St. PETER'S UNIVERSITY

St. Peter's Institute of Higher Education and Research
(Declared under section 3 of UGC Act 1956)
Avadi, Chennai – 600 054.

M.Sc. (CHEMISTRY) PROGRAMME

(Full Time)

(I to IV SEMESTERS)

REGULATIONS AND SYLLABI

REGULATIONS – 2014

(Effective from the Academic Year 2014-'15)

M.Sc. CHEMISTRY

Regulations -2014

Regulations and Syllabi

(Effective from the Academic Year 2014-'15)

1. **Eligibility:** A Candidate who has passed B.Sc. Examination with Chemistry as main subject of study of the University or any of the B.Sc. Degree Examination with specialization such as Industrial Chemistry, Applied Chemistry, or any other specialization in Chemistry of other University recognized by this University as equivalent thereto, are eligible for admission to Two Year M.Sc. Programme in Chemistry.

2. **Duration**: Two years

3. **Medium:** English is the medium of instruction and examination.

4. **Weightage for Continuous and End Assessment:** The weightage for Continuous assessment (CA) and End Assessment (EA) be 25: 75 unless the ratio is specifically mentioned in the scheme of Examinations.

5. **Credit System:** Credit system be followed with 18 credits for each semester and each credit is equivalent to 25 hours of effective study provided in the Time Table.

6. **Scheme of Examinations**

I Semester

Code No.	Course Title	Credit	Marks		
Theory			**CA**	**EA**	**Total**
114CMPT01	Organic Chemistry-I	4	25	75	100
114CMPT02	Inorganic Chemistry-I	4	25	75	100
114CMPT03	Physical Chemistry-I	4	25	75	100
114CMPE01	**Elective – I** Chromatographic Techniques	2	25	75	100
114CMPE02	**Elective – II** Bioorganic Chemistry	2	25	75	100
Practical					
114CMPP01	Inorganic Chemistry Practical	2	25	75	100
	Total	**18**	**150**	**450**	**600**

II Semester

Code No.	Course Title	Credit	Marks		
Theory			**CA**	**EA**	**Total**
214CMPT01	Organic Chemistry-II	4	25	75	100
214CMPT02	Inorganic Chemistry-II	4	25	75	100
214CMPT03	Physical Chemistry-II	4	25	75	100
214CMPE01	**Elective – III** Analytical Techniques in Chemistry	2	25	75	100
214CMPE02	**Elective – IV** Bioinorganic Chemistry	2	25	75	100
Practical					
214CMPP01	Organic Chemistry Practical	2	25	75	100
	Total	**18**	**150**	**450**	**600**

III Semester

Code No.	Course Title	Credit	Marks		
Theory			**CA**	**EA**	**Total**
314CMPT01	Organic Chemistry-III	4	25	75	100
314CMPT02	Inorganic Chemistry-III	4	25	75	100
314CMPT03	Physical Chemistry-III	4	25	75	100
314CMPE01	**Elective – V Nanoscience and Nanotechnology**	2	25	75	100
314CMPE02	**Elective – VI Polymer Chemistry**	2	25	75	100
Practical					
314CMPP01	Physical Chemistry Practical	2	25	75	100
	Total	**18**	**150**	**450**	**600**

IV Semester

Code No.	Course Title		Credit	Marks		
Theory				**CA**	**EA**	**Total**
414CMPT01	Organic Chemistry-IV		4	25	75	100
414CMPT02	Inorganic Chemistry-IV		3	25	75	100
414CMPT03	Physical Chemistry-IV		3	25	75	100
Practical						
414CMPP01	Analytical Chemistry Practical		2	25	75	100
Project						
414CMPP02	**Project Work**	Dissertation	6	25	65	100
		Viva			10	
	Total		**18**	**125**	**375**	**500**

LIST OF ELECTIVES

S.No.	Code No.	Subject	Credit
1.	114CMPE01	Chromatographic Techniques	2
2.	114CMPE02	Bioorganic Chemistry	2
3.	214CMPE01	Analytical Techniques in Chemistry	2
4.	214CMPE02	Bioinorganic Chemistry	2
5.	314CMPE01	Nanoscience and Nanotechnology	2
6.	314CMPE02	Polymer Chemistry	2
7.	314CMPE03	Industrial Electrochemistry	2
8.	314CMPE04	Corrosion and Corrosion Control	2
9.	314CMPE05	Supramolecular Chemistry and Crystal Engineering	2
10.	314CMPE06	Pharmaceutical Chemistry	2

Note: Any six subjects to be chosen as electives.

7. **Passing Requirements:** The minimum pass mark (raw score) be 50% in End Assessment (EA) and 50% in Continuous Assessment (CA) and End Assessment (EA) put together. No minimum mark (raw score) in Continuous Assessment (CA) be prescribed unless it is specifically mentioned in the Scheme of Examination.

8. **Grading System:** Grading System on a 10 Point Scale be followed with 1 mark = 0.1 Grade point to successful candidates as given below.

CONVERSION TABLE

(1 mark = 0.1 Grade Point on a 10 Point Scale)

Range of Marks	Grade Point	Letter Grade	Classification
90 to 100	9.0 to 10.0	O	First Class
80 to 89	8.0 to 8.9	A	First Class
70 to 79	7.0 to 7.9	B	First Class
60 to 69	6.0 to 6.9	C	First Class
50 to 59	5.0 to 5.9	D	Second Class
0 to 49	0 to 4.9	**F**	**Reappearance**

Procedure for Calculation

Cumulative Grade Point Average (CGPA) = $\frac{\text{Sum of Weighted Grade Points}}{\text{Total Credits}}$

$= \frac{\sum (CA+EA)\, C}{\sum C}$

Where Weighted Grade Points in each Course = Grade Points (CA+EA) multiplied by Credits

$= (CA+EA)C$

Weighted Cumulative Percentage of Marks(WCPM) = CGPAx10

C- Credit, CA-Continuous Assessment, EA- End Assessment

9. **Pattern of the Question Paper for Theory Subjects:** The question paper for End Assessment will be set for three hours and for the maximum of 100 marks with following divisions and details.

Part A: 10 questions (with equal distribution to all units in the syllabus). Each question carries 2 marks.

Part B: 5 questions with either or type (with equal distribution to all units in the syllabus). Each question carries 16 marks.

10. **Effective Period of Operation for the Arrear Candidates:** Two Year grace period is provided for the candidates to complete the arrear examination, if any.

Registrar

11. Syllabus

I Semester

114CMPT01 - ORGANIC CHEMISTRY - I

UNIT - I : STEREOCHEMISTRY

Optical activity and chirality. Classification of chiral molecules as asymmetric and dissymmetric. A brief study of dissymmetry of allenes, biphenyls, spiro compounds, trans cyclooctene and cyclononene and molecules with helical structures. Absolute configuration - R, S notation of biphenyls and allenes. Fischer projection. Inter conversion of Sawhorse, Newman and Fischer projections. Molecules with more than one asymmetric center (restricted to five carbons) E.g. Erythro and threo compounds. Asymmetric synthesis, Crams's rule. Geometrical isomerism. E, Z nomenclature of olefins, Geometrical and optical isomerism (if shown) of disubstituted cyclopropane, cyclobutane and cyclopentanes. Identification of enantiotopic, homotopic, diastereotopic hydrogens and prochiral carbons in compounds containing up to ten carbons only, Stereo specific and stereo selective reactions.

UNIT - II : CONFORMATIONAL ANALYSIS

Conformation of some simple, 1, 2-disubstituted ethane derivatives. Conformational analysis of disubstituted cyclohexanes and their stereo chemical features [geometric and optical isomerism (if shown) by these derivatives]. Conformation and reactivity of substituted cyclohexanols (oxidation andacylation), cyclohexanones (reduction) and cyclohexane carboxylic acid derivatives (esterification and hydrolysis). Conformation and stereochemistry of cis and trans decalin and 9-methyl decalin.

UNIT - III : ALIPHATIC NUCLEOPHILIC SUBSTITUTION REACTIONS

Kinetic and Non-Kinetic methods of determining organic reactions mechanisms. Hammet equation. Derivation and free energy relationship. Simple problems. Taft equation SN1, SN2 and SNi mechanism - Neighbouring group participation - reactivity, structural and solvent effects - substitution in norbornyl and bridgehead systems - substitution at allylic and vinylic carbons - substitution by ambident nucleophiles such as CN, N02, phenoxide and ambident dianions - substitution at carbon doubly bonded to oxygen and nitrogen - alkylation and acylation of amines, halogen exchange, Von-Braun reaction, alkylation and acylation of active methylene carbon compounds, hydrolysis of esters, Claisen and Dieckmann condensations.

UNIT - IV : NUCLEOPHILIC SUBSTITUTION REACTIONS

Nucleophilic substitution at carbon doubly bonded to oxygen and nitrogen - alkylation and acylation of amines, halogen exchange, Von-Braun reaction, alkylation and acylation of active methylene carbon compounds, hydrolysis of esters, Claisen and Dieckmann condensations Aromatic Nucleophilic Substitution Methods for the generation of benzyne intermediate and reactions of aryne intermediate - Nucleophilic substitution involving diazonium ions. Aromatic Nucleophilic substitution of activated halides. Ziegler alkylation. Chichibabin reaction.

UNIT - V : AROMATIC ELECTROPHILIC SUBSTITUTION REACTIONS

The arenium ion mechanism. Orientation and reactivity (ortho, meta and para directing groups). . Typical reactions to be studied - nitration, halogenation, alkylation, acylation and diazonium coupling. Formylation reactions - Gatterman, Gatterman-Koch, Vilsmeyer-Hack & Reimer-Tieman Reaction. Synthesis of di & tri substituted benzenes (symmetrical tribromobenzene, 2-Amino-5-methylphenol, 3-nitro-4-bromobenzoicacid, 3, 4-dibromonitrobenzene, 1, 2, 3 - trimethylbenzene) starting from benzene or any mono substituted benzene. Electrophilic substitution of furan, pyrrole, thiophene pyridine and pyridine-N-oxide.

References

1. D.Nasipuri, 1994, Stereochemistry of Organic Compounds, 2nd Edition, Wiley Eastern Ltd, New Delhi
2. PS.Kalsi, 1993, Stereochemistry,Conformation Analysis and Mechanism, 2nd Edition, Wiley Eastern Ltd, Chennai
3. P.S. Kalsi, 1994, Stereochemistry and Mechanism Through Solved Problems Wiley Eastern Ltd.
4. Niel Isaacs, 1987, Physical Organic Chemistry, ELBS Publications

114CMPT02 - INORGANIC CHEMISTRY - I

UNIT - I : BONDING IN INORGANIC COMPOUNDS

Poly acids: Isopolyacids and heteropolyacids of vanadium, chromium, molybdenum and tungsten. Inorganic Polymers: Silicates, structure - properties - correlation and applications - molecular sieves polysulphur - nitrogen compounds and poly - organophosphazenes.

UNIT - II: BORON CHEMISTRY

Boron hydrides: Polyhedral boranes, hydroborate ions, carboranes and metallo carboranes. Metal Clusters: Chemistry of low molecularity metal clusters (upto) trinuclear metal clusters; multiple metal-metal bonds.

UNIT - III : THEORIES OF COORDINATION COMPOUNDS

Crystal field theory and its limitations, d-orbital splittings, LFSE, spectro chemical series, evidences for metal ligand orbital overlap, molecular orbital theory and energy level diagrams, concept of weak and strong fields, Jahn-Teller distortion, charge-transfer spectra.

UNIT - IV : SPECTRAL STUDIES OF COMPLEXES

Spectral and magnetic properties of complexes.Term states for dn - ions, energy diagrams, d-d transitions, Orgel and Sugano - Tanabe diagrams, -spin orbit coupling, nephelauxetic effect, spectral and magnetic characteristics of transition metal complexes. Applications of IR, RAMAN,ESR, Massbauer, ORD to study of Coordination compounds.

UNIT - V : STABILITY AND STEREO ISOMERISM OF COORDINATION COMPLEXES

Stability of complexes: thermodynamic stability – stepwise and overall stability constants, their relationships, factors affecting the stability of the complexes, HSAB approach , chelate effect, importance of chelates. Macrocyclic ligands; types; schiff bases; crown ethers; cryptands; Chelating agents; types of EDTA titrations; direct and back titrations; replacement titrations; masking and demasking reagents. Determination of stability constants by spectrophotometric, polarographic and potentiometric methods. Stereochemical aspects; Stereoisomerism in inorganic complexes; isomerism arising out of ligand and ligand conformation; chirality and nomenclature of chiral complexes; optical rotatory dispersion and circular dichroism.

References

1. F.A. Cotton and G. Wilkinson, 1988, Advanced Inorganic Chemistry - A Comprehensive Text, V. Edition, John Wiley & Sons.
2. D.A. Skoog, 1985, Principles of Instrumental methods of Analysis, III Edition, Saunders College Publication.
3. Willard Merrit, Dean and Settle, 1986, Instrumental methods of Analysis, VI Edition CBS Publication.
4. A.I. Vogel, 1985, 1976, Text Book of Qualitative Inorganic Analysis, ELBS III Edition, and IV Edition.
5. K.V. Raman, 1993, Computer in Chemistry, Tata McGraw Hill, New Delhi.
6. K. Ebert, H. Ederes and T.L. Isenhowr, Computer Applications in Chemistry, VCH.

114CMPT03 - PHYSICAL CHEMISTRY - I

UNIT - I : CHEMICAL KINETICS - I

Effect of temperature on reaction rates-collision theory of reaction rates-molecular beams-collision cross sections-effectiveness of collisions-probability factors-potential energy surfaces-partition functions and activated complex. Eyring equation-estimation of free energy, enthalpy and entropy of activation and their significance.

UNIT - II : CHEMICAL KINETICS - II

Reactions in solutions-effect of pressure, dielectric constant and ionic strength on reactions in solutions-kinetic isotope effects-linear free energy relationships-Hammett and Taft equations-Acid base catalysis-mechanism of acid base catalysed reactions-Bronsted catalysis law.

UNIT - III : GROUP THEORY I

Symmetry elements and symmetry operations-point groups-identification and determination-reducible and irreducible representations-Direct product representation-orthogonality theorem and its consequences-character table.

UNIT - IV : GROUP THEORY II

Hybrid orbital in non-linear molecules (CH_4, XeF_4, BF_3, SF_6 and NH_3). Determination of representations of vibrational modes in non-linear molecules (H_20, CH_4, XeF_4, BF_3, SF_6 and NH_3) Symmetry selection rules for infrared, Raman and electronic Spectra. Electronic Spectra of Ethylene and formaldehyde-application of group theory.

UNIT - V: QUANTUM CHEMISTRY - I

Inadequacy of classical theory -, black body radiation, photo electric effect - the Compton effect - Bohr's Quantum theory and subsequent developments -wave particle duality- de Broglie equation, Heisenberg uncertainty principle.

References

1. G.K. Vemulapalli, 2000, Physical Chimistry, Prentice - Hall.
2. J. Rajaram and J.C. Kuriacose, 1993, Kinetics and mechanism of chemical transformations, MacMillan India
3. K. L. Kapoor, 2001, A Text book of Physical Chemistry, Macmillan India Ltd.
4. V. Ramakrishnan and M.S. Gopinathan, 1988, Group Theory in Chemistry, Vishal Publications.
5. P.W. Atkins, 1990, Physical Chemistry, Oxford., K.V. Raman, 1990, Group theory and its applications to Chemistry, Tata McGraw Hill.
6. D.A. McQuarrie, 1983, Quantum Chemistry, University Science Books, Mil Valley, California.

PRACTICAL

114CMPP01- INORGANIC CHEMISTRY PRACTICAL

Semi micro qualitative analysis of mixtures containing two common and two rare cations. The following are the rare cation to be included: W, Mo, Ti, Te, Se, Ce, Th, Zr, V, U and Li.

a. Complexometric titrations (EDTA) - Estimation of Ca, Mg and Zn.

b. Preparation of the following:

1. Tris (thiourea) copper (I) chloride
2. Potassium tris (oxalato) chromate (III) trihydrate
3. Sodium bis (thiosulphato) cuprate (I)
4. Tris (thiourea) copper (I) sulphate
5. Sodium hexanitrocobaltate (III)
6. Chloropentammine cobalt (III) chloride
7. Bis (acetylacetanato) copper (II)
8. Hexaminenickel (II) chloride
9. Bis (thiocynato) pyridine manganese, (ll)

c. Analysis of Ores:

1. Determination of tin and lead in solder.
2. Determination of chromium and nickel in stainless steel.

d. Colorimetric analysis:

(Using) Photoelectric method: Estimation of iron, nickel, manganese, copper.

References

1. Vogel, Text book of Inorganic quantitative analysis.
2. Dougles A. Skoog, Principles of Instrumental Analysis, 3rd Edition.

II Semester

214CMPT01 - ORGANIC CHEMISTRY - II

UNIT- I : ADDITION TO CARBON-CARBON AND CARBON-HETERO MULTIPLE BONDS:I

Electrophilic, nucleophilic and neighbouring group participation mechanism- Addition of Halogen and nitrosyl chloride to olefins. Hydration of Olefins and acetylenes. Hydroboration, Hydroxylations, Michael addition

UNIT - II :ADDITION TO CARBON-CARBON AND CARBON-HETERO MULTIPLE BONDS:II

Diels Alder Reaction, 1, 3-dipolar additions. Carbenes and their addition to double bonds - Simmon Smith Reaction. Mannich, Stobbe, Darzen, Wittig, Wittig-Horner and benzoin reactions. Stereochemical aspects to be studied wherever applicable. Nitrene : Methods for generating nitrenes and their reactions

UNIT - III : ELIMINATION REACTIONS

B_v E_2 and E1cB mechanism - E1, E2 and E1cB spectrum - Orientation of the double bond -Hoffman and Saytzeff rule - competition, elimination and substitution. Typical eliminations to be studied - dehydration, dehydro-halogenation and similar reactions. Stereochemistry of E2 eliminations in cyclohexane systems. Mechanism of pyrolytic eliminations. Examples : Chugaev and Cope Elimination.

UNIT - IV : MOLECULAR REARRANGEMENTS

A detailed study with suitable examples of the mechanism of the following rearrangements: Pinacol-Pinacolone (examples other than tetramethyl ethylene glycol) - Wagner-Meerwein, Demjanov, dienone-phenol, Favorski, Baeyer-Villiger, Wolf, Stevens (in cyclic systems) and Von Richter rearrangements. (A few examples in each rearrangement to be studied).

UNIT - V : OXIDATION AND REDUCTION

Mechanism - study of the following oxidation reactions - oxidation-of alcohols - use of DMSO in combination with DCC or acetic anhydride in oxidizing alcohols - oxidation of methylene to carbonyl -oxidation of aryl methanes - allylic oxidation of olefins- Reductions: Selectivity in reduction of 4-t-butyl cyclohexanone using selectrides hydride reductions - Synthetic importance of Clemensen and Wolf-Kishner reductions- Modifications of Wolf-Kishner reduction-Birch reduction, MPV reduction.

References

1. R.Bruckner, 2002, Advanced Organic Chemistry, Reaction Mechanism, Elsevier, New Delhi
2. J.March, 2002, Advanced Organic Chemistry, 4th Edition, John Wiley & Sons Singapore.
3. T.L. Gilchrist and C.W. Rees, Carbenes, Nitrenes and Arynes, Thomas Nelson and Sons Ltd., London.
4. Niel Issacs, 1987, Physical Organic Chemistry, ELBS Publications.
5. W. Carruthers, 1993, Some Modern Methods of Organic Synthesis, 3rd Edition, Cambridge University Press.

214CMPT02- INORGANIC CHEMISTRY - II

UNIT- I : COORDINATION CHEMISTRY - REACTION MECHANISMS

Electron transfer reactions; outer and inner sphere processes; atoms transfer reaction, complementary and non-complementary reactions. Formation and rearrangement of precursor complexes, the binding ligand, successor complexes, Marcus theory.

UNIT - II : SUBSTITUTION REACTIONS IN COORDINATION COMPOUNDS

Substitution Reactions : Substitution in square planar complexes, reactivity of platinum complexes, influences of entering, leaving and other groups, the trans-effect, substitution of octahedral complexes of cobalt and chromium, replacement, of coordinated water, solvolytic (acids and bases) reactions applications in synthesis (platinum and cobalt complexes only). Rearrangement in 4 and 6 coordinate complexes : reaction at coordinated ligands-template effect.

UNIT - III : THE CHEMISTRY OF SOLID STATE

Structure of Solids; Comparison of X-Ray, Neutron and Electron Diffraction; Structure of ZnS, Rutile, Per voskite, Cadmium iodide and nickel arsenide; spinels and inverse spinels; defects in solids, non-stoichometric compounds.Use of X-ray powder diffraction data in identifying inorganic crystalline solids, details for cubic systems. Band theory, Semiconductors, Superconductors, Solid State Electrolytes, Types of Magnetic Behaviour - Dia, Para,,Ferro, Antiferro and Ferrimagnetism, Hysterisis, Solid State Lasers, Inorganic Phosphorus, Ferrites, Garnets. Reactions in Solid State and Phase Transitions, Diffusion, Diffusion Coefficient, Diffusion Mechanisms, Vacancy and Interstitial Diffusion, Formation of Spinels. Solid Solutions: Order-Disorder Transformations and Super Structure.

UNIT- IV : NUCLEAR CHEMISTRY

Models of radioactive decay: orbital electron capture: nuclear isomerism, internal conversion, detection and determination of activity by cloud chamber, nuclear emulsion, bubble chamber, G.M., Scintillation and Cherenkov counters. Nuclear reaction: Types, reactions, cross section, Q-value, threshold energy, compound nucleus theory: high nuclear reactions, nuclear fission and fusion reactions as energy sources; direction reactions, photonuclear and thermo nuclear reactions. Components of nuclear reactors – the breeder reactor – nuclear reactors in India.

UNIT-V : LANTHANIDES AND ACTINIDES

Occurrence and isolation of the metals, electronic structure - Lanthanide contraction and significance. Oxidation states magnetic and spectral properties - Important co-ordination compounds of lanthanide -nuclear and non-nuclear applications of lanthanides including use of lanthanides as shift reagents. *Radioactive tracers:* Preparations - principles underlying tracer technique - application of tracers in the study of reaction mechanism and in analytical chemistry - neutron activation analysis, isotope dilution analysis - radio chemical determination of age of geological specimen. Tracers as applied to industry and agriculture - radioactive tracer in the diagnosis and treatment in the field of medicine.

References

1. F.A. Cotton and G.W. Wilkinson, 1988, Advanced Inorganic Chemistry - A Comprehensive Text; John Wiley & Sons.
2. B.E. Dogulas DH MX Daniels and Alexander, 1983, Concepts and Models of Inorganic Chemistry, Oxford IBH.
3. W.U. Mallik, G.D. Tul, R.D. Madan, 1992, selected topics in Inorganic Chemistry, S. Chand & Co., New Delhi.
4. A.R. West, 1991, Basic Solid State Chemistry, John Wiley
5. S. Glasstone, Source Book on Atomic Energy, East West Press.

214CMPT03 - PHYSICAL CHEMISTRY - II

UNIT- I : CHEMICAL KINETICS - III

Catalysis by Enzymes-rate of enzyme catalyzed reactions, effect of substrate concentration, pH and temperature on enzyme catalyzed reactions-inhibition of enzyme catalyzed reactions. Langmuir and BET adsorption isotherms- adsorption coefficient and its significance kinetics and mechanism of surface reactions-catalysis by metals, semiconductor oxides.

UNIT- II : CHEMICAL KINETICS - IV

Kinetics of complex reactions - reversible reaction, consecutive reactions, parallel reactions, chain reactions - general treatment of chain reactions. Rice Herzfeld Mechanism and explosion limits.Study of fast react ions-relaxation methods-temperature and pressure jump methods-stopped flow and flash photolysis, methods.

UNIT - III : QUANTUM CHEMISTRY - II

Quantum mechanical postulates-the Schrodinger equation-elementary applications of Schrodinger's equation-the particle in a box (one, two and three dimensional cases)- particle in a ring.

UNIT - IV : QUANTUM CHEMISTRY - III

The harmonic oscillator- the rigid rotor- the hydrogen atom- the Schrodinger equation for hydrogen atom (no derivation is required) -the solution- the origin of quantum number (angular momentum and spin) -their physical significance.

UNIT - V : QUANTUM CHEMISTRY - IV

Approximation methods-perturbation and variation method-application to hydrogen, helium atoms-R.S.Coupling and term symbols for atoms in the ground state - Slater orbital and HF-SCF methods.

Born-Oppenheimer approximation-valence bond theory for Hydrogen molecule-LCAO-MO theory for di and poly atomic molecules-concept of hybridization-Huckel theory for conjugated molecules (ethylene, butadiene and benzene) - semi-empirical methods.

References

1. J.Rajaram and J.C.Kuriakose, 1993, Kinetics and mechanism of chemical transformations, Macmillan India Ltd.
2. I.N. Levine, 1983, Quantum Chemistry, Allyn and Bacon, Boston.
3. R. Anantharaman, 2001, Fundamentals of quantum chemistry, Macmillan India Limited.
4. R.K. Prasad, 1992, Quantum Chemistry, Wiley Eastern, New Delhi.

PRACTICAL

214CMPP01– ORGANIC CHEMISTRY PRACTICAL

I. Analysis of organic mixture

a. Identification of components in a two component mixture and preparation of their derivatives.
b. Determination of b.p./ m.p. for components and m.p. for the derivatives.

II. Synthesis of an organic molecule involving one or two steps.

a. Any six preparations from the following.

1. Preparation of o-benzylbenzoic acid
2. p-Nitrobenzoic acid from p-Nitrotoluene
3. Anthroquinone from anthracene
4. Benzhydrol from benzophenone
5. m-Nitroaniline from m-dinitrobenzene
6. 1, 2, 3, 4-Tetrahydrocarbozole from cyclohexanone
7. p-chlorotoluene from p-toluidine
8. 2, 3-Dimethylindole from phenyl hydrazine and 2-butanone (boiling acetic acid)
9. Methyl orange from sulphanilic acid
10. Diphenyl methane from benzyl chloride

b. Any Six Preparations from the following involving two stages:

1. Syn-Tribromobenzene from aniline.
2. p-nitro aniline from acetanilide
3. m-Nitrobenzoic acid from methyl benzoate.
4. 2, 4-Dinitrobenzoic acid from p-nitro toluene.
5. m-Nitro benzoic acid from benzaldehyde
6. p-bromoaniline from acetanilide
7. Anthraquionone from phthalic anhydride.
8. Phthalide from phthalic anhydride
9. 2-phenyl indole from phenylhydrazine
10. 2-4, Dinitrophenyl hydrazine from p-nitrochlorobenzene.

III. Quantitative estimation of organic compounds using known methods, basic training for extraction of compounds from natural products and then chromatographic separations.

a. **Any Two Exercises In The Extraction Of Natural Products:**

1. Caffeine from tea leaves
2. Lactose from milk
3. Citric acid from lemon

b. Chromatographic separations

1. Column chromatography - separation of anthracene and acid from antharacene picrate.
2. Thin layer chromatography separation of green leaf pigments.
3. Paper chromatography

c. Estimation of organic compounds

1. Saponification of fat or an oil.
2. Iodine value of an oil.
3. Estimation of Ketone.
4. Estimation of amino group.

References

1. Arthur I. Vogel, A Text Book of Practical Organic Chemistry.
2. Raj K. Bansal, Laboratory Manual of Organic Chemistry, Wiley Eastern Limited.
3. Mann and Saunders, Laboratory manual of Organic Chemistry

III - Semester

314CMPT01 - ORGANIC CHEMISTRY – III

UNIT - I : PHYSICAL METHODS OF STRUCTURE DETERMINATION

Principles and applications of ultraviolet and infra – red spectroscopy in organic structure determination. Mass spectrometry and its applications. Optical rotatory dispersion and its applications. Cotton effect, axial haloketone rule and octant rule. Problem solving approach. (for molecules with a maximum number of C_{10}) Woodward Fieser Rule (only application).

UNIT – II : NMR SPECTROSCOPY

Nuclear magnetic resonance spectroscopy. Proton chemical shift, spin-spin coupling, coupling constants and applications to organic stuctures-FT NMR 13C resonance spectroscopy (elementary treatment).

UNIT - III : ORGANIC PHOTOCHEMISTRY AND AROMATICITY

Aromaticity of benzenoid, heterocyclic and non-benzenoid compounds, Huckel's rule-Aromatic systems with pi electron numbers other than six non-aromatic (cyclooctatetraene etc) and anti-aromatic systems (cyclobutadiene etc)-systems with more than 10pi electrons – Annulenes up to C18 (synthesis of these compounds is not expected). .Photo chemistry of ketones, photo reduction, photocycloaddition, Paterno - Buchi reaction, Di –p- methane rearrangement. cis- trans isomerisation, Barton reaction, photo- Fries reaction, photochemistry of cyclohexadienones synthesis of Vit - D.

UNIT - IV : ORBITAL SYMMETRY AND CORRELATION

Pericyclic reaction-classification-orbital symmety-Woodword Hoffman rules, FMO-Analysis of electrocyclic, cycloaddition and sigmatropic reactions-correlation diagram for, cycloaddition reaction ($\pi^{2s} + \pi^{2s}$) and ($\pi^{4s} + \pi^{2s}$) – butadiene – cyclobutene system and Inter conversion of hexatriene to cyclohexadiene. Structure of bulvalene, a fluxional molecule- Cope and Claisen rearrangements.

UNIT - V : HETEROCYCLIC COMPOUNDS , TERPENOIDS AND STEROIDS

Flavones, isoflavones, anthocyanins,.(Synthesis of parent and simple alkyl or aryl substituted derivatives are expected). Synthesis of carotenoids - licopenes and Vitamin A1 (Reformatsky and Wittig reaction methods only). Elucidation of structure of cholesterol (by chemical degradation). Conversion of cholestrol to progestrone, esterone and testosterone

References:

1. R.M. Silverstein, G.C. Bassler and Morril, 1991, Spectrometric identification of Organic Compounds, 5th Edition, John Wiley and Sons, New York.
2. I.L. Finar, 1986, Organic Chemistry – Vol.II, 5th edition, ELBS Publication.
3. P.S. Kalsi, 2002, Spectroscopy of Organic Compounds, Wiley Eastern Ltd, Chennai.
4. H. Depuy and Orville, Molecular reaction and Photochemistry Charles, L.Chapman, Prentice Hall of India Pvt. Ltd., New Delhi
5. L.A. Pacquette, 1978, Principles of Modern Heterocyclic Chemistry, Benjamin Cummings Publishing Co., London.
6. J. March, 1992, Advanced Organic Chemistry, 4th Edition, Singapore

314CMPT02 - INORGANIC CHEMISTRY - III

UNIT - I : SOLID STATE CHEMISTRY I

Structure of Solids; Comparison of X-Ray, Neutron and Electron Diffraction.Structure of ZnS, Rutile, Pervoskite,Cadmium iodide and nickel arsenide; spinels and inverse spinels.Defects in solids, non-stoichometric compounds.Use of X-ray powder diffraction data in identifying inorganic crystalline solids, details for cubic systems.

UNIT - II : SOLID STATE CHEMISTRY II

Band theory, Semiconductors, Superconductors, Solid State Electrolytes. Magnetic Behaviour - Dia, Para,,Ferro,Antiferro and Ferrimagnetism, Hysterisis, Ferrites, Garnets.Solid State Lasers, Inorganic Phosphorus Diffusion in solids , types, Diffusion Coefficient, Diffusion Mechanisms, Vacancy and Interstitial Diffusion, Formation of Spinels. Reactions in Solid State and Phase Transitions. Solid Solutions: Order-Disorder Transformations and Super Structure.

UNIT - III : SPECTROSCOPY OF METAL COMPLEXES

Term states for d^n - ions, energy diagrams, d-d transitions, Orgel and Sugano - Tanabe diagrams, spin- orbit coupling, nephelauxetic effect.Applications to inorganic systems of the following: Ultraviolet, visible, Infrared and Raman spectroscopy of metal complexes, organometallic and simple inorganic compounds with special reference to coordination sites, isomerism.

UNIT – IV : SPECTROSCOPY IN INORGANIC SYSTEMS

Applications to inorganic systems of the following: NMR, NQR, Mossbauer spectra: NMR spectra of ^{31}P, ^{19}F, NMR shift reagents, NQR-Nitrosyl compounds. Mossbauer of Fe and Sn systems.

UNIT - V : ESR AND PHOTOELECTRON SPECTROSCOPY

ESR introduction-Zeeman equation, g value, nuclear hyperfine splitting, Interpretation of the spectrum, simple carbon centered free radicals. Anisotropy in g value and hyperfine splitting constant. McConnels equation, Kramer's theorem, esr of transition metal complex of copper, manganese and vanadyl complexes. Photoelectron spectroscopy – UPS and XPS-Photoelectron spectra – Koopman's theorem,-Fine structure in PES, Chemical shift and Correlation with electronic charges..

References

1. L.Smart, E.Moore – Solid State Chemistry – An Introduction-2nd Edition
2. A.R.West – Basic Solid state Chemistry 1961 – John Wiley
3. A.R.West – Solid state Chemistry and its applications 2007 – John Wiley
4. W.E Addison, 1961, Structural principles in Inorganic Chemistry, Longman
5. R.B.Heslop and K.Jones, inorganic Chemistry, Elsevier Scintific Publ .1976.
6. H.A.O Hill and P.Day, physical methods in dvanced Inorganic Chemistry, John wiley 1968.
7. C.N.R Rao, J.R.Ferraro, Spectrosopy in inorganic chemistry, Vol.I and Vol II, Academic press, 1970.
8. G.Aruldhas, molecular structures and spectroscopy-Prentice hall.
9. M.F.Lappert –Physical inorganic Chemistry-inorganic Electron Spectrosopy 1968

314CMPT03 - PHYSICAL CHEMISTRY – III

UNIT- I : THERMODYNAMICS - I

Partial molar properties - Partial molar free energy (Chemical potential) - Partial molar volume and partial molar heat content - their significance and determination of these quantities. Variation of chemical potential with temperature and pressure.Thermodynamics of real gases - gas mixture - fugacity definition - determination of fugacity variation of fugacity with temperature and pressure - thermodynamics of ideal and non ideal binary solutions-dilute solutions-excess functions for non-'ideal solutions and their determination-the concepts of activity and activity coefficients-determination of standard free energies.Choice of standard states - determination of activity and activity coefficients for non-electrolytes.

UNIT - II : SPECTROSCOPY I

Interaction of matter with radiation-Einstein's theory of transition probability-rotational spectroscopy of a rigid rotor- non-rigid rotor-diatomic and polyatomic molecules. Vibrational spectroscopy-harmonic oscillator-anharmonicity-vibrational spectra of polyatomic molecules-vibrational frequencies-group frequencies-vibrational coupling-overtones-Fermi resonance. Raman Spectra.Electronic spectra of polyatomic molecules, selection rules-types of transition in saturated and unsaturated hydrocarbons, effect of conjugation,and solvent effects .

UNIT - III : SPECTROSCOPY II

Resonance spectroscopy-Zeeman effect-equation of motion of spin in magnetic fields-chemical shift-spin-spin coupling-NMR of simple AX and AMX type molecules- H^1 -^{13}C, ^{19}F, ^{31}P NMR spectra - a brief qualitative discussion of Fourier transform spectroscopy.

UNIT – IV : ELECTROCHEMISTRY OF SOLUTION

Mean ionic activity and activity coefficient-concept of ionic strength, Debye-Huckel theory of strong electrolytes-activity coefficient of strong electrolytes-determination of activity coefficient -Debye Huckel limiting law at appreciable concentration of electrolytes - Debye Huckel Bronsted equation-qualitative and quantitative verification.

UNIT –V : SURFACE PHENOMENA AND KINETICS

Surface Phenomena: Gibbs adsorption isotherm – solid- liquid interfaces – contact angle and wetting – solid-gas interface – physisorption and chemisorption – Langmuir, BET isotherms – surface area determination. Kinetics of surface reactions involving adsorbed species – Langmuir-Hinshelwood mechanism, Langmuir – Rideal mechanism – Rideal –Eley mechanism. Some interfacial aspects on Micelles, Reverse micelles, Micro emulsions and Membranes. 28- Application of ARRT to solution kinetics - Effect of solvent and ionic strength, influence of pressure on rates in solution - Enzyme catalysis- Mechanism of single substrate reactions – Michaelis Menton law – Kinetics of processes in micellar and reverse micellar systems.

References

1. S. Glasstone, 1960, Thermodynamics for chemists, Affiliated East West Press, New Delhi.
2. J. Rajaram and J.C. Kuriacose, 1986, Thermodynamics for students of chemistry, Lal Nagin Chand, New
3. A. Caringtion and A.D Mc Lachlan, 1967, Introduction to Magnetic Resonance Harper and Row
4. G. Aruldas, 2002, Molecular structure and spectroscopy, Prentice Hall.
5. C.N. Banwell, 2003, Fundamentals of Molecular ,Spectroscopy Tata McGraw Hill.
6. D.N. Sathyanarayana vibrational spectroscopy and electronic spectroscopy
7. Puri and Sharma, 1988, physical chemistry
8. J.O.M. Bokris and A.K.N. Reddy, 1977, Electrochemistry, VoIs1 and 2 Plenum, New York..
9. J. Robbins -1993, Ions in Solution-An Introduction in electrochemistry, Clarendon press, Oxford

PRACTICAL

314CMPP01 – PHYSICAL CHEMISTRY PRACTICAL

1.Study of the adsorption of acetic acid or oxalic acid on charcoal , verification of Freundlich isotherm and determination of concentration of given acetic acid or oxalic acid.

2.Construction of phase diagram for a simple binary system ;naphthalene – biphenyl, naphthalene – p-dichlorobenzene , naphthalene-diphenylamine.

3.Construction of phase diagram for the three component system(partially miscible liquid system) acetone – chloroform – water ; chloroform –aceticacid – water.

4.Determination of the equilibrium constant of the reaction between iodine and potassium iodide by partion method ..

5. Determination of the concentration of given potassium iodide solutions by partition method.

6.Determination of molecular weight of benzoic acid in benzene and the degree of association of benzoic acid in benzene using partition method .

7.Kinetic study and comparison of rate constant for the inversion of cane sugar in presence of acid using polarimeter

8.Kinetic study of the reaction between acetone and iodine in acidic medium and determination of the order with respect to iodine and acetone

.9.Kinetic study of saponification of ethylacetate by sodium hydroxide conductometrically and determination of order of the reaction.

10.Kinetic study and comparison of acid strengths using acid catalysed hydrolysis of methyl acetate

11.Determination of temperature coefficient and energy of activation for the acid catalysed hydrolysis of methylacetate.

12.Determination of the rate constant and order for the reaction between potassium persulphate and potassium iodide

13.Study of the primary salt effect on the kinetics of oxidation of iodide by persulphate

14.Kinetic study of the decomposition of sodium thiosulphate by mineral acid.

References

1. Arthur I. Vogel, A Text Book of Practical Organic Chemistry.
2. V K Ahluwalia etal sunita Dhingra Adarsh Gulati, College Practical Chemistry, 2008

IV - Semester

414CMPT01 - ORGANIC CHEMISTRY - IV

UNIT - I : BIO-ORGANIC CHEMISTRY

Pyrimidines (cytocine and uracil) and purines (adenine and guanine only) Structure and role of nucleic acids. DNA and RNA Genetic code. Biosynthesis of Cholestrol , phenanthrene alkaloids and bile acids

UNIT -II : ALKALOIDS AND PROTEINS

Peptides and their synthesis (Synthesis of tripeptide using the Amino acids - Glycine, Alanine, Lysine, Cysteine, Glutamic acid, Arginine).Merrified synthesis, Determination of primary, secondary and tertiary structure of proteins. Total synthesis of , morphine, resperine and cocaine.

UNIT- III : MODERN SYNTHETIC METHODOLOGY

Retro synthetic analysis and Synthesis of simple organic molecules using standard reactions like acetylation and alkylation of enamines and active methylene compounds, Grignard reactions, Phosphorus and sulphur ylides, Robinson annulation. Formation of C-C and C=C bonds.

UNIT - IV :USE OF REAGENTS IN ORGANIC SYNTHESIS

Diels-Alder reactions ENE reaction, protection and deprotection of functional groups (R-OH, RCHO, R-CO-R, R-NH2 and R-COOH). Uses of the following reagents : DCC, trimethyl silyl iodides, 1, 3-dithiane (Umpolung), diisobutyl aluminimumhydride (DIBAL), 9BBN, trimethylsilylchloride. and tributyl tinhydride .Application of synthetic methodology for the synthesis of simple cyclic and acyclic target molecules -synthesis of cubane, 5 - hexenoicacid , bicyclo (4, 1, 0) heptane-2-one.,trans 9-methyl-1- decalone ,longifolene and onocerin

UNIT – V : FREE RADICAL REACTIONS

Long lived and short lived free radicals, methods of generation of free radicals. Adddition of free radicals to olefinic double bonds. The following aromatic radical substituents are to be studied decomposition of diazocompounds, phenols-coupling - Sandmayer reaction - Gombereg-Gauchmann reaction, Pschorr reaction, Ulmann reaction, mechanism of Hunsdicker reaction Detection of free radicals by ESR.

References

1. R.K. Mackie and D.M. Smith. 1998, Guide book to organic synthesis, ELBS Publication.
2. I. L. Finar, 1986, Organic Chemistry, 5th Edition, Vol .II, ELBS Publication.
3. L. Smith, Robert L. Hill .1. Robert Lehman, Robert J .Iet Rowitz, Philp Handler and abrahim white principles of Biochemistry General aspects, 7th Edition, McGraw Hill Int.
4. L. Stryer, Biochemistry, W.H.Freeman and Co., New York.
5. Agarwal, Chemistry of Organic Natural Products, Goel Publishing House.
6. B.l. Smith, 1980, Organic synthesis, Chapman and Hall, NY.
7. Francis.A. Carey, Richard J. Sundbreg, 2001, Advanced Organic Chemistry, 4th Edition, Plenum Press, New York.
8. N.J. Turro, 1978 Modern Molecular Photochemistry, Benjamin, Cummings, California.

414CMPT02 - INORGANIC CHEMISTRY - IV

UNIT - I : COORDINATION CHEMISTRY - REACTION MECHANISMS

Electron transfer reactions; outer and inner sphere processes; atoms transfer reaction, complementary and non-complementary reactions. Formation and rearrangement of precursor complexes, the bridging ligand, successor complexes, Marcus theory.

UNIT - II : SUBSTITUTION REACTIONS IN COORDINATION COMPOUNDS

Substitution Reactions : Substitution in square planar complexes, reactivity of platinum complexes, influences of entering, leaving and other groups, the trans-effect. Substitution of octahedral complexes of cobalt and chromium, replacement of coordinated water, solvolytic (acids and bases) reactions applications in synthesis (platinum and cobalt complexes only). Rearrangement in 4 and 6 coordinate complexes : reaction at coordinated ligands- template effect.

UNIT- III : ORGANO METALLIC COMPOUNDS

Carbon donors: Alkyls and Aryls, metalation, bonding in carbonyls and nitrosyls, chain and cyclic donors, olefin, acetylene, and allyl systems, synthesis, structure and bonding, metallocenes.Reactions: Asscociation, Substitution, Addition, Eleimination, Ligand protonation, Electrophilic and Nucleophilic attack on ligands, carnonylation and decarboxylation, oxidative addition and fluxionality.

UNIT - IV: REACTION MECHANISMS

Catalysis – Hydrogenation of olefins(Wilkinson's catalyst), hydroformylation of olefins using cobalt or rhodium catalyst(Oxo process), oxidation of olefins to aldehydes and ketones(Wacker process):polymersisation(Ziegler-Natta catalyst); Cyclo oligomerisation of acetylene using nickel catalyst(Reppe's catalyst), polymer bound catalysts.

Unit – V : LANTHANIDES AND ACTINIDES

Lanthanides and actinides: Occurrence and isolation of the metals, electronic structure – Lanthanide contraction and significance. Oxidation states magnetic and spectral properties - Important co-ordination compounds of lanthanide -nuclear and non-nuclear applications of lanthanides including use of lanthanides as shift reagents. Inorganic Photochemistry – Photoredox reactions and photosubstitution reactions in coordination complexes with particular reference to Co(III), Cr(III) and Pt(II) complexes. Photosensitisation reactions of $[Ru(bpy)_3]^{2+}$ complex and its applications in solar energy conversions.

References:

1. N,J,Turro, 1978, molecular photochemistry.
2. K.K.Rohatgi Mukherjee
3. Purcell, K.F. and Kotz, J.C., - Inorganic Chemistry
4. D.F.Shrivers, Atkins.Inorganic Chemistry
5. J.E. Huheey, 1993, Inorganic Chemistry - Principles, Structure and Reactivity; IV Edition, Harper Collins,.
6. S.F.A. Kettle, 1973, Coordination Chemistry, ELBS
7. G.Coates, M.L.green and K.Wade, Priciples of Organometallic Chemistry, !988
8. R.B.Jordan, Reaction Mechanism of Inorganic and Organo Metallic systems – OUP 1991.
9. P.Powell, Principles of Organometakkic chemistry, Chapman and hall 1998.
10. R.C.Mehothra, A.Singh, Organo Metallic Chemistry, Wiley Eastern Comp.1992.
11. V.Balzani & Carrasitti – Photochemistry of coordination compounds

414CMPT03 – PHYSICAL CHEMISTRY – IV

UNIT - I : FUNDAMENTALS

Absorption and emission of radiation-Franck-Condon Principle-decay of electronically excited states-radiative and non radiative processes-fluorescence and phosphorescence-spin forbidden radiative transition internal conversion and intersystem crossing-energy transfer process-excimers and exciplexes-static and dynamic quenching-Stern Volmer analysis.

UNIT - II : TECHNIQUES AND PHOTOCHEMICAL REACTIONS

Quantum yield and Life time measurements, Flash photolysis, Actinometry. Photo physical process and kinetics of photochemical reactions.Photoredox reactions and photosubstitution reactions in coordination chemistry - photovoltaic and photogalvanic cells. photoelectrochemistry, Aspects of solar energy conversion

UNIT - III : ELECTRODE KINETICS

Electrode-electrolyte interface - electrical double layer-electrocapillary phenomena - Lippmann equation-Structure of double layer-Helmholtz -Perrin, Guoy Chapmann and Stern models of electrical double layer.

Mechanism of electrode reaction - polarization and overpotential, the Butler - Volmer equation for one step and multistep electron transfer reactions- significance of exchange current density and symmetry factor-transfer coefficient and its significance-mechanism of hydrogen and oxygen evolution reactions. :Corrosion and passivation of metals- Pourbaix diagram - fuel cells-electrodeposition - principle and applications.

UNIT - IV : THERMODYNAMICS - II

Concept of thermodynamic probability - distribution of distinguishable and non-distinguishable particles .Maxwell-Boltzmann, Fermi-Dirac and Bose Einstein statistics - modes of contribution to energy-. Partition function - translational, vibrational and rotational partition functions for mono, diatomic and polyatomic ideal gases.

UNIT- V : THERMODYNAMICS – III

Thermodynamic functions in terms of partition functions, equilibrium constant for isotope exchange and dissociation of diatomic molecules; heat capacity of solids (Einstein and Debye Models) ortho and para hydrogen -Planck's radiation law - electron in metals

References

1. J.O.M. Bokris and A.K.N. Reddy, 1977, Electrochemistry, VoIs1 and 2 Plenum, New York.
2. P. Delahay - 1965, Electrode Kinetics and Structure of Double layer, Interscience, New York.
3. S. Glasstone, 1960, Introduction to Electrochemistry, Affiliated East West Press, New Delhi.
4. D.R. Crow, 1991, Principles and Applications of Electrochemistry, Chapman and Hall.
5 N.J. Turro, 1978, Modern Molecular Photochemistry, Benjamin, Cummings, Menlo Park, California.
6 K.K. Rohatgi Mukherjee, 1978, Fundamentals of Photochemistry, Wiley Eastern Ltd.
7. J.G. Calvert and J.N. Pitts, 1966, Photochemistry, Wiley, London.
8. R.P. Wayne, 1970, Photochemistry, Butterworths, London.
9. R.P. Cundell and A. Gilbert, 1970, Photochemistry, Thomas Nelson London

PRACTICAL

414CMPP01 - ANALYTICAL CHEMISTRY PRACTICAL

I . ESTIMATION OF ORGANIC COMPOUNDS

1. Estimation of Phenol and Aniline – Bromination method
2. Estimation of ethyl methyl Ketone
3. Estimation of Glucose – Bertrand's method

II . QUANTITATIVE ANALYSIS

Gravimetric estimation of

a. magnesium in the mixture of Iron and magnesium –
b. Nickel in the mixture of copper and nickel –
c. Zinc in the mixture of copper and zinc –
d. Nickel in the mixture of iron and Nickel.

III . ANALYSIS OF ORES AND ALLOYS

a. Determination pf percentage of calcium and magnesium in dolomite
b. Determination of percentage of MnO_2 in pyrolusite
c. Determination of copper and zinc in brass.

IV. ANALYSIS OF INORGANIC COMPLEX COMPOUNDS:

a. Preparation of cis and trans potassium bis (oxalato) diaquochromate and analysis of each of these for chromium.
b. Preparation of potassium tris (oxalato) ferrate (III) and analysis for iron and oxaiate.

V. CHROMATOGRAPHIC SEPARATIONS

a. Separation of a mixture of two metal ions by paper chromatography
b. Separation of zinc and magnesium on an anion exchanger
c. Column chromatography – separation of o-nitro and p-nitro phenol

VI . SPECTRAL INTERPRETATION

List of inorganic spectra to be given for interpretation.

a. IR Spectra of the sulphato ligand
b. IR Spectra of the nitro and nitritopentaminecobalt (III) chloride
c. IR Spectra of the dimethylglyoxime ligand and its Nickel (II) complex.
d. IR Spectra of carbonyls

Special interpretation of organic compounds.using UV and IR spectroscopy

1. 1, 3, 5-Trimethylbenzene
2. Pinacolonen0
3. prophyl amine
4. p-Methoxybenzyl alcohol
5. Benzyl bromide

References

1. Vogel, Text book of Inorganic quantitative analysis.
2. Dougles A. Skoog, Principles of Instrumental Analysis, 3rd Edition.
3. Arthur I. Vogel, A Text Book of Practical Organic Chemistry

Electives

114CMPE01 – CHROMATOGRAPHIC TECHNIQUES

UNIT- I : **INTRODUCTION**
Chromatographic methods, general aspects of chromatography, classification and types, mechanism.

UNIT - II: COLUMN CHROMATOGRAPHY
Column chromatography, construction and operation of column, choice of adsorbent elements, applications. Ion exchange chromatography : Anion & cation exchangers techniques applications.

UNIT - III : PAPER CHROMATOGRAPHY
Paper chromatography: Mechanism of separation, development & applications. Thin layer chromatography: Techniques, choice of adsorbent solvents &applications.

UNIT – IV : GAS- LIQUID CHROMATOGRAPHY
Gas-liquid Chromatography, Principles, Retention Volumes, Instrumentation, Carrier Gas, Columns, Stationary Phase, Detectors, Thermal Conductivity, Flame Ionization, Electron Capture, application of G.L.C.

UNIT V :HIGH PERFORMANCE LIQUID CHROMATOGRAPHY
High Performance Liquid chromatography: Scope, Column efficiency, Instrumentation, Pumping Systems, Columns, Column packing, Detectors, Applications.

References

1. Vogel's, 2000, Text book of Quatitative Chemical Analysis, Sixth Edition, Pearson Education Limited, London.
2. D. A. Skoog and J. J.Leary, 1971, Principles of Instrumental Analysis, Fourth Edition, Saunders College Publishing, US.

114CMPE02 – BIOORGANIC CHEMISTRY

UNIT - I : CHEMISTRY AND METABOLISM CARBOHYDRATES

Definition, classification and biological role of carbohydrates. Monosaccharides Linear and ring structures (Haworth formula) of ribose, glucose, fructose and mannose (structural determination not required) physical and chemical properties of glucose and fructose.Disaccharides: Ring structures (Haworth formula) - occurrence, physical and chemical properties of maltose, lactose and sucrose. Polysaccharides: Starch, glycogen and cellulose - structure and properties. Glycolysis of carbohydrates.

UNIT - II ; CHEMISTRY AND METABOLISM OF AMINO ACIDS AND PROTEINS

Amino acids : Various classifications, essential amino acids, physical properties (amphoteric nature and isoelectric point) and reactions. Proteins : Classifications (based on shape, composition and solubility), physical properties. Primary structure - End group analysis (N- terminal analysis- Edman's method, dansyl chloride method ; C - terminal analysis- hydrazinolysis and bio - chemical methods) Biological functions of proteins, Deamination, transamination reactions, Urea cycle.

UNIT - III : CHEMISTRY AND METABOLISM OF LIPIDS

Definition, classification- simple lipids (fatty acids), compound lipids and derived lipids. Properties : saponification number, Acetyl number.Sterols : Cholesterol (structure not needed), biological importance and chemical properties. Bile acids- functions. Biological functions of lipids.

UNIT - IV : NUCLEIC ACIDS

Purine and pyrimidine bases, nucleosides, nucleotides, polynucleotides, DNA structure - various types, RNAstructure - various types. Biological functions of DNA and RNA, Genetic code.

UNIT- V :VITAMINS

Vitamins: Definition, classification- water-soluble vitamins (B_v B_2, B_3, B_6, B_{12} and vitamin-C) and fat-soluble vitamins (A, D, E and K) - occurrence, structure, deficiency diseases, biochemical rules and daily requirements

References

1. Biochemistry C.B. Powar and G.R. Chatwal.
2. Elements of Biochemistry Ragunatha Rao
3. Essential Biochemistry U. Sathyanarayanan
4. Essential Biochemistry J.L. JAIN

214CMPE01 - ANALYTICAL TECHNIQUES IN CHEMISTRY

UNIT - I : UV-VISIBLE, IR AND RAMAN SPECTROSCOPY

Colorimetric analysis and UV-Visible spectroscopy: Beer Lambert's law, Principles of single and double beam instruments – applications for analysis of inorganic and organic samples.Infrared spectrophotometric analysis – principle and instrumentation and molecular structure determination.Raman Spectra – principle, basic instrumentation – structural analysis.

UNIT - II : NMR SPECTROSCOPY

Nuclear Magnetic Resonance – Principle, instrumentation, structure determination. NMR of ^{1}H, ^{13}C, ^{31}P, ^{19}F.

NQR - Nitrosyl compounds, Mossbauer of Fe and Sn systems.

UNIT- III : ELECTRON SPIN RESONANCE SPECTROSCOPY

Electron Spin Resonance – Principle, instrumentation, applications to coordination compounds**.** Magnetic Susceptibility and measurements- Guoy method, Faraday method-applications

UNIT - IV : THERMAL ANALYSIS AND MASS SPECTROSCOPY

Thermo gravimetric and differential thermal analysis, thermometric titrations, differential scanning colourimetry – basic instrumentation and applications.Mass Spectrometry- Principle, basic instrumentation, fragmentation patterns – organic molecular structural determination

UNIT - V : ABSORPTION SPECTROSCOPY

Atomic absorption spectroscopy:Theory, Atomizers, Flame and Electro thermal. Radiation sources, Instrumentation, spectral and chemical interferences, applicationPhotoelectron spectroscopy (UV and X-Ray)-photo electron spectra-Koopman's theorem, fine structure in PES, chemical shift and correlation with electronic charges.

References

1. D.A .Skoog, 1985, Principles of Instrumental Methods of analysis, III Edition, Saunders College Publ.
2. Willard Merrit, Dean and Settle, 1986, Instrumental methods of analysis, VI Edition, CBS Publ.
3. A.I. Vogel, 1976, Textbook of Qualitative Inorganic Analysis, III Edition, ELBS.
4. D.A. Skoog and D.M. West, 1982, Fundamentals of Analytical Chemistry, IV Edition, old Reinhord & Winston, Publication.

214CMPE02 - BIOINORGANIC CHEMISTRY

UNIT-I : INTRODUCTION

Thermodynamics and biology – Basic concepts of structure and functionality – membranes – structure, function transport properties, aspects of electrochemical phenomena – active transport, ionophores, biological energy storage and Phosphate hydrolysis.

UNIT-II : ENZYME CHEMISTRY

Enzymes - Nomenclature and classification, chemical kinetics, the free energy of activation and the effects of catalysts, kinetics of enzyme catalysed reactions – Michelis - Menton equation - Effect of pH, temperature on enzyme reactions, Factors contributing to the catalytic efficiency of enzymes, Study by spectroscopic methods.

UNIT -III : COENZYMES

Essential and trace metal ions.Coenzymes - Vitamin B_{12} coenzymes, carboxypeptidase and Superoxide dismutase.Heme-enzyme - Peroxidase and catalases.- Oxygen carriers - Hemeproteins - Hemoglobin, myoglobin - Structure Oxygenation and stereochemistry - Bohr effect. Non-heme oxygen carriers - Hemerythrin and hemocyanin.

UNIT- IV : BIOLOGICAL SYSTEMS

Nitrogen fixation - Introduction, types of nitrogen fixing micro organisms. 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. Biological redox systems: Cytochromes -Classification, cytochrome a, b and c. Cytochrome P-450. Iron - sulphur proteins - rubredoxin and ferredoxin.
Photosynthesis and chlorophyll's.

UNIT-V : BIO ANALYTICAL CHEMISTRY

Toxicity & medicine.Toxicity of Hg, Cd, Zn, Pb, As, Sb. Anti cancer agents.Metal ion poisoning : Failure of metal ion control systems, role of metal ion in diagnosis and treatment - use of radio isotopes.- Pollution studies : Effluents and treatment.Inorganic plant nutrition and indicator plants for mineral exploration.

References

1. Williams, D.R. - Introduction to Bioinorganic Chemistry
2. Fiabre, F.M., and Williams D.R. - The Principles of Bioinorganic Chemistry, Royal Soceity of Chemistry, Monograph for Teachers - 31.
3. Purcell, K.F. and Kotz, J.C., - Inorganic Chemistry
4. Elements of Bioinorganic Chemistry - G.N. Mugherjee and Arabinda Das, 1993.
5. Bioinorganic Chemistry - M. Satake and Y. Mido, Discovery Publishing House, New Delhi (1996).

314CMPE01 - NANOSCIENCE AND NANOTECHNOLOGY

UNIT – I: NANOMATERIALS – AN INTRODUCTION AND SYNTHETIC METHODS

Definition of nanodimensional materials - Historical milestones - unique properties due to nanosize,Quantum dots, Classification of Nanomaterials .General methods of synthesis of nanomaterials – Hydrothermal synthesis,Solvothermal synthesis,Microwave irradiation, sol – gel and Precipitation technologies, Combustion Flame-Chemical Vapor Condensation Process, gas Phase Condensation Synthesis,Reverse Micelle Synthesis, Polymer – Mediated Synthesis, Protein Microtube – Mediated Synthesis Synthesis of Nanomaterials using microorganisms and other biological agents, Sonochemical Synthesis, Hydrodynamic Cavitation. Inorganic nanomaterials – Typical examples – nano TiO2 / ZnO/CdO/CdS , Organic nanomaterials – examples – Rotaxanes and Catenanes

UNIT – II: TECHNIQUES FOR CHARACTERISATION OF NANOSCALE MATERIALS

Principles of Atomic force microscopy (AFM)- Transmission electron microscopy (TEM)-Resolution and scanning transition electron microscopy (STEM) Scanning Tunneling Microscopy (STM) Scanning nearfield optical microscopy (SNOM),Scanning ion conductance microscope, scanning thermal microscope, scanning probe microscopes and surface Plasmon spectroscopy.

UNIT – III: REACTIONS IN ENVIRONMENT ON NANOSCALE

Reactions in Nanospace / Nanoconfinement / Nanocapsules- Cavitands, Cucurbiturils, Zeolites, M.O.Fs, Porous silicon, Nanocatalysis.

UNIT – IV: CARBON CLUSTERS AND NANOSTRUCTURES

Nature of carbon bond – New carbon structures – Carbon clusters: Discovery of C60 – Alkali doped C60 – Superconductivity in C60 – Larger and smaller fullerenes. Carbon nanotubes: Synthesis – Single walled carbon nanotubes – Structure and characterization – Mechanism of formation – Chemically modified carbon nanotubes – Doping – Functionalizing nanotubes –Application of carbon nanotubes. Nanowires – Synthetic strategies – Gas phase and solution phase growth – Growth control – Properties.

UNIT- V: NANOTECHNOLOGY AND NANODEVICES

DNA as a nanomaterial, DNA – knots and junctions, DNA – nanomechanical device designed by Seeman. Force measurements in simple protein molecules and polymerase – DNA complexes. Molecular recognition and DNA based sensor. Protein nano array, nanopipettes, molecular diodes, self assembled nano transistors, nanoparticle mediated transfection.

References

1. C.N.R. Rao, A. Muller, A.K. Cheetam (Eds), The Chemistry of Nanomaterials, Vol.1, 2, Wiley – VCH, Weinheim, 2004.
2. C.P. Poole, Jr: F.J. Owens, Introduction to Nanotechnology Wiley Interscience, New Jersey, 2003
3. Kenneth J. Klabunde (Ed), Nanoscale materials in Chemistry, Wiley- Interscience, New York, 2001.
4. T. Pradeep, Nano: The Essentials in understanding nanoscience and nanotechnology,
Tata McGraw Hill, New Delhi, 2007

314CMPE02 - POLYMER CHEMISTRY

UNIT – I : POLYMERIC MATERIALS

Introduction – Classification –types – thermoplastics – cellulose derivatives – LDPE, HDPE, PVC, PMMA, PTFE, PET and Nylons – thermosetting resins – phenolic resins, epoxy resins – silicones and polyurethanes – polymer blends and alloys – reinforced plastics.

UNIT - II: ELASTOMERS

Nutural rubber – processing – vulcanization – synthetic rubber – SBR, neoprene, butyl reclaimed rubbers – thermoplastic elastomers – high performance polymers – polyethers – polysulphones and polyimides.

UNIT- III : MOULDING TECHNIQUES

Moulding constituents – functions – moulding techniques – compression – injection extrusion – blow moulding – thermoforming – vacuum forming – casting – calendaring - lamination

UNIT – IV: : POLYMER PROPERTIES AND CHARACTERISATION

Effect of structure on mechanical, chemical, thermal, electrical and optical properties.
Characterisation of polymers by IR and UV – Visible and NMR – Thermal properties by TGA and DSC.

UNIT – V: MOLECULAR WEIGHT AND ITS DISTRIBUTION

Molecular weight of the polymer-number, weight and viscosity average molecular weights-molecular weight distribution- molecular weight determination by GPC and viscometry. Poly dispersity index and its significance-Polymerisation techniques-homogeneous and heterogeneous polymerization.

References

1. Michael L. Berine – Plastics Engineering Hand Book, 5th Edn. Chapman & Hall, New York, 1991.
2. Jacqueline. I Kroschwitz – concise encyctopedia of polymer science and engineering John Wiley & sons, New York 1998.
3. R.W. Iyson – specialty polymers, blackie academic & professional, London, 19992.
4. Mourice Morton – Rubber Technology, Van Nostrand, Reinhold New York, 1987.

314CMPE03 - INDUSTRIAL ELECTROCHEMISTRY

UNIT – I : CHLORALKALI INDUSTRY

General concepts of brine electrolysis – modern technological developments – chlorine cell technologies – mercury and diaphragm cell – membrance cell.

UNIT – II : ELECTROMETALLURGY

Metal extraction and refining – electrowinning – aluminium extraction – manufacture of sodium, lithium and magnesium – hydrometallurgical processes – electrorefining aqueous and molten salt electrorefining.

UNIT – III : METAL FINISHING

Pretreatment – conversion coatings – phosphating – types, methods, properties and influencing factors – evaluation and testing – applications – anodizing – principle and applications. Electroplating – objectives, theory and method- electroplating of nickel electroless plating – galvanizing – tinning.

UNIT – IV : ELECTROSYNTHESIS

Electrolytic preparation of inorganic compounds – fluorine – peracids and their slats – $KMnO_4$, $K_2Cr_2O_7$. Organic Electrosynthesis – hydromerisation of acrylonitrile – Monsanto process – manufacture of ethylene glycol – electrolysis of organic compounds with the use of ion – exchange membranes.

UNIT – V : INDUSTRIAL ELECTROCHEMICAL PROCESSES

Water treatment and environmental protection – metal ion removal and metal recovery – electro – filtration of particulates form gases – electrodialysis – desalination – electroflotation.

Reference

1. P.H. Rieger – Electrochemistry, prentice hall, inc. New York 1987
2. D. Fletcher – Industrial electrochemistry, Chapman and Hall London 1982
3. J. Bockris and A.K. M. Reddy – Modern electrochemistry, Vol II. Mac Donold, London 1970
4. C. Rajagopal and K. Vasu – conversion coatings, 1st Edn. Tata McGraw Hill, New Delhi 2000.

314CMPE04 - CORROSION AND CORROSION CONTROL

UNIT I : CORROSION

Causes and effects of corrosion – theories of corrosion – oxidation – direct atmospheric effect – electrochemical corrosion – hydrogen evolution – presence and absence of oxygen corrosion by gaseous reduction.

UNIT II: FORMS OF CORROSION

Galvanic bimetal corrosion – differential aeration corrosion – concentration cell corrosion – erosion corrosion – pitting corrosion – underground soil corrosion – intergranular corrosion – stress corrosion – seasonal cracking of alloys – gaustic embrittlement – corrosion fatigue.

UNIT III: CORROSION TESTING

Rate of corrosion – calculation of G and other related thermodynamic parameters – potential measurement – electrochemical series – redox reactions – emf measurement and corrosion current – anodic and cathodic behavior of metals – passivity – testing of virgin metals – alloy – pourbaix and evans diagrams.

UNIT IV: FACTORS INFLUENCING CORROSION

Nature of metal – overvoltage – areas of anodic / cathodic – purity of metal – physical state of metals – passive nature of metal – solubility – volatility of corrosion products – corroding environment – influence of pH – ions – formations of cells – polarization of electrodes.

UNIT V: CORROSION CONTROL

Design – selection of materials – pure metals and alloys – annealing – elimination of galvanic action – cathodic protection – sacrificial anodic protection – impressed currect cathodic protection – modification of environment – deaeration – dehumidification – inhibitors – protective coatings – preparation of materials for coating – metallic and non metallic – organic coatings – special paints – varnish, enamel and lacquers.

References

1. M.G. Fontana and n.G. Green - Corrosion Engineerig, McGraw Hill Book Company, New York 1984.
2. J.H. Brophy R.M. Rose and J.Walf – The structure and properties of materials, wiley inter science inc, New York 1984
3. B.T. Kelly 0 irradiation diamagneto solids, pergamon press, New York 1992
4. D.R. Cross – Principles and applications of electrochemistry, chapman and hall U.K. 1988.

314CMPE05 - SUPRAMOLECULAR CHEMISTRY & CRYSTAL ENGINEERING

UNIT- I:Introduction of supra molecular chemistry

Concepts and Languages of supramolecular chemistry. Various types of non-covalent interactions. Hydrogen bonds, C-H…X interactions, Halogen bonds. π – π interactions,non –bonded interactions. Various types of molecular recognition. Crystal engineering of Organic solids: Hydrogen bonded supramolecular patterns involving water / carboxyl / halide motifs. Concepts of different types of synthons based on non-covalent interactions. Principles of crystal engineering and non-covalent synthesis. Polymorphism and Pseudopolymorphism. Supramolecular isomorphism / polymorphism. Crystal engineering of pharmaceutical phases.

UNIT –II: Organometallic systems

M.O.F (Metallo Organic Frame works) Combinations of different interactions to design molecular rods, triangles, ladders, networks, etc. Design of nanoporous solids. Inter ligand hydrogen bonds in metal complexes – implications for drug design. Crystal engineering of NLO materials,OLED.

UNIT –III: Coreceptor Molecules

Coreceptor Molecules and Multiple Recognition: Dinuclear and ploynulclear Metal ion Cryptates. Linear recognition of molecular length by Ditopic Coreceptors. Heterotopic Coreceptors- Cyclophane Receptors, Amphiphillic Receptors, Large molecular cages. Multiple Recognition in Metalloreceptors. Supramolecular dynamics.

UNIT- IV: Supramolecular Reactivity and Catalysis

Supramolecular Reactivity and Catalysis by Reactive Macrocyclic Cation Receptor Molecules. Catalysis by Reactive Anion Receptor Molecules. Catalysis with Cyclophane Type Receptors.Supramolecular Metallocatalysis. Cocatalysis: Catalysis of Synthetic reactions. Biomolecular and Abiotic catalysis Supramolecular Chemistry in solution: Cyclodextrin, Micelles, Dendrimmers, Gelators. Classification and typical reactions- Applications.

UNIT- V: Supramolecular Devices and Sensors

Various types of supramolecular devices – an overview. Supramolecular Photochemistry: Molecular and Supramolecular Photonic Devices – Light conversion and Energy transfer Devices. Molecular and Supramolecular Electronic Devices – Electronic conducting Devices - Molecular wires, Modified and Switchable Molecular wires. Molecular and Supramolecular Ionic Devices – Tubular Mesophases, Molecular Protonics. Switching Devices: Photo switching and Electro switching. Ion and molecule sensors. Role of supramolecular chemistry in the development of nanoscience and technology.

References

1. Lehn, J.M. Supramolecular Chemistry, VCH, Wienheim, 1995.
2. Desiraju, G.R. Crystal Engineering: The Design of Organic Solids, Elsevier, Amsterdam, 1989.
3. Desiraju, G.R. & Steiner, T. The weak Hydrogen Bond in Structural Chemistry and Biology: Oxford University press: Oxford, 1999.
24
4. Jeffrey, G. A. Introduction to Hydrogen Bonding ; Oxford University press: New York, 1997.
5. Lehn, J.M. Transition metals in supramolecular chemistry : John Wiley & sons: New York, 1999.
6. Desiraju, G.R. (2001). Current Science, 81, 1038.
7. Rao, C.N.R. (2001). Current Science, 81, 1030.
8. "Molecule Matters" Saravanakumar, k & Sankararaman, S,(2007).Resonance,Vol.12, No 11,

314CMPE06 - PHARMACEUTICAL CHEMISTRY

UNIT I: INTRODUCTION TO DRUG DESIGN

Factors governing drug design – advantages – types of drug – literature survey for preparation of drugs – characterization and structural elucidation of drugs using different spectral methods. Analgesics – narcotic analgesics – morphine analogues – synthesis of codeine – synthetic narcotic analgesics – synthesis and use of pethidines, methodones, dexdtropropoxyfene – narcotic antagonists – nalorphine – naloxone- antipyretic analogeics – salicylic acid analogues – methyl salicylate, phenyl salicylate – para amino phenol derivatives – structure synthesis and use of paractamol, phenacetin, aspirin and salol.

UNIT II: ANTIHIST AMINES AND ANTIMALARIALS

Anthithistamines – classification H1 & H2 receptor antagonists – structure, synthesis, activity and use of diphenhydramine, cyclizinc, chlorpheneraminemaleate and promethazine. Antimalerials – classification – quinine 4-amino and 8-amino quinolines – chloroquine phosphate – pyrimidines and acidines sedatives – barbiturats – structure, synthesis, action and use of phenodarbitol – benzodiazepines – mode of action structure and synthesis of diazepam and nitrazepam.

UNIT III: ANTIBIOTICS AND ANTIBACTERIALS

Antibiotics – penicillin, D-Pencillamine, phenoxy methyl pencillin – chloramphenicol- antibacterials – norfloxacin, ciproflozacin, trimethoprimsulphadrugs – mode of action preparation of sulphanilamide, sulphadiazine, sulphathiazole, sulphapyridine, sulphadimidine, sulphaguidines and sulphamethoxazole, antifungals – action, use and synthesis of clotrimazole, micronazole and isoconazole.

UNIT IV: ANTIHYPERTENSIVE AND ANTITUBERCULAR DRUGS

Antihypertensive drugs – synthesis and mode of action of methyldopa, pargyline, bertyline, hydralazine and propranolol – Antitubercular drugs – synthesis of PAS, ethambutol, pyrazinamide and isoniazid.

UNIT V: ANTIDIARRHEAL AGENTS

Antitussives and antineoplastic drugs – antidiarrheal agents – cimetidine , domperidone and loperamide, expectorants – antitussives – guaiphenesin, ambroxal bromohexine and dextromethorphan, antineoplastic drugs – alkylating agents – nitrogen mustards – sulphonic acid esters.

References

1. A. Berger – Medicinal chemistry, wiley interscience, New York, vol 1&2,1990
2. Asutoshkar – Medicinal chemistry, wiley eastern ltd, Chennai , 1992
3. Bentely and driver's textbook of pharmaceutical chemistry, Oxford Univ. press, 1985
4. H.J. Roth and A. Keleemann – pharmaceutical chemistry col. 1 drug synthesis.

Registrar