers, Some modern methods of organic synthesis, Cambridge University Press, 3rd edition, 1986. **(Unit I)**
4. O.P. Agarwal, Chemistry of Organic Natural products-volume II, Prentice Hall, 33rd edition, 2008. **(Unit II)**
5. I.L. Finar, Organic Chemistry, volume II, Dorling Kindersley, 5th edition, 2008. **(Unit II - V)**
6. Gurdeep R Chatwal, Organic Chemistry of natural products-volume II, Himalaya Publishing house, New Delhi, 4th edition, 2006. **(Unit II - V)**

PHYSICAL CHEMISTRY - IV

Semester: IV **Hours: 6**
Code : 17PCH4C10 **Credits: 5**

COURSE OUTCOMES:

- Formulate the theories of reaction rates in chemical kinetics and apply the theories to decomposition of acetaldehyde and N_2O_5.
- Explain the concepts of catalysis and surface chemistry.
- Apply the principles of catalysis and adsorption for their practicals and research project.
- Discuss the various features of chemical thermodynamics and different phenomena in irreversible thermodynamics.
- Formulate the distribution of molecules by Maxwell Boltzmann, Fermi Dirac and Bose Einstein statistics and explain Debye and Einstein model of heat capacity of solids.

UNIT I: THEORIES OF REACTION RATES

Kinetic theory of collisions - steric factor - theory of absolute reaction rate - theory of unimolecular reactions: Lindemann - Christianson hypothesis, Hinshelwood's treatment Rice - Rampserger-Kassel (RRK) treatment and Marcus extension of RRK treatment (RRKM) - reactions in solutions: transition state theory - substituent and correlation effects - Hammett equation - chain reactions: general characteristics - study of kinetics of chain reactions like decomposition of acetaldehyde and N_2O_5.

(18 Hours)

UNIT II: CATALYSIS AND SURFACE CHEMISTRY

Homogeneous Catalysis: mechanism of acid base catalysis - acidity function - catalysis by enzyme - Michaelis - Menten kinetics - reactions in flow systems: techniques for very fast reaction -stopped flow method- relaxation methods - T - jump and P- jump methods - reactions on surface: physical and chemical adsorption - Langmuir and BET adsorption isotherm - Gibbs adsorption isotherm - micelles: surface active agents - classification of surface active agents - micellization. **(18 Hours)**

UNIT III: CHEMICAL THERMODYNAMICS

Fugacity - methods of determining the fugacity of a real gas - activity - choice of standard states - determination of activity and activity coefficients of electrolytes and non - electrolytes by vapor pressure measurement - determination of activity of electrolytes by cryoscopic method - determination of activity coefficients from solubility measurements - introduction to irreversible thermodynamics - phenomenological laws and Onsager's reciprocal relations - conservation of mass and energy in closed and open systems - microscopic reversibility and Onsager reciprocal relations - verification of the Onsager relation. **(18 Hours)**

UNIT IV: STATISTICAL THERMODYNAMICS - I

Probability and most probable distribution - Ensemble averaging - permutations - combinations - Maxwell - Boltzmann statistics - negative temperature - partition functions:translational, rotational, vibrational and electronic partition functions - Thermodynamic properties in terms of partition function:Internal energy, Entropy, Enthalpy and Free energy - equilibrium constant of an ideal gas in terms of partition function. **(18 Hours)**

UNIT V: STATISTICAL THERMODYNAMICS - II

Quantum statistics - Fermi Dirac and Bose Einstein statistics - Heat capacities of diatomic gas - quantum statistical theory of specific heat - rotational partition function of hydrogen molecule and nuclear spin - statistical thermodynamics of ortho and para hydrogen - application of Bose - Einstein statistics to black body radiation - heat capacity of solids - Einstein and Debye models of heat capacity of solids. **(18 Hours)**

BOOKS FOR REFERENCE:

1. K.J. Laidler, Chemical Kinetics, Pearson Education Inc., 3rd edition, 2007. **(Unit I - III)**
2. Kuriacose and Rajaram, Thermodyamics, Jalandar Shoban Lal Co.,1993 **(Unit IV and V)**
3. B.R. Puri, L.R. Sharma and Madan S.Pathania, Principles of Physical chemistry, Vishal Publishing Co, 47th edition, 2016. **(Unit I - V)**

FOR FURTHER REFERENCE:

1. M.C. Gupta, Statistical Thermodynamics, Wiley-Eastern Limited, Madras 1997.
2. Rajaram and Kuriacose, Kinetic and mechanism of chemical transformation, Macmillan, India, 1993.

INORGANIC CHEMISTRY - IV

Semester: IV **Hours: 6**

Code : 17PCH4C11 **Credits: 5**

COURSE OUTCOMES:

- Explain the role of inorganic substances in living systems and the use of metal ions in medicinal therapy and diagnosis.
- Acquire knowledge in organometallic compounds
- Apply the organometallic catalysts in industrial sector
- Classify the toxification and detoxification of metal
- Explain the principles involved in inorganic photochemistry

UNIT I: BIOINORGANIC CHEMISTRY I

Introduction - role of Na, K(sodium pump), Mg , Ca(calcium pump), V, Cr, Mn, Fe, Co, Ni, Cu, Zn, Mo, Pt, Hg and Pb metal ions in biological systems - metalloenzymes: Zn enzymes - carboxy peptidase A and carbonic anhydrase - vitaminB_{12} - photosynthesis - chlorophyll - nitrogen fixation - metal toxification, detoxification and chelate therapy - anticancer drug: cis-platin. **(18 Hours)**

UNIT II: BIOINORGANIC CHEMISTRY II

Energy sources for life - metalloporphyrins and respiration: cytochrome P450 - dioxygen binding, transport and utilization: interaction between heme and dioxygen - binding of dioxygen to myoglobin - structure and function of hemoglobin - other biological dioxygen carriers: hemerythrin - hemocyanine -

electron carriers: Fe-S proteins (rubredoxin and ferridoxin) - blue copper proteins - iron storage and transport: ferritin and transferring. **(18 Hours)**

UNIT III: ORGANO METALLIC CHEMISTRY-I

The 18 electron rule - metal carbonyl complexes - structures of mono and poly nuclear metal carbonyls - concept of isolobality and isolobal analogies - nitrosyl complexes - dinitrogen complexes - metal alkyls - carbenes- carbines - carbides - non - aromatic alkene- alkyne complexes - allyl and pentadieny complexes - metallocenes - molecular orbital of metallocenes - structure of cyclopenta dienyl complexes - synthesis of cyclopentadienyl complexes-arene complexes. **(18 Hours)**

UNIT IV: ORGANO METALLIC CHEMISTRY - II

Reactions of organo metallic compounds: Substitution reactions in carbonyl complexes - oxidative addition and reductive elimination-insertion and elimination - nucleophilic and electrophilic attack of coordinating ligands

Catalysis by organometallic compounds: homogenous and heterogenous catalysts - alkene hydrogenation- synthesis gas - hydroformaylation - wacker process - Zeigler - Natta catalyst. **(18 Hours)**

UNIT V: INORGANIC PHOTOCHEMISTRY

Electronic transitions in metal complexes: metal - centred, intra ligand and charge transfer transitions - photophysical processes of coordination compounds - Jablonski diagram - photochemical reactions of coordination compounds: oxidation - reduction, photo isomerisation, photo substitution, photoanation, unimolecular charge transfer reactions - photochemistry of cobalt(III) complexes - ligand field photochemistry of chromium(III) complexes - Adamson's rules - photochemistry of ruthenium - polypyridine complexes, organometallic compounds and metal carbonyl compounds - bimolecular reactions - unimolecular reactions - photochemistry of compounds with metal - metal bonding. **(18 Hours)**

BOOKS FOR REFERENCE:

1. E. Huheey James, Inorganic Chemistry, Principles of structure and reactivity, Dorling Kindersley India Pvt. Ltd., 4th edition, 2007. **(Unit I - IV)**
2. B.R. Puri, L.R. Sharma and K.C. Kalia, Principles of Inorganic Chemistry, Milestone Publishers 32nd edition, 2015. **(Unit I- IV)**

3. A. Abdul Jameel, Applications of physical methods to inorganic compounds, 2007. **(Unit V)**
4. S. Arunachalam, Inorganic photochemistry, Kala publications, 2002. **(Unit V)**
5. E. Douglas, H.Mc Daniel, J. Alexander, Concepts and Models of Inorganic Chemistry, 3rd Edition, 2006. **(Unit V)**

PROJECT

Semester: IV **Hours: 12**

Code : 17PCH4R01 **Credits: 6**

COURSE OUTCOMES:

- Identify the thrust areas in Research
- Demonstrate the different analytical skills used in characterization of compounds
- Compile the project work
- Develop the presentation skills through reviews
- Provide confidence to take up a task

GROUP PROJECT - MAXIMUM 3 STUDENTS

THE INTERNAL COMPONENTS OF PROJECT WORK- MAXIMUM 50 MARKS

Components	Marks
First review	10
Second review	10
Final review (Internal viva voce)	30
Total	**50**

COMPREHENSIVE EXAMINATION

Semester: IV

Code : 17PCH4A01 **Credits: 2**

COURSE OUTCOMES:

- Gain in depth knowledge in chemistry
- Develop problem solving skills in organic, inorganic, physical and interdisciplinary chemistry
- Discuss the different aspects of learning
- Gain confidence to take up CSIR- NET/ SET examinations
- Appear for various competitive examinations

QUESTION PATTERN

M.Sc. Chemistry

Blue print of question paper (External)

Time 3 hours **Max. Marks: 60**

Section	Types of Question	Number of Qns.	Number of Qns. to be answered	Marks for each Qn.	Total
A Q. No(1-10)	Two from each unit	10	10	1	**10**
B Q. No(11-15)	Five either or qn - one from each unit	5	5	4	**20**
C Q. No(16-20)	Open choice - One from each unit	5	3	10	**30**