MANGALORE UNIVERSITY
M. Sc. Degree Programme in Chemistry:

CHOICE BASED CREDIT SYSTEM (CBCS) SEMESTER SCHEME

C O U R S E P A T T E R N AND S C H E M E OF E X A M I N A T I O N
(Year 2014-2015 onwards)

Semester	Paper	Instruction hrs/week	Duration of Exam(hrs)	Marks			Credits
				IA	Exam	Total	
I/II	4 Theory Papers	4x4	4x3	4x30	4x70	4x100	4x4
	3 Practicals. and 1 theory paper of 2 hrs duration per week in each semester	3x4 1x2	3x4 1x2	3x15 1x15	3x35 1x35	3x50 1x50	3x2 1x2
	Semester Total 18T+12P		180	420	600		24
III/IV	4Theory Papers	4x4	4x3	4x30	4x70	4x100	4x4
	3 Practicals	3x6	3x5	3x25	3x50	3x75	3x3
	Seminar	1	-	25	-	25	1
	Semester Total	16T+18P	220	430	650		26
					Grand Total		100
In the III / IV Semester, there may be project work/dissertation in lieu of 1 or 2 Practicals.							

M. Sc. DEGREE PROGRAMMES IN CHEMISTRY

The First, Second and Third Semesters of the course involve theory and practicals, while the IV Semester involves theory, practicals and project work. The project work shall be carried out for 6 to 8 weeks (at least 30 hrs per week), after the Second Semester of the course, either in the concerned Department or in an Approved Industry or in both, under the supervision of a teacher and submit a project report. Experts from the industries may also be involved in the project work as co-guides and in the evaluation of project reports.

BASIS FOR INTERNAL ASSESSMENT:

Internal assessment marks in theory papers shall be based on tests. The tests may be conducted 8 and 12 weeks after the start of a semester. Practical internal assessment marks shall be based on test and records. The practicals test may be conducted 10 weeks after the start

of a semester. The Seminar shall be of at least 45 minutes duration. The project report shall be evaluated for 75 marks. The Seminar in IVSemester shall be related to the project.

THEORY QUESTION PAPERS PATTERN

The Syllabus of each paper shall be grouped into units of 14 teaching hours. All the papers, except, Environmental Chemistry (1st semester) and Diffraction & Electroanalytical Techniques (2nd Semester) shall contain four such units each. Question Papers in all the four semesters shall consist of Parts A and B. Part A shall contain twelve (12) very short answer objective type questions carrying 2 marks each drawn from all the four units of the syllabus (3 questions per unit). Ten (10) questions out of Tweleve (12) are to be answered. Part B shall contain eight (8) brief and/or long answer questions carrying 10 marks each drawn from all the four units of the syllabus (2 questions per unit). There may be a maximum of three sub-divisions per question, carrying 3 or more marks per sub-division. Five (5) out of eight (8) questions are to be answered.

The Syllabi of the papers, in AC 405/OC 405/CA 405 - Environmental Chemistry (1st semester) and in in AC 455/OC 455/CA 455 - Diffraction & Electroanalytical Techniques (2nd Semester) shall also be grouped into units of 14 teaching hours. They shall contain two such units each. Question Papers in AC 405/OC 405/CA 405 and AC 455/OC 455/CA 455 shall also consist of Parts A and B. Part A shall contain six (6) very short answer objective type questions carrying 2 marks each drawn from both the units of the syllabus (3 questions per unit). Four (4) questions are to be answered. Part B shall contain five (5) brief and/or long answer questions carrying 9 marks each drawn from both the units of the syllabus (2 questions per unit and a combined question from both the units). There may be a maximum of three sub-divisions per question, carrying 3 or more marks per sub-division. Three (3) out of five (5) questions are to be answered.

PRACTICALS EXAMINATION PATTERN

In the I& II semesters, the 35 marks shall be awarded based on the experiment. But in the III & IV semesters, out of 50 marks, 10 marks are for the viva to be conducted during the practical examinations and 40 marks for the experiment.

Description of Papers	Teaching Hrs/week	Hrs.of Exam	Max Marks: Exam+IA	Credits for the Course
I Semester: i) Theory				
CH 401 : Inorganic Chemistry	4	3	70+30	4
CH 402 : Organic Chemistry	4	3	70+30	4
CH 403 : Physical Chemistry	4	3	70+30	4
CH 404 : Molecular Spectroscopy	4	3	70+30	4
CH 405: Environmental Chemistry	2	2	35+15	2
ii) Practicals				
CH 406 : Inorganic Chemistry Practicals-I	4	4	35+15	2
CH 407 : Organic Chemistry Practicals-I	4	4	35+15	2
CH 408 : Physical Chemistry Practicals-I	4	4	35+15	2
II Semester: i) Theory				
CH 451 : Advanced Inorganic Chemistry	4	3	70+30	4
CH 452 : Advanced Organic Chemistry	4	3	70+30	4
CH 453 : Advanced Physical Chemistry	4	3	70+30	4
CH 454 : Molecular Symmetry & Spectroscopy	4	3	70+30	4
CH 455: Diffraction and Electroanalytical Techniques	2	2	35+15	2
ii) Practicals				
CH 456 : Inorganic Chemistry Practicals-II	4	4	35+15	2
CH 457 : Organic Chemistry Practicals-II	4	4	35+15	2
CH 458 : Physical Chemistry Practicals-II	4	4	35+15	2
III Semester: i) Theory				
CH 501 : Choice Based Paper	4	3	70+30	4
CH 502 : Co-ordination and Bioinorganic Chemistry	4	3	70+30	4
CH 503 : Reaction Mechanism & Heterocyclic Chemistry	4	3	70+30	4
CH 504: Electrochemistry and Polymers	4	3	70+30	4
ii) Practicals				
CH 505 : Inorganic Chemistry Practicals-III	6	5	50+25	3
CH 506 : Organic Chemistry Practicals-III	6	5	50+25	3
CH 507 : Physical Chemistry Practicals-III	6	5	50+25	3
CH 508 : Seminars	2		25	1
IV Semester: i)Theory				
CH 551 : Organometallic Chemistry	4	3	70+30	4
CH 552 : Organic Synthetic Methods	4	3	70+30	4
CH 553 : Solid State Chemistry & Reaction Dynamics	4	3	70+30	4
CH 554 : Bioorganic and MedicinalChemistry **ii) Practicals**	4	3	70+30	4
CH 555 : Inorganic Chemistry Practicals-IV	6	5	50+25	3
CH 556 : Organic Chemistry Practicals-IV	6	5	50+25	3
CH 557 : Physical Chemistry Practicals-IV	6	5	50+25	3
CH 558 :Seminars	2		25	1

BASIS FOR INTERNAL ASSESSMENT:

Internal assessment marks in theory papers shall be based on tests. The tests may be conducted 8 and 12 weeks after the start of a semester. Practical internal assessment marks shall be based on test and records. The practical tests may be conducted 10 weeks after the start of a semester. The Seminar shall be of at least 45 minutes duration.

THEORY QUESTION PAPERS PATTERN

The Syllabus of each paper shall be grouped into units of 14 teaching hours. All the papers, except CH 405-Environmental Chemistry(1st Semester) and CH 455-Diffraction and Electroanalytical Techniques (2nd Semester), shall contain four such units each. Question Papers in all the four semesters shall consist of Parts A and B. Part A shall contain twelve (12) very short answer objective type questions carrying 2 marks each drawn from all the four units of the syllabus (3 questions per unit). Ten (10) out of twelve (12) questions are to be answered. Part B shall contain eight (8) brief and/or long answer questions carrying 10 marks each drawn from all the four units of the syllabus (2 questions per unit). There may be a maximum of three sub-divisions per question, carrying 3 or more marks per sub-division. Five (5) out of eight (8) questions are to be answered.

The Syllabi of the papers, CH 405 and CH 455, shall also be grouped into units of 14 teaching hours. They shall contain two such units each. Question Papers in CH 405-Environmental Chemistry and CH 455-Diffraction and Electroanalytical Techniques shall also consist of Parts A and B. Part A shall contain six (6) very short answer objective type questions carrying 2 marks each drawn from both the units of the syllabus (3 questions per unit). Four (4) questions are to be answered. Part B shall contain five (5) brief and/or long answer questions carrying 9 marks each drawn from both the units of the syllabus (2 questions per unit and a combined question from both the units). There may be a maximum of three sub-divisions per question, carrying 3 or more marks per sub-division. Three (3) out of five (5) questions are to be answered.

PRACTICALS EXAMINATION PATTERN

In the first and second semesters, the 35 marks shall be awarded based on the experiment. But in the third and fourth semesters, out of 50 marks, 10 marks are for the viva to be conducted during practicals and 40 marks for the experiment.

FIRST SEMESTER M. Sc. Course in Chemistry

CH 401: INORGANIC CHEMISTRY

UNIT- I: **[14 Hours]**

Ionic bond: Properties of ionic substances, coordination number of an ion, structures of crystal lattices- NaCl, CsCl, ZnS and rutile. Lattice energy- Born Lande equation, Born-Haber cycle, Uses of Born-Haber type of calculations. Ionic radii, methods of determining ionic radii, factors affecting ionic radii, radius ratio rule, covalent character in ionic bonds, hydration energy and solubility of ionic solids.

Covalent bond: valence bond theory, resonance, hybridisation, Bent's rules and enregetics of hybridization, Deduction of molecular shapes – VSEPR theory.

M.O.theory, application to homo- and hetero-diatomic and -triatomic molecules.

UNIT -II: **[14 Hours]**

Alkali and alkaline earth metal complexes of crown ethers, cryptands and calixarenes and their biological significance.

Halogens and Noble gas chemistry –interhalogens, psuedohalogens, polyhalide ions, oxyhalogen species, xenon oxides and fluorides. Oxy- and peroxy acids of N, P and S.

Graphitic compounds, carbides, pure silicon, silica and silicates, zeolites.

UNIT- III: **[14 Hours]**

Theories of acids and bases – Lux-Flood theory, Bronsted and Lewis acids and bases, gas phase vs. solution acidity, solvent leveling effects, hardness and softness, HSAB concept. super acids. Reactions in non-aqueous media: Liquid ammonia, anhydrous sulphuric acid, glacial acetic acid, anhydrous HF, bromine trifluoride, liquid sulphur dioxide and dinitrogen tetroxide. Reactions in molten salts.

UNIT- IV: **[14 Hours]**

Sampling techniques, preparation of samples for analysis. Nature of errors, statistical treatment of errors, the t- and F-tests, significant figures, rejection of data.

Precipitation phenomena: precipitation from homogeneous solutions, organic precipitants in inorganic analysis. Solvent extraction of metal ions, nature of extractant, distribution law, partition coefficients, types of extractions and applications.

Theories of redox indicators, titration curves, feasibility of redox titrations.

Chelometric titrations- titration curves with EDTA, feasibility of EDTA titrations, indicators for chelometric titrations, selective masking and demasking techniques, industrial applications of masking.

References:

1. J.E Huheey,Keiter, Keiter and Medhi: Inorganic Chemistry (4th ed.), Pearson Education, 2006.
2.Shriver, Atkins and Langford : Inorganic Chemistry (3rd edn.) OUP, 1999.
3.J.D.Lee: Concise Inorganic Chemistry, (5th edn.) Blackwell Science, 2000.
4.B.E.Douglas, D.McDaniel & A Alexander: Concepts & Models of Inorganic Chemistry, Wiley 2001
5.W.W.Porterfield: Inorganic chemistry – A Unified Approach, Elsevier, 2005.

CH 402: ORGANIC CHEMISTRY

UNIT –I: [14 Hours]

Nature of Bonding in Organic Molecules: Hybridization and Index of Hybridization, Localized and delocalized bonding: Conjugation crossconjugation, resonance, hyper-conjugationandtautomerism.Huckel rule, Homo-aromatic, non-aromatic and anti-aromatic systems. Aromaticity in benzenoid and non-benzenoid molecules. Annulenes and hetero-annulenes. Physical methods to study aromaticity-UV, IR &^{1}H NMR. 7 hrs

Bonds weaker than covalent: Addition compounds, crown ether complexes, cryptands,inclusioncompounds, catenanes, fluxionalmolecules.2hrs

Acids and Bases: Introduction to acids and bases, Bronsted-Lowry and Lewis acid- bases concept, organic acids and bases, pKa and pH, effect of solvent on acid and base strength, effect of structure of organic compound on acid & base strength. Running scale of acidity, General & specific acid-base catalysis. 5 hrs

UNIT-II: [14 Hours]

Methods of Determining Reaction Mechanism: Kinetic and non-kinetic methods, Identification of products, detection of intermediates, isotopic labeling, stereochemical evidences, cross-over experiments, Limitation of reactions, kinetic evidences and kinetic isotopic effects. 4 hrs

Reaction Intermediates: Generation, structure, stability, reactivity and detection of classical and non-classical carbocations, carbanions, free radicals, carbenes, nitrenes and arynes. Singlet oxygen-generation and reactions with organic molecules. 4 hrs

Aliphatic Nucleophilic Substitution Reactions: Mechanism and scope of aliphatic nucleophilic substitution reactions-S_N1, S_N2 and S_Ni. Stereochemistry of nucleophilic substitution reactions, allylic nucleophilic substitution reactions, Walden inversion, neighbouring group participation and anchimeric assistance. Factors influencing the rates of nucleophilic substitution reactions. 6 hrs

UNIT-III:Stereochemistry [14Hours]

Optical Isomerism: Conformation and configuration of molecules, projection formulae, Fischer, Saw-horse, Newman and Flying wedge representations.Interconversion of these formulae. Absolute configuration (D,L) and (R,S) systems. Elements of symmetry,Psedoassymmetric centres, chirality, molecules with more than one chiral centre, threo and erythro isomers, methods of resolution, stereospecific and stereoselective synthesis, asymmetric synthesis, Cram's and Prelog's rules. Optical activity in the absence of chiral carbon-biphenyls, allenes and spiranes. Conformational analysis of cycloalkanes and decalins. Effect of conformation on reactivity. Acyclic & cyclic systems-Substituted cyclohexanes, cyclohexanones, cyclohexanols, Curtain-Hammet Principle.Stereochemistry of compounds containing nitrogen, sulphur and phosphorus. 11hrs

Geometrical Isomerism: Cis-trans isomerism resulting from double bonds, monocyclic compounds & fused ring systems. E,Z-notations, determination of configuration of geometrical isomers, syn & anti isomers.3hrs

UNIT-IV: Carbohydrates& Heterocycles [14Hours]

Carbohydrates: Introduction, Configuration and conformation of monosaccharides, Chemistry of important derivatives of monosaccharides-ethers, esters, acetals, ketals, deoxysugars,

aminosugars, Structure of disaccharides-maltose, cellobiose and sucrose. General methods of structural degradation of polysaccharides-methylation, partial hydrolysis, periodate oxidation, Smith degradation and alkaline degradation techniques. Structures of cellulose, chitin, starch and glycogen.
8 hrs

Heterocycles: Introduction, Biologically important heterocycles, Synthesis and reactions of five membered simple and fused heterocycles-furan, pyrrole, thiophene, pyridine,benzofuran, benzothiophene & indole. 6 hrs

References:

1.Organic Chemistry-P.Y.Bruice (Pearson Education Pvt. Ltd.,New Delhi),2002.
2.Stereochemistry,Conformation and Mechanism-P.S.Kalsi (Wiley Eastern,New Delhi)1993.
3.Stereochemistry of Carbon Compounds-E.L.Eliel (Tata McGraw Hill, New. Delhi) 1994.
4.Advanced Organic Chemistry-Reactions, mechanisms & structure-J.March(Wiley, NY)2000.
5.Organic Chemistry-Vol. -1,2 &3-Mukherji, Singh and Kapoor. (Wiley Eastern,) 1994.
6.A guide book of mechanisms in Organic Chemistry-P.Sykes (Orient- Longman) 1985.
7.Organic Chemistry-R.T. Morrison and R.N. Boyd (Prentice Hall, New Delhi) 1994.
8.Organic Chemistry 4th Edn.–S.H. Pine et al (McGraw-Hill, London) 1987.
9.Advanced Organic Chemistry- R.A. Carey and R.J. Sundberg (Plenum, New York)1990.
10.Modern Concepts of Advanced Organic Chemistry-R.P. Narein (Vikas, Delhi) 1997.
11.A Text book of Organic Chemistry-Tewari, Vishnoi and Mehrotra (Vikas, New Delhi)1998.
12.A Text book of Organic Chemistry-3rd Edn.-R.K. Bansal, (New Age, New Delhi) 1997.
13.Organic Chemistry-3rd Edn- F.A. Carey (Tata McGraw Hill, New Delhi) 1996.
14.Stereochemistry by K.Mislow.

CH 403: PHYSICAL CHEMISTRY

UNIT – I : [14 hours]

Catalysis: Homogeneous catalysis-equilibrium and steady state treatments, activation energies of catalysed reactions. Acid-base catalysis (general and specific), protolytic and prototropic mechanisms, catalytic activity and acid strength measurements. Kinetics of enzyme catalysed reactions-Michaelis-Menten equation. Effect of pH, temperature & inhibitors 7 hrs.

Surface reaction kinetics: A review of adsorption isotherms, uni- and bi-molecular reactions. multilayer adsorption-BET equation- application in surface area determination. Harkin–Jura equation-application. Desorption & heterogeneous catalysis–catalytic activity at surfaces, semiconductor catalysis, n-&p-type. Mechanism of surface reactions. . 7 hrs.

UNIT - II: [14hours]

Chemical Kinetics: Complex reactions- parallel, consecutive and reversible reactions. Chain reactions (H_2-halogen reactions). Branched chain reactions- general rate expression, explosion limits and Oscillatory reactions. 4 hrs.

Reactions in solution: Ionic reactions - salt and solvent effects. Substituent effects on the rates of reactions - Hammett and Taft equations, linear free energy relationships. 4 hrs.

Fast reactions-Introduction, Study of fast reactions by-flow, relaxation, molecular beam and photolysis and line broadening methods. 4 hrs

Theories of Reaction Rates: Collision theory of reaction rates, limitations and an introduction to transition state theory. 2hrs

UNIT-III : [14hours]

Electrochemistry of solutions: Ionic atmosphere-introduction, derivation and its effect on the theory of conductivity. Walden`s rule. Debye-Huckel limiting law (DHL)- Concept of Ionic strength and activity coefficient, derivation of DHL equation, modifications to DHL equation-qualitative tests and verification of DHL equation. Bjerrum theory of ion association, triple ion formation and significance, abnormal conductance 5hrs.

Corrosion: Introduction, principles, loss due to corrosion, Forms of corrosion (Galvanic, Atmospheric, stress, microbial, and soil). Corrosion rate measurement, EMF series &Galvanic series and their limitations. Thermodynamics (Pourbaix diagram) and Kinetics (mixed potential theory) of corrosion. Kinetics of passivity. Protection against corrosion (Design improvement, Anodic and cathodic protection, inhibitors, coating).Corrosion failure and its treatment. 9hrs.

UNIT-IV : **[14hours]**

Photochemistry: Introduction to photochemistry. Actinometry. Frank-Condon principle. Absorption and emission spectra- effect of solute solvent interactions on electronic spectra-spectral shifts. Physicochemical properties of electronically excited molecules-excited state dipole moments, acidity constants. Flash photolysis technique.

Photophysical pathways- Jablonski diagram, Radiationless transitions and selection rules. Photochemical kinetics of unimolecular and bimolecular processes. Quenching-collisions in the gas phase, solution (Stern-Volmer equation). Photoisomerization, photo Fries rearrangement and Norrish type cleavage reactions with specific examples.

REFERENCES :

1. Physical Chemistry, 5th Ed., - Atkins (ELBS) 1995.
2. Physical chemistry – G. M. Barrow (McGraw Hill, Int. St. Ed) 1988.
3.Fundamentals of Physical Chemistry – Maron and Lando (Collier, Macmillan) 1974.

4. Chemical Kinetics - K. J. Laidler (Harper and Row) 1987.
5. Kinetics of Chemical Reactions, S K Jain (Vishal Publications, Delhi) 1982.
7. Principles and Applications of Electrochemistry–Crow (Chapman hall, New York) 2014.
8.Electrochemistry and Corrosion Science-Nebtor Ferez (Springer Pvt.Ltd.), Delhi, 2010.
9. Fundamentals of Photochemistry – Rohatgi and Mukherje (New Age Bangalore), 2000.

CH 404: MOLECULAR SPECTROSCOPY

UNIT–I: [14 hours]

Unifying Principles -Electromagnetic radiation, dual nature, regions of the spectrum, interaction of electromagnetic radiation with matter - absorption, emission, transmission, reflection, refraction, dispersion, polarization and scattering. Natural line width and broadening, intensity of spectral lines. Rotational, vibrational and electronic energy levels, selection rules.

Microwave Spectroscopy- The rotation and classification of molecules, rotation spectra of diatomic and polyatomic molecules. Rigid and non-rigid rotator models. Determination of bond lengths, isotope effect on rotation spectra. Stark effect, nuclear and electron spin interaction. Microwave Spectrometer.

Vibrational Spectroscopy: Vibration spectra of diatomic molecules - linear harmonic oscillator, vibrational energies, zero point energy, force constants & bond strengths; anharmonicity of molecular vibrations- Morse PE diagram, selection rules, fundamental, overtones and hot bands. Vibrations of polyatomic molecules- normal modes of vibrations & nature of molecular vibrations (Ex-CO_2& H_2O).

UNIT–II :[14 hours]

Vibration-rotation spectra of diatomic and polyatomic molecules, selection rules, PQR branches. IR Spectrophotometer-Instrumentation, sample handling techniques, FTIR Spectroscopy. Far IR region.

Raman Spectroscopy: Classical and quantum theories of Raman effect, concept of polarizability and polarizability ellipsoid. Rotational and vibrational Raman spectra, selection rules, Raman activity of vibrations, vibrational - rotational Raman spectra, selection rules, mutual exclusion principle, polarization of Raman lines. An introduction to Laser Raman Spectroscopy. Raman Spectrometer – instrumentation. Applications of IR and Raman spectroscopy in elucidation of molecular structure (Ex - H_2O, N_2O & CO_2 molecules).

UNIT–III: [14 hours]

Application of infrared spectroscopy in the structural study-identity by fingerprinting and identification of functional groups. Characteristic vibrational frequencies of common functional groups (alkanes, alkenes, alkynes, aromatic compounds, alcohols, ethers, phenols and amines). Study of vibrational frequencies of carbonyl compounds (ketones, aldehydes, esters, amides and acids). Factors affecting band positions and intensities such as effect of hydrogen bonding, phase and solvent on vibrational frequencies, overtones, combination bands and Fermi resonance.

Polarimetry: Plane polarized light, instrumentation, acid-catalyzed muta rotation of glucose, inversing of cane sugar-relative strengths of acids. Optical rotatory dispersion &circular dichroism–introduction, selection rules, deduction of absolute configuration, octant rule for ketones and cotton effect.

UNIT-IV: Nuclear Magnetic Resonance Spectroscopy [14 hours]

Magnetic properties of nuclei, theory and measurement techniques, NMR spectrometer, FT NMR and its advantages. Solvents used, chemical shift and its measurements, factors affecting chemical shift. Integration of NMR signals, spin-spin coupling, coupling constant. Shielding and deshielding. Chemical shift assignment of major functional groups, Classification (ABX, AMX, ABC, A_2B_2), spin decoupling; effects of chemical exchange, fluxional molecules, Hindered rotation through NMR spectrum, Karplus relationships (Karplus curve–variation of coupling constant with dihedral angle), double resonance techniques, NMR shift reagents,

solvent effects and Nulear Overhauser Effect. High resolution ^{1}H NMR. Applications of NMR spectroscopy in structure elucidation of simple organic and inorganic molecules. ^{1}H NMR in the structural study of complex organic compounds. Pulse techniques in NMR, two dimensional and solid state NMR.Use of NMR in Medical diagnostics.

REFERENCES:

1.Fundamentals of Molecular Spectroscopy, Banwell & McCash (Tata McGraw Hill, New Delhi)2007.
2. Spectroscopy, H. Kaur (Pragathi Prakashana,Meerut), 2012.
3.Spectroscopy, Donald L.Pavia (Cengage learning India Pvt.Ltd., Delhi), 2007.
4.Spectroscopy, B.K.Sharma (Goel prakashan, Meerut), 2013.
5. Organic Spectroscopy-3rd ed.-W.Kemp (Pagrave Publishers, New York), 1991.
6.Spectrometric Identification of Organic Compounds-
Silverstein,Bassler&Monnill(Wiley)1981.

CH 405: ENVIRONMENTAL CHEMISTRY

UNIT-I: **[14 hours]**

Environmental segments, evolution of earth's atmosphere. Air pollution : Air pollutants, prevention and control, Green house gases and acid rain. Carbon monoxide, industrial sources and tranportation sources. SO_x- sources, ambient concentration, test methods, control techniques - scrubbing, , limestone injection process. Ozone hole and CFC's. Photochemical smog and PAN. NO_x - Sources, ambient concentration, test methods, NO_x, control techniques. Particulates : Size distribution, , particulate collection - settling chambers, centrifugal separators, wet scrubbers, electrostatic precipitators & fabric filters. Catalytic converters for mobile sources. Bhopal gas tragedy.

UNIT-II: **[14 hours]**

Hydrologic cycle, sources, chemistry of sea water, criteria and standards of water quality- safe drinking water, maximum contamination levels of inorganic and organic chemicals, radiological contaminants, turbidity, microbial contaminants. Public health significance and measurement of colour, turbidity, total solids, acidity, alkalinity, hardness, chloride, residual chlorine, sulphate, fluoride, phosphate and different forms of nitrogen in natural and polluted water. Chemical sources of taste and odour, treatment for their removal, sampling and monitoring techniques. Determination and significance of DO, BOD ,COD and TOC. Water purification for drinking and industrial purposes, disinfection techniques, demineralization, desalination processes and reverse osmosis.

REFERENCES :

1. A.K. De : Environmental Chemistry, (Wiley Eastern).
2. S.K.Banerji : Environmental Chemistry, (Prentice Hall India), 1993.
3 S.D. Faust and O.M. Aly : Chemistry of Water Treatment, (Butterworths),1983.
4. G.D. Christian : Analytical Chemistry, (4th Ed.), (John Wiley)
5. Sawyer and McCarty, Chemistry for Environmental Engineering(McGraw Hill) 1978
6. I.Williams, Environmental Chemistry, John Wiley, 2001

CH 406: INORGANIC CHEMISTRY PRACTICALS - I

1. Analysis of Hematite-insoluble residue by gravimetry and Iron by volumetry using Ce^{4+}.
2. Analysis of Dolomite - insoluble residue be gravimetry and Ca, Mg by complexometry.
3. Pyrolusite - Insoluble residue by gravimetry and Manganese content by oxalate method.
4. Analysis of solder - Pb and Sn by EDTA method.
5. Complexometric determination of Mn, Cu, Ni and Fe-Cr mixture
6. Hardness of water
7. Analysis of Halide Mixture - Iodide by KIO_3 and total halide by gravimetrically.
8. Colorimetric Determination of Iron by thiocyanate and Cu by aqueous ammonia.
9. Gravimetric Determinations of Mn, Ni, Mo, Pb/Cr, sulphide, thiocyanate.
10. Statistical Analysis of Data.

Reference :

1. Vogel's Text Book of Quantitative Chemical Analysis(5^{th} Ed), G.H.Jeffrey, J.Bassette, J.Mendham and R.C.Denny, Longman, 1999.

CH 407 : ORGANIC CHEMISTRY PRACTICALS - I

Single and two stage organic preparations

1. Electrophilic substitution reactions–Preparations of p-bromoaniline, p-nitroaniline, and picric acid
2. Alkylations–Preparations of nerolin and N-methyl anthranilic acid.
3. Acetylations–Preparations of β-D-glucose penta-acetate and 2-naphthyl acetate.
4. Reactions with ring formation–Preparations of 1,2,3,4–tetrahydrocarbazole and 7–hydroxy-4-methyl-coumarin.
5. Diazotisation reactions–Preparations of iodo, chloro and azo compounds.
6. Dehydration reactions–Preparations of cyclohexene and succinic anhydride
7. Condensation reactions–Condensations involving diethylmalonate and ethyl acetoacetate. Aldol condensation and Perkin reactions.
8. Halogenation reactions-Preparation of n-butylbromide &α,β-dibromocinnamic acid.
9. Reduction reactions–Reductions of nitro compounds and carbonyl compounds.
10. Oxidation reactions-Preparation of p-nitrobenzoic acid, p-benzoquinone and adipic acid.

References :

1. Laboratory Manual in Organic Chemistry–R. K. Bansal (New Age, New Delhi)1990.
2. Experimental Organic Chemistry–Vol. I & II–P. R. Singh et al (TMH New Delhi)1981
3. Laboratory Manual in Organic Chemistry–Dey &Sitaraman(Allied , New Delhi)1992.
4. Vogel's Text Book of Practical Organic Chemistry including Qualitative Organic Analysis-B. S. Furniss et al., (Longman - ELBS, London), 1989.

CH 408 : PHYSICAL CHEMISTRY PRACTICALS - I

Any 12 experiments are to be carried out

1. Potentiometric titration of halides in mixtures (Cl^-, Br^- and I^-) with silver nitrate
2. Potentiometric determination of redox potentials (Fe^+ Vs. I^- Mn^{+7}, Ce^{+4}).
3. Potentiometric and conductometric acid –base titrations in partial,aqueous & non-aqueous media.
4. Conductometric titrations of displacement and precipitation reactions.
5. Determination of equivalent conductances and dissociation constants of weak acids.
6. Determination of solubility of lead iodide at different T & hence molar heat of solution
7. Determination of pH of buffer solutions with a pH meter & evaluation of pK_a of acids
8. Verification of Walden`s rule (relation between viscosity of a solution and the electrical conductivity.
9. Study of variation of viscosity of a liquid with temperature

10. a)Determination of parachor value for CH_2 group by S.T method,
    b)Determinationof the composition of a solution by S.T measurement and
    c) Determination of CMC of a soap solution by S.T measurement
11. Potentiometric determination of solubility of insoluble silver halide and the standard electrode potential using quinhydrone electrode
12. Determination of degree of hydrolysis of CH_3COONa and NH_4Cl.
13. Determination of hydrolysis constant of aniline hydrochloride.
14. Verification of Nernst equation for Ag^+, $Cu^{2+}$and Zn^{2+} species.

References:

1. Findlay's Practical Physical Chemistry- B. P. Levitt (Longman, London).
2. Experiments in Physical Chemistry–James and Prichard.
3. Experimental Physical Chemistry - Daniels et al.
4. Experimental Physical Chemistry-Das & Behera(Tata McGraw Hill, New Delhi)1983.
5. Advanced Practical Physical Chemistry–Yadav (1989).
6. Experiments in Physical Chemistry–J. C. Ghosh(Bharathi Bhavan)1974.

SECOND SEMESTER M. Sc. Course inChemistry

CH 451: ADVANCED INORGANIC CHEMISTRY

Unit -I: **[14 Hours]**

Chemistry of higher boranes, classification, structures and M.O. description of bonding, framework electron counting, Wade's rules, chemistry of B_5H_9, $B_{10}H_{14}$ and $B_nH_n^{2-}$. Carboranes and metallocarboranes. Cyclophosphazenes, phosphazene polymers, P-O and P-S cage compounds. S-N compunds : binary sulphur nitrides- S_4N_4, S_2N_2 and $(SN)_x$. Borazines and boron nitride, Isopoly and heteropoly acids of transition metals.

Unit -II: **[14 Hours]**

Coordination numbers 2-10 and their geometry, crystal field theory of coordination compounds, d-orbital splittings in octahedral, square planar and tetrahedral fields, spectrochemical series, and Jahn-Teller effect.

Structural evidences for ligand field splittings – hydration, ligation and lattice energies, site preference energies. MO theory of coordination compounds- MO energy level diagrams for octahedral and tetrahedral complexes.

Stepwise and overall formation constants, factors affecting stability of metal complexes, determination of binary formation constants by pH-metry and spectrophotometry.

Unit-III: **[14 Hours]**

Metal Pi-acceptor complexes: metal carbonyls – preparative methods, structure and bonding, vibrational spectra of metal carbonyls for bonding and structural elucidation, magnetic and X-ray evidences of structures, M.O.representation of bi- and tri-nuclear carbonyls,. Reactions of metal carbonyls. Metal carbonylates and carbonyl halides – preparation and important reactions. Chemistry of metal nitrosyls – preparation, structure and bonding; dinitrogen and dioxygen complexes. Metal-metal bonding in carbonyls and halides evidences for M-M bonding, factors favouring M-M bond formation. Metal clusters- bi-, tri-, tetra-, penta- and hexanuclear metal clusters, bonding in metal clusters. Zintl ions and Chevrel phases.

Unit -IV: **[14 Hours]**

Methods of reduction of oxide ores, Ellingham diagram, chemical and electrolytic reductions, reduction potentials, Latimer and Frost diagrams, effect of complexation on potential.

Trends in oxidations states, stereochemistry and ionic sizes of metals, comparison of 3d, 4d and 5d series by taking Ti subgroup as example. Lanthanides and actinides: electronic structure, oxidation states, extraction and separation of lanthanides, stereochemistry, spectral and magnetic properties of lanthanide and actinide complexes, lanthanide complexes as NMR shift reagents. Comparison with d-block ions.

References:

1.J.E Huheey, E.A..Keiter, R.L.Keiter & O K Medhi: Inorganic Chemistry (4th edn.), Pearson, 2006.
2.Shriver, Atkins and Langford : Inorganic Chemistry (3rd edn.) OUP, 1999.
3.J.D.Lee: Concise Inorganic Chemistry, (5th edn.) Blackwell Science, 2000.
4.B.E.Douglas, D.McDaniel &A Alexander: Concepts & Models of Inorganic Chemistry, Wiley 2001
5.W.W.Porterfield: Inorganic chemistry – A Unified Approach, Elsevier, 2005.

CH 452: ADVANCED ORGANIC CHEMISTRY

UNIT - I: [14 Hours]

Aliphatic Electrophilic Substitution Reactions: Bimolecular mechanisms-S_E1, S_E2 and S_Ei mechanism. Electrophilic substitution reactions accompanied by double bond shifts. 3 hrs

Aromatic Electrophilic and Nucleophilic Substitution Reactions: Mechanism of aromatic electrophilic substitution reactions, Arenium ion mechanism, orientation and reactivity, energy profile diagram. The ortho/para ratio, ipso attack, orientation in other ring systems. Mechanism of Vilsmeir-Haack reaction, Pechmann reaction and Fries rearrangement. Mechanisms of aromatic nucleophilic substitution reactions- S_NAr, S_N1 &aryne mechanism. Von-Richter rearrangement, Sommelet-Houser rearrangement, Smiles rearrangement. 11 hrs

UNIT- II: [14 Hours]

Free Radical Reactions: Types, mechanisms of free radical substitution reactions & neighbouring group assistance. Reactivity for the aliphatic and aromatic substances at a bridgehead. Reactivity of attacking radical. Effect of solvent on reactivity. Auto-oxidation, coupling of alkynes. Arylation of aromatic compounds by diazonium salts. Sandmeyer, Ullmann & Hunsidiecker reactions. 5 hrs

Elimination Reactions: Discussions of E1, E2 and E1cB mechanisms. Orientation during elimination reactions. Saytzeff and Hofmann rules. Reactivity-effects of substrate structures, attacking base, leaving group and solvent medium. 5 hrs

Pyrolytic Eliminations: Mechanisms of pyrolysis of esters of carboxylic acids. Chugaev reactions, Hofmann degradation, Cope elimination and xanthate pyrolysis. 4 hrs

UNIT- III: [14 Hours]

Formation and Hydrolysis of Esters: Plurality of mechanism. Mechanism of esterification reactions. Ester hydrolysis-$A_{AC}2$, $B_{AC}2$, $A_{AC}1$ & $A_{AL}1$ mechanism. Transesterification.4 hrs

Addition to Carbon-Carbon Multiple Bonds: Addition reactions involving electrophiles, nucleophiles and free radicals. Cyclicmechanisms. Orientation and stereochemistry. Addition of halogens, hydrogen halides, carboxylic acids and amines. Addition to cyclopropanes, hydroboration, Michael addition. Addition of oxygen across double bonds. 6 hrs

Addition to Carbon-Hetero Multiple Bonds: Electrophilic, nucleophilic and free radical additions to C=O and C=N systems. Addition of Grignard reagents. Reformasky reaction, aldol condensation, Knoevenagel condensation, Perkin reaction and Wittig reactions. 4 hrs

UNIT- IV: Chemistry of Heterocyclic Compounds [14 Hours]

Synthesis and reactions of three membered heterocycles-aziridines, oxiranes, episulfides, diaziridines, oxazirines and diazirines. Synthesis and reactions of four membered heterocycles-oxetanes, azetidines and thietanes.Synthesis & reactions of selenophenes, tellurophenes, oxazoles, imidazoles, thiazoles and oxazines..

References:

1.Organic Reactions and Their Mechanisms- P.S. Kalsi (New Age, New Delhi),1996.
2.Advanced Organic Chemistry 4th Edn- J. March (Wiley, NY) 2000.
3.Organic Reaction Mechanisms- Bansal (Tata McGraw Hill, New Delhi) 1978.
4.Organic Chemistry-Vol.–I & II-Mukherji, Singh and Kapoor(Wiley Eastern, New Delhi) 1985.
5.Mechanism and Theory in Organic Chemoistry-Lowry and Richardson Harper and Row, 1987.
6.An Introduction to the Chemistry of Heterocyclic Compounds-Acheson (Wiley–Eastern) 1987.
7. Heterocyclic Chemistry-J. Joule & G. Smith, (Van-Nostrand, ELBS), 1978.

8. Reaction Mechanisms in Organic Chemistry-Mukherji, Singh and Kapoor (McMillan) 1978.
9. Organic Chemistry-P.Y. Bruice (Pearson Education, New Delhi) 2002.

CH 453: Advanced Physical Chemistry

UNIT - I: [14 hours]

Chemical Thermodynamics : Entropy, dependence of entropy on variables of a system (S,T & V; S,T and P). Thermodynamic equations of state. Irreversible processes-Clausius inequality.

Free energy, Maxwell relations and significance, temperature dependence of free energy-Gibbs Helmholtz equation, applications of Gibbs Helmholtz equation.

Partial molar quantities, chemical potential and Gibbs-Duhem equations, determination of partial molar volume and enthalpy.

Fugacity, relation between fugacity and pressure, determination of fugacity of a real gas.

Activity. variation of fugacity and activity with temperature and pressure.

Thermodynamics of mixing, Gibbs-Duhem-Margules equation, Henry's law.

Excess thermodynamic functions-free energy, enthalpy, entropy and volume, Determination of excess enthalpy and volume.

Chemical affinity and thermodynamic functions, effect of temperature and pressure on chemical equilibrium-vant Hoff reaction isochore and isotherm.

Third law of thermodynamics, Nernst heat theorem, determination of absolute entropies using third law, entropy changes in chemical reactions.

UNIT - II: Statistical and Irreversible thermodynamics [14 hours]

Statistical Thermodynamics : Basic terms: Probability, cell, phase space, micro and macro states, thermodynamic probability, statistical weight factor, statistical equilibrium, assembly, ensemble and its classification, Derivation of Boltzmann-Maxwell, Bose-Einstein and Fermi-Dirac statistics, partition function and derivations of translational, rotational, vibrational and electronic partition functions, thermodynamic functions such as internal energy, heat capacity, entropy, work function, pressure, heat content, etc. Partition function and third law of thermodynamics, applications of partition function to mono atomic gases, diatomic molecules, equilibrium constant.Heat capacity of solids -the vibrational properties of solids, Einsteins theory and its limitations, Debye theory and its limitations. 9hrs.

Irreversible Thermodynamics-Thermodynamics of irreversible processes with simple examples. Uncompensated heat and its physical significance. Entropy production-rate of entropy production, entropy production in chemical reactions, the phenomenological relations. The principle of microscopic reversibility, Onsager reciprocal relations – validity (linear and non-linear rections) and application (Electrokinetic, Thermoelectric phenomena).

UNIT-III:Quantum Chemistry-1 [14 hours]

Particle waves and Schrödinger wave equation, wave functions, properties of wave functions, Normalization and orthogonality of wave functions. Operators and their algebra, linear and hermitian operators, operators for the dynamic variables of a system such as, position, linear momentum, angular momentum, total energy, eigen functions, eigen values and eigen value equation. Quantum numbers and their characteristics.

Shrodinger wave equation- significance and derivation. Eigen values and eigen functions. Statistical interpretation of ψ. Solution of SWE for simple systems-particle in a box(1D & 3D), particle in a ring, harmonic oscillator, rigid rotor, the H atom (solution of r,θ,Φ

equations), tunneling the harmonic oscillator, the rigid rotator, and the hydrogen atom.Quantum numbers and their characteristics.

UNIT-IV:Quantum Chemistry-II [14hours]

Approximates methods of solving SWE- Principle of Variation and Perturbation methods. Application of variation method to H and He atoms. Secular equations and determinants.

Chemical Bonding: Covalent bond-Valence bond and molecular orbital approaches with comparison. Application of VBT to H_2.

MO theory applied to homonuclear and heteronuclear diatomic molecules –calculation of BO.

Hybridisation-construction of wave function of hybrid orbitals (sp, sp^2 and sp^3). Calculation of bond angle between hybrid orbitals.

Huckel molecular orbital theory of conjugated systems - secular equations and determinants. Applications to linear (ethane, allyl, 1-3 butadiene) and cyclic (benzene) systems.

Calculation of charge density, bond order, free valence and delocalisation energy.

References:

1. Physical Chemistry, 5th Ed., - Atkins, (ELBS) 1995
2. Physical Chemistry, 4th ed.,Ignacia Tinowa Jr, Kenneth Sauer etal., (Pearson), 2011.
3. Chemical Themodynamics, Rajaram and Kuriokose (East-West)Pearson, Chennai, 2013.
4. Thermodynamics, 3rd Ed., R.C. srivastava and Subit K Saha (Prentice-Hall of India, Delhi), 2007.
5. Statistical Thermodynamics, M. C. Gupta (Wiley eastern Ltd.) 1993.
6. Advanced Physical Chemistry- Gurdeep R Chatwal (Goel Publishes, Meerut), 1992.
7. Introductory Quantum Chemistry – A.K.Chandra (Tata McGraw Hill) 1994.
8.Quantum Chemistry, A.B.Sannigrahi (Book and Allied Pvt.Ltd., Kolkatt), 2013.
9. Quantum Chemistry, Donald A.P (Viva Books, Delhi), 2013.
10. Physical Chemistry, 4th Edn., K.J. Laidler, J.H. Meiser, B.C.Sanctuary(Houghton Mifflin), 2003

CH 454: MOLECULAR SYMMETRY AND SPECTROSCOPY

UNIT- I: Symmetry and Group Theory [14 Hours]

Definitions of group, subgroup, relation between orders of a finite group and its subgroup. Conjugacy relation and classes, symmetry elements and symmetry operations, Schonflies symbols, Matrix representations of symmetry operations, products of symmetry operations, some properties of matrices and vectors, classification of molecules into point groups. Reducible and irreducible representations. The Great Orthogonality theorem (without proof), character tables. The direct product. Applications of group theory - Molecular vibrations, group theoretical selection rules for electronic transitions, for infra red and Raman spectra. Hybrid orbitals and Molecular orbitals, transformation properties of atomic orbitals.

UNIT- II:[14 Hours]

Electron Spin Resonance Spectroscopy: Basic principles, hyperfine couplings, the 'g' values, factors affecting 'g' values, isotropic and anisotropic hyperfine coupling constants, Zero Field splitting and Kramer's degeneracy. Measurement techniques and Applications to simple inorganic and organic free radicals and to inorganic complexes. 4 hrs

NQR Spectroscopy: Quadrupolar nuclei, electric field gradient, nuclear quadrupole coupling constants, energies of quadrupolar transitions, effect of magnetic field. Applications.3 hrs

Mössbauer Spectroscopy: The Mössbauer effect, chemical isomer shifts, quadrupole interactions, measurement techniques and spectrum display, application to the study of Fe^{2+} and Fe^{3+} compounds, Sn^{2+} and Sn^{4+} compounds(nature of M-L bond, coordination number and structure), detection of oxidation states and inequivalent Mössbauer atoms. 4 hrs

Photoelectron spectroscopy: Basic principles, valence &core binding energies, shifts in energies due to chemical forces, Photoelectron spectra of simple molecules, Auger transitions, measurement techniques. Applications. 3 hrs

UNIT- III: [14 Hours]

UV/Electronic Spectroscopy: Basic principles, Beer-Lambert law, molar absorptivity, energy levels, types of electronic transitions. Franck - Condon principles, ground and excited electronic states of diatomic molecules. Chromophores, auxochromes, electronic spectra of polyatomic molecules. Emission spectra, spectra of transition metal complexes, charge transfer spectra. Instrumentation and application. Factors affecting the positions of UV bands. Electronic transitions and empirical correlations of predicting λ_{max} of organic compounds. Woodward–Fieser rules. UV absorption of aromatic compounds - effect of substituents and solvent effects. Emperical rules to calculate $\lambda_{max.}$ Application of UV spectroscopy in the structural study of organic molecules.

7 hrs

NMR of nuclei other than proton: ^{13}C chemical shift & factors affecting it Coupling constants. Decoupling-Noise decoupling & broad band decoupling. Off-resonanceproton decoupling-some representative examples. ^{19}F &^{31}P NMR- Predicting the spectra of simple inorganic compounds, NMR of paramagnetic complexes. 7 hrs

UNIT- IV:[14 Hours]

Mass Spectrometry:Basic principles, Instrumentation -Mass spectrometer, interpretation of mass spectra, resolution, exact masses of nucleides, molecular ions, meta-stable ions and isotope ions. Fragmentation processes-representation of fragmentation, basic fragmentation

types and rules. Factors influencing fragmentations and reaction pathways. McLafferty rearrangement. Fragmentations (fragmentation of organic compounds with respect to their structure determination) associated with functional groups- alkanes, alkenes, cycloalkanes, aromatic hydrocarbons, halides, alcohols, phenols, ethers, acetals, ketals, aldehydes, ketones, quinines, carboxylic acids, esters, amides, acid chlorides, nitrocompounds, amines & nitrogen heterocycles. Fragmentation patterns of carbohydrates, terpenoids, alkaloids, steroids, peptides & proteins-some representative examples, ion analysis, ion abundance, retro Diels-Alder fragmentation. Application in structure elucidiation and evaluation of heats of sublimation & ionization potential. Nitrogen rule. High resolution mass spectroscopy. 9 hrs

Composite problems involving the applications of UV, IR, ^{1}H and ^{13}C NMR and mass spectroscopic techniques. Structural elucidation of organic molecules. 5 hrs

REFERENCES:

1. Fundamentals of Molecular Spectroscopy, Banwell & McCash (Tata McGraw Hill)2001.
2. Organic Spectroscopy-3rd Ed.-W.Kemp(Pagrave Publishers, New York), 1991.
3. Spectrometric Identification of Organic Compounds - Silverstein, Bassler & Monnill (Wiley)1981.
4. Applications of Absorption Spectroscopy of Organic Compounds-Dyer(Prentice Hall,NY) 1965.
5. Spectroscopy of Organic Compounds-3rd Ed.-P.S.Kalsi (New Age, New Delhi) 2000.
6. E.A.V.Ebsworth, D.W.H.Ranklin and S.Cradock: Structural Methods in Inorganic Chemistry, Blackwell Scientific, 1991.
7. R.S.Drago: Physical Methods for Chemists, Saunders College Publishing, 1992.
8. D.N.Satyanarayana: ElectronicAbsorption Spectroscopy and Related Techniques,
9. G.Aruldhas, Molecular Structure and Spectroscopy, Prentice Hall, 2001
10. J. A. Iggo: NMR Spectroscopy in Inorganic Chemistry, Oxford University Press, 1999.
11. C.N.R.Rao and J.R. Ferraro: Spectroscopy in Inorganic Chemistry, Vol I&II(Academic)1970
12. Analytical Chemistry-Open Learning : Mass spectrometry.
13. Spectroscopic Methods in Organic Chemistry - Williams and Fleming, TMH.

CH455: Diffraction and Electroanalytical Techniques

UNIT-I: **[14 hours]**

Diffraction Techniques: Introduction, production of X-ray, X-ray diffraction-Bragg`s law, Laue equations, Ewald`s diagram, X-Ray diffraction experiments-Powder method (Debye-Scherrer and photographic methods), Interpretation of power patterns. Single crystal technique- :Laue and Rotation photographic methods). Moving Film method (Weissenberg method). X-ray diffractometers. Systematic absences. Intensities of diffracted X-rays and structural analysis, X-ray scattering by atoms and molecules, Factors affecting X-ray intensities,Crystalstructureanalysis.

10 hrs

Electron Diffraction: Scattering intensity vs. scattering angle, qualitative aspects of Wierl equation, measurement technique,Elucidation of structure of simple gas molecules, Low Energy Electron Diffraction and structure of surfaces.

Basic theory and applications of Neutron diffraction.4 hrs

UNIT- II: **[14 hours]**

Electroanalytical Techniques: Theory of classical polarography, polarograhic measurements, polarograms, polarographic currents. Factors influencing diffusion currents, advantages and limitations of using dropping mercury electrode. half wave potential, oxygen interference, Applications ofpolarographic measurements. Modern Polarography : Necessity and development of new voltammetric techniques and their comparison with classical polarography. Fundamentals of DC polarography (Tast), oscilliography, differential and derivative voltammetry, cyclic, pulse, alternating current and square wave polarography.

Cyclic Voltammetry: Principle, Instrumentation, current-potential relation applicable for Linear Sweep Voltammetry (LSV) and Cyclic Voltammetry (CV), interpretation of cyclic voltammograms and parameters obtainable from voltammograms.

Principle, measurement technique and the applications of Coulometry, Amperometry and Electrogravimetry.

Chrono Methods: Basic concepts and applications of chronopotentiometry, chronoampermetry.

References:

1. A Basic Course in Crystallography, JAK Tareen and TRN Kutty, University Press, Hyderabad (2001).
2. Essentials of Crystallography, M.A. Waheb, Narosa Publishing House, New Delhi (2009),
3. Polarography and Allied Techniques, V. Suryanarayana Rao (University Press, Hyderabad), (2002).
5. Principles of Instrumental Analysis, D.A. Skoog, F.J. Holler and T.A. Nieman, 5th Ed. , (Saunders College Publishing, Harcourt Brace & Company, U.S.A.) 1998.
6. Electrochemical Methods: Fundamentals and Applications, A.J. Bard and L.R. Faulkner, 2nd Ed. (Wiley, New York), 2000.

CH 456 : INORGANIC CHEMISTRY PRACTICALS-II

Qualitative Analysis of mixtures of Inorganic Salts containing 4 metal ions and 2 anions (2 less common metal ions like Tl, W, Mo, V, Zr, Th, U, Ce, Ti and Li to be included among anions organic acid radicals, phosphate, borate and fluoride separation included).

References:

1. Vogel's Text Book of Quantitative Chemical Analysis(5th Ed), G.H.Jeffrey,J.Bassette, J.Mendham and R.C.Denny, Longman, 1999
2. Vogel's Qualitative Inorganic Analysis(7thEd), G. Svehla, Longman (2001).

CH 457: ORGANIC CHEMISTRY PRACTICALS-II

SEPARATION AND SYSTEMATIC QUALITATIVE ANALYSIS OF BINARY MIXTURES OF ORGANIC COMPOUNDS CONTAINING BOTH MONO AND BIFUNCTIONAL GROUPS AND PREPARATION OF SUITABLE DERIVATIVES.

References:

1.Practical Organic Chemistry-F .G. Mann and B. C. Saunders (ELBS, England), 2001.
2. Practical Organic Chemistry - A. I. Vogel (Longman-ELBS, England), 1971.
3. Experimental Organic Chemistry–Vol.I&II Singh et al(TMH, New Delhi)1981.
4. Semimicro Qualitative Organic Analysis–Cheronis etal Wiley-Eastern, New Delhi) 1964.
5. Vogel's Text Book of Practical Organic Chemistry Including Qualitative Organic Analysis- B. S. Furniss et al (Longman-ELBS, England), 1978.

CH 458 : PHYSICAL CHEMISTRY PRACTICALS - II

At least 12 experiments are to be carried out

1. Determination of cryoscopic constants of solvents and molecular weight of non volatile substances by thermal method.
2. Determination of degree of dissociation & Vant Hoff factor of an electrolyte by cryoscopic method.
3. Heat of solution of substances by solubility method.
4. Phase diagram of two component systems by thermal analysis.
5. Kinetics of acid catalysed hydrolysis of methyl acetate and determination of (a) order and rate constant, (b) Relative strength of two acids and (c) Energy of activation.
6. First and second order kinetics of reaction between potassium persulphate and KI.
7. Kinetics of (a) inversion of cane sugar, (b) sodium formate–iodine reaction.
8. Determination of heat of neutralisation, integral and differential heat of solution calorimetrically. 9. Thermometric titration of an acid with a base.
10. Direct determination of the latent heat of evaporation of carbon tetrachloride.
11. Measurement of the vapour pressure and latent heat of vapouration of Benzene using tensemeter.
12. Detn.of association constants carboxylic acids in organic solvents by distribution method.
13. Preparation of colloidal solutions.
14. Verification of F & L adsorption isotherms for acetic acid on activated charcoal.
15. To study the adsorption of iodine on charcoal from alcoholic solution.
16. To study the effects of gelatin solution on the precipitation values.
17. To determine the surface and interfacial tension and the effect of detergents.

18. Thermodynamic prediction and measurement of the solubility of naphthalene in benzene.
19.
Study of association of benzoic acid in benzene/toluene.

Any other relevant experiments of interest.

References:

1. Findlay's Practical Physical Chemistry- B. P. Levitt (Longman, London).
2. Experiments in Physical Chemistry–James and Prichard.
3. Experimental Physical Chemistry - Daniels et al.
4. Experimental Physical Chemistry-Das & Behera(Tata McGraw Hill, New Delhi)1983.
5. Advanced Practical Physical Chemistry–Yadav (1989).
6. Experiments in Physical Chemistry–J. C. Ghosh (Bharathi Bhavan)1974.

THIRD SEMESTER M.Sc. Course in CHEMISTRY

CH 501: CHOICE BASED COURSE

CH 502: CO-ORDINATION AND BIOINORGANIC CHEMISTRY

UNIT- I: [14 Hours]

Spectral and Magnetic properties of complexes: Term symbols for d^n ions, spectroscopic ground states, selection rules, nature of spectral bands- band shapes, band intensities, band widths, spin-orbit coupling, vibrational structures.

Orgel diagrams, Tanabe-Sugano diagrams, interpretation of spectra of octahedral, distorted octahedral, tetrahedral and square planar complexes. Charge transfer bands – origin, types, and characteristics. Photochemistry of metal complexes- photosubstitution and photoredox reactions, ligand photoredox reactions, photoreactions and solar energy conversion.

Type of magnetic behaviour, orbital contribution, spin orbit coupling, measurement of magnetic susceptibility – Gouy and Faraday methods, diamagnetic corrections, ferro- and antiferromagnetic coupling, spin cross-over systems.

UNIT- II: [14 Hours]

Reaction Mechanisms in Transition Metal Complexes**:** Energy profile of a reaction, inert and labile complexes, kinetics of octahedral substitution and mechanistic aspects. Acid hydrolysis, factors affecting acid hydrolysis, base hydrolysis, conjugate base mechanism and evidences in its favour. Anation reactions, reactions without M-L bond cleavage. Substitution reactions in square planar complexes, trans effect, mechanisms of substitution. Electron transfer reactions- inner sphere and outer sphere reactions, complimentary and non-complimentary reactions.

UNIT -III: [14 Hours]

Metal ions in biological systems-essential and trace metals, ion transport across membranes, active transport of ions, ionophores.

Metalloproteins as enzymes – carboxy peptidase, carbonic anhydrase, alcohol dehydrogenase, catalases, peroxidases, cytochrome P 450, superoxide dismutase, copper oxidases, vitamin B_{12} coenzyme.

UNIT-IV: [14 Hours]

Transport and storage of dioxygen- heme proteins, oxygen uptake, functions of haemoglobin, myoglobin, hemerythrin and hemocyanins, synthetic oxygen carriers.

Metal storage and transport – ferritin, transferrin and ceruloplasmin. Electron transfer proteins- cytochromes, iron-sulphur proteins. Biological nitrogen fixation, nitrogenase.

Metals in medicine- metal deficiency, metal toxicity, metal complexes as drugs.

References:

1. D.N.Satyanarayana:Electronic absorption Spectroscopy and Related Techniques, OUP, 2001.
2. F.Basolo and R.G.Pearson: Inorganic Reaction Mechanisms, Wiley Eastern, 1979.
3. W.W.Porterfield: Inorganic chemistry – A Unified Approach, Elsevier, 2005.
4. R.L.Dutta and A Syamal : Elements of Magnetochemistry, Affiliated east-West, 1993.
5. J.E Huheey, R.L.Keiter and A.L.Keiter: Inorganic Chemistry(4^{th} edn),Addison Wesley, 2000.
6. M.N.Hughes: Inorganic Chemistry of Biological Processes, (2^{nd} edn.) Wiley, 1988.
7. I.Bertini. H.B.Gray, S.J.Lippard and J.S.Valentine: Bioinorganic Chemistry, Viva Books, 1998.

CH 503: REACTION MECHANISM AND HETEROCYCLIC CHEMISTRY

UNIT-I: [14 Hours]

Organic Name reactions: Reactions, Mechanisms and synthetic uses of the following: Stobbe condensation, Darzen condensation, Gattermann-Koch reaction, Cannizzaro reaction, Chichibabin reaction, Benzoin condensation, Claisen-Schmidt condensation, Claisen reaction, Simon-Smith reaction, Stork Enamine reactions, Sharpless asymmetric epoxidation, Hofmann-Loffler-Freytag reaction, Suzuki coupling, Woodward and Prevost Hydroxylation, Bucherer reaction, Ullmann reaction. Wittig reaction,Mitsunobu reaction.

UNIT –II:[14 Hours]

Molecular rearrangements: Classification and general mechanistic treatment of nucleophilic, electrophilic and free radical rearrangements. Intermolecular and Intramolecular migration, nature of migration and migratory aptitudes. Mechanism of Wagner-Meerwein, Dienone-Phenol, Pinacol-Pinacolone, Demaynov, Benzil-Benzilic acid, Fries, Wolff, Favorskii, Neber, Benzidine, Baeyer-Villiger, Beckmann, Lossen, Curtius, Schmidt, Stevens, Shapiro, Baker-Venkatraman and Amadori rearrangement.

UNIT-III:[14 Hours]

Heterocyclic Chemistry: Nomenclature of Heterocycles, Replacement and systematic nomenclature, Hantzsch-Widman system for monocyclic, fused and bridged heterocycles. Structure, synthesis and reactions of six membered heterocycles- α- and γ-Pyrones, Pyrazines, Pyridazines, Pyrimidines. Synthesis and reactions of seven membered heterocycles-Azepines, Oxepines and Thiepines. Synthesis and reactions of fused heterocycles-Quinolines, Isoquinolines, Coumarins, Naphthyridines and Purines.

UNIT- IV:[14 Hours]

Pericyclic Reactions: Molecular orbital symmetry, Frontier orbitals of ethylene, 1,3-butadiene, 1,3,5-hexatriene and allyl systems. Classifications of Pericyclic reactions. Woodward-Hoffmann correlation diagram and FMO approach.

Electrocyclic Reactions: Introduction, Con-rotatory & dis-rotatory Process, 4n & 4n+2 systems.Electrocyclic reactions with odd number of atoms.

Cycloaddition reaction: Suprafacial and Antrafacial addition, 2+2 and 4+2 systems.,cycloaddition of ketenes. 1,3-dipolar cycloaddition reactions and their applications in the synthesis of five membered heterocycles.

Sigmatropic reactions: Suprafacial and Antrafacial shift of H, [1,3] & [1,5] -sigmatropic shifts. Claisen, Cope, Oxy-Cope and Aza-Cope rearrangements.

References:

1. O.L. Chapman, Organic Photochemistry. Vol I & II. Marcel Decker.
2. Francis A Carey and R. J. Sundberg, Advanced Organic Chemistry-Part A & (Plenum).
3. Mukherji Singh and Kapoor , Organic Chemistry, Vol 1-3, (Wiley Eastern, New Delhi)
4. Synthetic Organic Chemistry- G.R.Chatwal (Himalaya, Bombay), 1994.
5. Organic Reaction Mechanisms , V.K.Ahluwalia & R.K.Parashar (Narosa) 2006
6. Organic Chemistry, Vol I-II, I.L.Finar,(Longmann ELBS, London), 1973.
7. Advanced Organic Chemistry- Reaction Mechanisms, Reinhard Bruckner(Academic) 2005.
8. Pericyclic reactions, S.M Mukherji(The McMillan Bangalore), 1979.
9. Organic Reactions and their mechanisms- P.S.Kalsi (New Age, New Delhi), 1996.

CH 504: ELECTROCHEMISTRY AND POLYMERS

UNIT-I: [14 hours]

The Electrified Interface: Thermodynamics of double layer, Electrocapillary equation, Determination of surface excess, electrocapillarity, excess charge capacitance and relative surface excesses. Metal/water interaction-Contact adsorption, its influence on capacity of interface. Structure of electrified interface (assumptions, merits and limitations Helmholtz - Perrin, Guoy-Chapmanand Stern model). Competition between water and organic molecules at the electrified interface. Semiconductor-electrolyte solution interface. Effect of light at semiconductor interface. Capacity of space charge-Mott-Schottky plot. 6hrs

Ion-solvent Interaction : Ion-Solvation- Introduction, evidence for solvation, Structural aspects of ion-solvent interaction -Born model and its limitations, structural treatment : ion-dipole and ion-quadruple models. Solvation number–Introduction, methods of determination (compressibility, Spectroscopic and thermochemical approach). Ion solvent –nonelectrolyte interactions. 4hrs. .

Electrocatalysis-Introduction. Electrogrowth of metals on electrodes, its importance and consequences. Importance of oxygen reduction and hydrogen evolution reactions and their mechanisms. 4hrs.

UNIT –II: [14hours] Electrochemical Energy System : Introduction to electrochemical energy systems. Electricity storage-Importance, storage density; Primary battery (Laclanche-dry cell and Alkaline cell). Secondary battery (acid and alkaline). Reverse batteries. Fuel cells (H_2-O_2 , methanol, bio-cells). Introduction to Li batteries and Solar energy systems (Photoelectrochemical and and Galvanic cells).4hrs.

Electrode processes: Charge transfer across the interface and its application. Quantum aspects of charge transfer(qualitative aspects only). Polarization, Overvoltage – Types(Ohmic, concentration and activation), theory of hydrogen and oxygen overvoltage.Electrode kinetics, Polarizable and non-polarizable interfaces. Multistep reactions- near equilibrium relation between current density and over potential-Butler-Volmer equation,Concept of rate determining step. Mechanism of cathodic and anodic reactions, Tafel equation. 6hrs. **Ionic liquids**-Introduction, characteristics of ionic liquids, models of simple ionic liquids, mixtures of simple ionic liquids. Hole model for liquid electrolytes. Transport phenomena in liquid electrolytes. Electronic conductance of alkali metals dissolved in alkali halides. 4hrs.

UNIT-III: [14 hours]

Terminology and basic concepts of Polymers: Monomers, Functionality, repeat units, degree of polymerization.General structure and naming of polymers. Average molecular weight and average chain dimension concept.Expressions for average molecular weighs. Molecular weight distribution and Polydispersity.

Classification based on various considerations-source, preparation methods, thermal behavior, chain structure etc.

Types –Homopolymers and copolymers; linear, branched and network polymers.

Techniques of polymerization: Techniques of preparation of addition and condensation polymers.

Kinetics of polymerization: Kinetics and mechanism of addition and condensation polymerization. Kinetics of copolymerization-reactivity ratio and copolymer equation.

UNIT- IV: 14 hours]

Stereochemistry of polymers: Geometric and optical isomerism in polymers. Structure, properties and preparation of stereoregular polymers.

Determination of molecular weight: Osmometry and viscometry.

Thermal Characterization: Glass Transition and melting-correlation with structure- Factors affecting Tg and Tm. Techniques of thermal characterization: DSC, DTA , DTG and TGA techniques.

Structural features, properties and uses of commercial polymers: Polyethylene, polystyrene, PVC, polyesters, polyamides, polyurethanes and polycarbonates. Conducting polymers, liquid crystal polymers and biomedical polymers.

REFERENCES:

1. Modern Electrochemistry, 2nd Ed. Vol.1, 2A &2B, J O M Bockris and A K N Reddy, (Plenum, New York) 1998.
2. Chemical and Electrochemical Energy Systems, Narayan & Viswanathan (Univ. Press, Hyderabad) 1998.
3. Fundamentals of Electrochemistry, Fulkner and A. J. Bard, Wiley India, 2006.
4. Ions in solution-Basic principles of chemical interactions, J. Burgeess (Chichester) 1999.
5. Electrochemistry-Principles, Methods and Applications, Brett and Brett, Oxford Science1993.
6. Text book of Polymers- F.W.Billmeyer (Wiley)
7. Contemporary Polymer Chemistry-H.R. Allcock and F.W. Lampe (Prentice Hall).
8. Polymer Science and Technology-J.R. Frird (Prentice Hall).
9. Polymer Science: V.R. Gowariker, N.V.Viswanathan & T.Sreedhar
10. Principles of Polymer Science- P.Bahadur and N.V.Sastry(Narosa Publishers)

CH 505: INORGANIC CHEMISTRY PRACTICALS – III

A. Any five of the following experiments are to be carried out:

1. Analysis of brass-Cu gravimetrically using ∝-Benzoinoxime & Zinc complexometrically.
2. Analysis Cu-Ni alloy.
3. Analysis of Stainless Steel – Insoluble residue by gravimetry, Ni gravimetrically using DMG, Fe volumetrically using Ce(IV) & Cr(III) volumetrically by persulphate oxidation.
4. Analysis of Type metal–Sn gravimetrically, Pb electrogravimetrically and Sb titrimetrically using $KBrO_3$
5. Quantitative analysis of the constituents & mixtures containing the following radicals
   (i) Cu(II) + Fe(II) - Cu gravimetrically as CuSCN and Fe using Ce(IV).
   (ii) Fe(II) + Ni(II) - Fe gravimetrically as Fe_2O_3 and Ni using EDTA.
   (iii) Fe(III) + Ca(II) - Fe gravimetrically as Fe_2O_3 and Ca using EDTA.
   (iv) Cr(III) + Fe(III) – Using EDTA by Kinetic masking method.
6. Analysis of chalcopyrites, magnetite and ilmenite.
7. Ion-exchange chromatography: Separation and determination of Mg^{2+}/Zn^{2+}, Zn^{2+}/Cd^{2+}&Cl^-/ Br^-.

B. Any five of the following experiments are to be carried out:

8. Determination of COD of a water sample
9. Determination of Phosphorus.
10. Determination of dissolved oxygen (DO) by Winkler's method
11. Determination of nitrate & nitrite in water samples and sea water.
12. Analysis of heavy metals in waste water, sea water (Pb, Hg etc. By spectrophotometry)
13. Determination of available K in soil,
14. Nephelometric determination of sulphate/phosphate.
15. Determination of alkalinity of water samples
16. Determination of fluoride in drinking water by spectrophotometry and ion selective electrode
17. Determination of phosphates in detergents
18. Spectrophotometric determination of sulphur and phosphorus present in soil.

REFERENCES:
1. A..I. Vogel : A Text book of Quantitative Inorganic Analysis, (ELBS), 1978.
2. APHA, AWWA and WPCF: Standard Method for the Examination of water and Waste Water (WashingtonDC),1989,
3. I. M. Kolthof and E.P. Sandell: Quantitative Chemical Analysis.McMillan,1980
4. I.Williams, Environmental Chemistry, Wiley, 2001
5. Lobinski and Marczenko, Comprehensive Analytical Chemistry, Vol.30, Elsevier,1996.

CH 506: ORGANIC CHEMISTRY PRACTICALS - III

Quantitative determination of sugars, amino acids, phenols, amines, carboxylic acids, amides, esters, aldehydes, ketones, urea by various methods.
Determinations of acid & ester and acid &amide in the given mixtures.
Determination of functional groups like hydroxyl, vic-hydroxyl, enol, amino, amide, nitro and unsaturation.
Applications of computers in the study of conformation and geometry of some simple organic molecules.

References:
1. Elementary Practical Organic Chemistry-Vol. III quantitative Organic Analysis- A.I. Vogel
2. Experimetal Organic Chemistry- Vol. I &II- P.R.Singh, Tata McGraw-Hill, 1981.
3. Practical Organic Chemistry- IV Ed- Dey &.Sitaraman (Allied)
4. Laboratory Experiments in Organic Chemistry-Adam, Johnson & Wicon(McMillan, London), 1979.
5. Experimental Organic Chemistry- H.D.Durst & G.E.Goke (McGraw-Hill)1980.

CH 507: PHYSICAL CHEMISTRY PRACTICALS – III

A. Electrochemistry:
a. Conductometry (At least three experiments to be carried out)
1. Titration of a mixture of acetic acid, monochloro and trichloacetic acids with NaOH.
2. Determination of concentrations/amounts of sulphuric acid, acetic acid and coppersulphate by conductometric titration with sodium hydroxide.
3. Measurements of the conductance of a weak acid, (a) HOAC and of the strong electrolytes NaOAc, HCl and NaCl and (b) HCOOH and of the strong electrolytes HCOONa, HCl and NaCl) and to calculate the ionisation constant of the acid and
4. Titration of mixture of strong acid and weak acid with weak base (HCl + HAC against NH_4OH.
5. Determination of pK_a of a given weak acidby pH measurements at various dilutions.
6. Conductometric titration of the mixture of (a) HCl and NH_4Cl and (b)HCl and acetic acid.
7.Determination of activity coefficient of Zinc ions in 0.002M $ZnSO_4$.8. Conductometric determination of Critical Micelle Concentration.

b. Potentiometry (At least three experiments are to be carried out)
1. Determination of pK values of maleic acid/malonic and phosphoric acid bypotentiometric titration with sodium hydroxide using glass electrode.
2. Composition of Zinc Ferrocyanide Complex by potentiometric Titration.
3. Potentiometric titration of (a) Non aqueous sytem and (b) mixture of strong (HCl) and weak (HAC) acid with NaOH / NH4OH and find the strength of the acids in mixture.
4. Determination of decomposition potential of an aqueous electrolytic solution.
5. Determination of the potential of an electrochemical cell and mean ionic activity coefficient.
6. Determination of pKa values of di and tri-acid base potentiometrically and pH metrically.

7. Determination of acidic and basic dissociation constants and isoelectric point an amino acid pH metrically..
8. pH titration of (a) HCl versus NaOH, (b) HOAC versus NaOH and (c) lead nitrate versus potassium chromate, and Titration of mixture of bases (Na_2CO_3& $NaHCO_3$) with standard HCl and find the concentration of bases.
9. Determination of pK_a values of functional groups in amino acids using a pH meter.
10. Determination of Hammett constants of o-, m-, p- amino/nitro benzoic acidby pH measurements.
11. Determination of activity coefficient of an electrolyte at different molalities.
12. Verification of Tafel equation of hydrogen evolution reaction.
13. Study of rate of corrosion (with and without inhibitir) by weight loss method.
14. Thermodynamics of an Electrochemical Cell: Free Energy, Enthalpy and Entropy of Reaction: Standard Cell

B. Radiochemistry Experiments (At least Three experiments to be carried out)

1. Study of (a) Characteristic plateau, (b) Geometry effects and Statistics of G.M counter
2. Determination of (a) Dead time by single source&double source method. (b) E_{max} of β - source (c) Back scattering of β and (d) β energy emitted by C-14.
3. Verification of the inverse square law.
4. Determination of half life of radionuclides.
5. Determination of Linear and mass attenuation coefficient.
6. Preparation of Fricke and Ceric sulphate dosimeters & calculation of G-value&dose rate.
7. Study of isotope dilution analysis; 8. Radiochemical Determination of I-131 in sea water.
8. Detrmination of β-particle range and, axmum energy (by half thickness method).

C. Photochemistry(Any Two experiments are to be carried out**)**

1. Irradiation of a reaction mixture and calculation of the quantum yield.
2. Determination of the quantum yield of chloride in the photohydrolysis ofaqueous solution of monochloroacetic acid
3. Photochemical study of decomposition of hydrogen peroxide.
4. Photochemical study of Bleaching of dyes.
5. Photochemical reaction between threonine and ferrous sulphate.

D. Voltammetry & Polarography (Any Three experiments are to be carried out)

1. Determination of the half-wave potential of Cd (II), Cu(II)& Zn(II) ions in 0.1M solutions.
2. Determination of metal ions individually and in mixtures,
2. Determination of the formula and the stability constant of a lead oxalate.
3. Study of the polarogram of supporting electrolyte with and without dissolved oxygen,
5. Determination of Huckel β value of aromatic hydrocarbon reduction at dropping mercury electrode.
6. Amperometric titrations.
7. Coulometric titration
8. Percentage purity of copper sulphate by electrogravimetric method.

References:

1. Findlay's Practical Physical Chemistry- B. P. Levitt (Longman, London).
2. Experiments in Physical Chemistry–James and Prichard.
3. Experimental Physical Chemistry - Daniels et al.
4. Experimental Physical Chemistry-Das & Behera(Tata McGraw Hill, New Delhi)1983.
5. Advanced Practical Physical Chemistry–Yadav (1989).
6. Experiments in Physical Chemistry–J. C. Ghosh(Bharathi Bhavan)1974.
7. Nucleonix systems Pvt. Ltd, Hyderabad.

FOURTH SEMESTER M.Sc.Course in CHEMISTRY

CH 551: ORGANOMETALLIC CHEMISTRY

UNIT- I: [14 Hours]

Historical development- classification and nomenclature, bond energies and stability.

Transition metal alkyls and aryls- types, routes of synthesis, stability and decomposition pathways,. Nucleophilic and electrophilic cleavage of metal-carbon sigma bonded compounds. Alkane activation.

Transition metal to carbon multiple-bonded compounds- carbenes, carbynes, synthesis, nature of bond, agostic interactions, structural characteristics and reactivity. Transition metal hydrides – synthetic routes, structure and reactivity, synthetic applications.

UNIT-II: [14 hours]

Transition metal-carbon pi complexes: Preparative methods, nature of bonding, structural features of olefinic, acetylenic, allylic, butadiene, cyclobutadiene, η^5- cyclopentadienyl, η^6-benzene and other arenes, cycloheptatriene and cyclooctatetraene complexes.

Important reactions relating to nucleophilic and electrophilic attack on ligands.

Fluxional isomerism in olefin, allyl, dienyl and cyclopentadienyl complexes.

Isolobal concept.

UNIT- III: [14 hours]

Catalysis by organometallic compounds:16- and 18-electron rules, oxidative addition, insertion, deinsertion and reductive elimination reactions.

Homogeneous catalysis by organometallics- hydrogenation, hydrosilation, hydrocyanation and isomerization of olefins, immobilisation of homogeneous hydrogenation catalysts,

Hydrocarbonylation of olefins (oxo reaction–cobalt and rhodium oxo catalysts), carbonylation of alcohols- Monsanto acetic acid process. Polymerization of olefins and acetylenes: Ziegler-Natta catalyst systems. Fischer – Tropsch reaction , Water Gas Shift reactions.

Unit IV: [14 Hours]

Organometallics in Organic Synthesis: Main group organometallics- preparation, properties and applications of organometallic compounds of Li, Mg, Hg, Zn, Cd and Sn. Synthetic applications of organo-transition metal compounds: organocuprates. Hydrozirconation, transmetallation reactions by organopalladiums and organonickels, carbonylation by metal carbonylates, decarbonylation, carbene complexes and metallacycles, arene complexes.

References:

1. J.P.Collman, L.S.hegedus, J.R.Norton and R.G.Finke: Principles and Applications of
2.Organotransition Metal Chemistry, University Science Books, 1987.
3. R.C.Mehrotra and A.Singh: Organometallic Chemistry, New Age International, 1999.
4. R.H.Crabtree:Organometallic Chemistry of Transition Metals, Wiley , 1999.
5. F.A.Cotton and G.Wilkinson : Advanced Inorganic Chemistry, Wiley, 1991.

CH 552: ORGANIC SYNTHETIC METHODS

UNIT–I: **[14 Hours]**

Reduction Reactions: Catalytic hydrogenation: Introduction, catalysts and solvents employed reduction of functional groups, mechanisms and stereochemistry of catalytic hydrogenations, Hydrogenolysis, and homogeneous catalytic hydrogenation.

Metal hydride reduction: Reduction with $LiAlH_4$ and $NaBH_4$, Stereo chemistry of reduction, Functional group transformation during reduction, Reduction with diborane and related reactions.Reduction in Biological systems-NADH,FAD.

Dissolving Metal Reductions: Mechanisms of reduction of conjugated system and carbonyl compounds, Bimolecular reductions of esters, Birch reduction, Wolf-Kishner reduction and related reactions, Reaction with diimide and related compounds.

UNIT- II: **[14 Hours]**

Oxidation reactions: Introduction and different oxidative processes, Mechanism of oxidation reaction with chromium and manganese salts, peracids and peresters, periodic acid, Lead tetra acetate, Ozone, Osmium tetroxide and their synthetic importance in functional group transformation.

Halogenation: Halogenation of olefins, carbonyl compounds, Benzyllic and Allylic halogenation, Dehalogenation reactions. Dehydrogenation with S, Se, Pt, Pd, Ni.

UNIT- III: **[14 Hours]**

Synthetic Design: Carbon skeleton frame work, Classification of carbon-carbon single bond and double bond forming reaction and their use in carbon skeleton ring formation. Ring forming and ring cleaving reactions, use of Thorpe condensation, Carbene insertion reaction, Friedel-Crafts reaction, 1,3-dipolar addition and Ene reaction in ring formation, Oxidative cleavage of rings and Retro Diel's-Alder reactions.

Planning of Organic Synthesis: Selection of starting materials and key intermediates during the synthesis. Synthesis of Cubane and Iswarane. Use of Robinson annulation, Dieckmann cyclisation, Arndt-Eistert synthesis, Diel's- Alder reaction in organic synthesis.

Functionality: Synthesis of 6- and 7- methoxy tetralones, biotin and penicillin-V with special reference to the introduction of functional groups. Stereo chemical consideration and stereo selectivity during organic synthesis.

UNIT- IV: **[14 Hours]**

General introduction to disconnection approach. Basic principles and technologies used in disconnection approach. Synthons and synthetic equivalents. Interconversion of functional groups. One group C-X and two group. C-X disconnections.

Protecting groups: Principle of protection of hydroxyl amino carboxylic and carbonyl groups.

Retrosynthetic analysis: Analysis of alcohols, carbonyl compounds cyclic and acyclic alkanes, benzocaine, p-methoxyacetophenone, acetonecyanohydrin, 2-methyl-6-methoxy-indole-3-aceticacid, 6-methylquinoline & 1-phenyl-4-p-methoxyphenyl-1,3-butadiene, Limonene, Danishefsky's pentalenolactone, Benziodarone, nitrofurazone, Warfarin and Juvabione.

References:

1. Modern Organic Reactions- H.O.House.
2. Organic Synthesis- R.E.Ireland (Prentice Hall India), 1969.
3. Art in Organic Synthesis- Anand, Bindra & Ranganath-(Wiley New Delhi), 1970.
4. Organic Synthesis a Disconnection Approach- Stuart Warren

5. Advanced Organic Chemistry-IV-Ed. Part A &B-F.J.Carrey & R.J.Sundberg(Kluwer) 2001.
6. Modern Methods of Organic Synthesis-N.Carruthers(Cambridge University), 1996.

CH 553: SOLID STATE CHEMISTRY AND REACTION DYNAMICS

UNIT–I: [14 hours]

Crystal Defects and Non-Stoichiometry: Perfect and imperfect crystals, intrinsic and extrinsic defects- point, line and plane defects.Vacancy, Schottky and Frenkel defects. Thermodynamics of Schottky and Frenkel defect formation, colour centres, non-stoichiometry and defects – Structures of UO_2, FeO and TiO_2.
5 hrs

SolidState Reactions: General Principles, Wagner's theory. Order - disorder transitions in solids- Bragg- William's theory Mechanism of diffusion , Kirkendall effect 4 hrs

Preparative Methods: Ceramic, sol-gel, precursor and chemical vapour deposition (CVD) methods. Nucleation & crystal growth techniques-pulling, zoning, flame fusion & skull melting. Basic methods of preparation of thin films
5 hrs

UNIT- II : [14 Hours]

Electronic Properties and Band Theory: Free electron theory to band theory of solids, electrical conductivity, Hall effect. Metals, Insulators and Semiconductors. Intrinsic and extrinsic semiconductors, hopping semiconductors. Metal – semiconductor and p-n junctions.
6 hrs

Insulators-Dielectric, ferroelectric, pyroelectric & piezoelectric properties and their applications
3hrs

Magnetic properties: Classification of magnetic materials – dia, para, ferro, ferri, antiferro & antiferri magnetic types Langevin diamagnetism. Selected magnetic materials such as spinels & garnets. 5 hrs

UNIT - III : [14 Hours]

Ionic Conductors: Types of ionic conductors, mechanism of ionic conduction, diffusion superionic conductors; phase transitions and mechanism of conduction in superionic conductors, examples- β-alumina, AgI, halide and oxide ion conductors
5 hrs

Superconductivity: Meisner effects; Types I and II superconductors, Features of super-conductors, isotope effect, high T_c materials. Principle of low temperature superconductivity.
.
4hrs

Liquid Crystals: Mesomorphic behaviour, thermotropic liquid crystals, positional order, bond orientational order, nematic and smectic mesophases; smectic – nematic transition and clearing temperature- homeotropic, planar and schlieren textures, twisted nematics chiral nematics, molecular arrangements in smectic A and smectic C phases. Optical properties of liquid crystals.
.
5hrs

UNIT-IV: [14 Hours]

Reactions at Surfaces: Structures of solid surfaces & adsorbed layers. Mechanisms of surface reactions- kinetic effects of surface heterogeneity & interactions – surface inhibition and activation energies –reactions between two adsorbed molecules – surface exchange reactions –

Transition state theory of surface reactions – unimolecular and bimolecular reactions. Comparison of homogeneous and heterogeneous reaction rates.7 hrs

Micelles: Surface active agents-micellisation, hydrophobic interactions, critical micellar concentration (CMC), factors affecting the CMC of surfactants. 2 hrs

Pharmaco kinetics: Introduction,Plasma concentration - time curve, protein binding and drugs, drug dissolution rate, pharmacokinetics applied to one compartment open model (calculation of elimination rate constant & metabolism constant).
5hrs

REFERENCES:

1. D. K. Chakrabarty, Solid state chemistry (New Age) 1996.
2. H.V.Keer, Principles of the solid state (Wiley Eastern) 1993.
3. A.R.West, Solid state chemistry and its applications (Wiley) 1984.
4. L.Smart and E. Moore, Solid State Chemistry –An Introduction (Chapman &Hall)1992.
5. L. Azaroff, An Introduction to Solids (Mc Graw Hill).
6. V. Raghavan, Material science and Engineering (3rd Ed), (Prentice Hall India)1993.
7. Thermotropic Liquid Crystals, Ed. G.W. Gray, Wiley.
8. S. Chandrasekhar, Liquid Crystals, Cambridge University Press (2nd ed), 1994.
9. Chemical Kinetics, K. J. Laidler, Pearson Education, Anand Sons(India) 3rd edition (2008)
10. Physical Chemistry at surfaces, 6th ed., A.W Adamson and A P Gast, John Wiley, Canada, 1997.

CH 554: **BIOORGANIC AND MEDICINAL CHEMISTRY**

UNIT- I: **[14 Hours]**

Drugs: Introduction, Classification and nomenclature of drugs. Theories of drug action-Occupancy theory, Rate theory, Induced fit theory and Perturbation theory. Analogues and Prodrugs, Factors governing drug design. Rational approach to drug design, Variation method of drug designing, tailoring of drugs, Physico-Chemical factors and biological activities. Factors governing the ability of drugs, Isosterism and Bio-isosterism.

Antipyretic Analgesics: Classification, synthesis of Phenacetin, Aspirin, Cinchophen, Phenazone and Mefenamic acid, mode of action.

General Anesthetics: Introduction and classification, synthesis of anesthetic ether-methoxyfluorane, Thiopental sodium and Fentanyl citrate, Mode of action.

Local anesthetics: Introduction and classification, synthesis of benzocaine, α-Eucaine, Lignocaine hydrochloride and Dibucaine hydrochloride, Mode of action.

UNIT- II: **[14 hours]**

Cardiovascular drugs: Introduction, classification, Synthesis of Hydralazine, Methyldopa, Diazoxide, Procainamide, Propranolol, Bretylium tosylate, Isoxsupurine, Prenylamine & their mode of action.

Antimalarials: Introduction and classification, Synthesis of Chloroquine phosphate, Pamaquine, Meparine hydrochloride, Proguanil hydrochloride, pyrimethanine and dapsone, mode of action.

Antineoplastic agents: Introduction and classification, Synthesis of Mechlorethamine hydrochloride, Busalfan triethylenemelamine, Methotrexate, Mercaptopurinum and Flurouracil, Mode of action.

Antiviral drugs: Introduction, classification, mechanism of action study of some representative drugs like Methisazone, Idoxuridine, Amantidine hydrochloride.

UNIT- III:Chemistry of Bio Molecules **[14 hours]**

Peptides & Proteins: Peptide bond formation and synthesis of polypeptides, Amino and carboxy protecting groups in peptide synthesis, Solid phase peptide synthesis-Merrifield method, Peptide structure determination-Sequence and End group anaysis (N-Terminus and C-Terminus), Secondary, Tertiary and Quaternary structure of proteins.

Nucleic acids: Nucleosides and Nucleotides, Occurrence, Classification of nuleosides and nucleotides. Chemical synthesis of nucleosides and nucleotides. Poly nucleotides- Structure and functions of DNA and RNA.Solid phase synthesis of oligonucleotides.

Non steroidal hormones: Study of the Oxytocin, Vasopressin and synthetic analogs, General study of ACTH, Growth hormones, Somotropin and Insulin.

UNIT IV: Vitamins and Antibiotics **[14 hours]**

Vitamins: Introduction, Classification and Nomenclature-Source and Deficiency diseases-Biological, functions of Vitamins- Study of the following Vitamins: VitaminA_2, VitaminB_3, B_4, B_5 and B_{12}, Vitamin C, Vitamin K_1 and K_2.

Antibiotics: Introduction, Classification, Chemistry of Pencillin V, Cephalosporine C, Streptomycin, Chloramphenicol and Tetracyclin.

References:

1.Medicinal Chemistry- Ashutosh Kar (New Age.), 2005,
2. Medicinal Chemistry- G. R.Chatwal (Himalaya) 2002.
2. Natural Products Chemistry, Vol-I-II- G.R.Chatwal (Himalaya), 1990.
4. Principles of Drug Action- II Ed. A.Goldstein Lewis Arnold & Suner M.Kalman (Wiley Int.Ed.)
5. Organic Chemistry by I.L.Finar,Vol.1 & Vol.2

CH 555: INORGANIC CHEMISTRY PRACTICALS - IV

1. Colorimetric determination of Ti(IV) and Zr(IV)
2. Simultaneous colorimetric determination of two metal ions – Mn and Cr.
3. Flame photometric determination of Na, K, Li and Ca individually and in mixtures.
4. Electrogravimetric determination of (a) Cu-Ni alloy and (b) Pb in Type Metal.
5. Solvent extraction of Ni(II) and UO_2(II).
6. Preparation of any three of the following complexes, checking the purity of the prepared samples by chemicals analysis, structural study of the prepared complexes using conductance and magnetic susceptibility measurements, recording the electronic and infrared spectra:
   i) Chloropentamminecobalt(III) chloride, ii) Hexamminecobalt(III)chloride.
   iii) Potassium trisoxalatoferrate(III) and iv) Potassium hexathiocyanatochromate(III)
   v) $K_3Cr(OX)_3.3H_2O$ vi) $Cu(tu)_3Cl$ vii)$Zn(tu)_3OSO_3$
7. Determination of composition of complexes:
   a) Job's method: Fe-phenanthroline complex
   b) Mole ratio method: Zr-Alizarin red S complex,
   c) Slope ratio method: Cu ethylenediamine complex,
   d)Limiting logarithmic method:Uranyl-sulphosalicyclic acid complex.
8. Determination of stability constants
   a) Turner Anderson method : Fe-Tiron system,
   b) Bejrrums's method : Cu – sulphosalicyclic acid system,
   c) Polarographic method :Cu-glycinate or Pb -oxalate system.

References:

1. J. Rose, Physicochemical Experiments
2.Vogel's Text Book of Quantitative Chemical Analysis(5^{th} Ed), G.H.Jeffrey, J. Bassette, J. Mendham and R.C. Denny, Longman, 1999.

CH 556: ORGANIC CHEMISTRY PRACTICALS –IV

Multi Step Organic Synthesis

Preparation of Ethyl resorcinol from Resorcinol, 3-Bromo-4-methyl benzaldehyde from p-Toluedine, ε-Caprolactam from cyclohexanone, p-Aminobenzoic acid from p-Nitrotoluene, s-Tribromobenzene from aniline, o-hydroxyacetophenone from phenol, Benzanilide from Benzophenone, Benzylic acid from Benzoin, Benzopinacolone from Benzophenone, p-Chlorotoluene from p-Toludine, 2,5-Dihydroxyacetophenone from Hydroquinone, 2,4-Dinitrophenylhydrazine from Chlorobenzene, m-Nitrobenzoic acid from Benzoic acid, 2,4-Dinitrophenol from Chlorobenzene, o-Aminobenzoic acid from Phthalic acid, 2-Carbethoxycyclopentanone from Adipic acid, α-Acetylaminocinnamic acid from Glycine, p-Aminoazobenzene from Aniline.

Separation of components from mixture of organic compounds by fractional crystallization, fractional distillation, adsorption, Paper, TLC and column chromatography. The purification and characterizationof organic compounds.

References:

1. Elementary Practical Organic Chemistry-Vol. III quantitative Organic Analysis- A.I Vogel
2. Experimetal Organic Chemistry- Vol. I &II- P.R.Singh, Tata McGraw-Hill , 1981.
3. Practical Organic Chemistry- IV Ed- Dey &.Sitaraman (Allied)
4. Laboratory Experiments in Organic Chemistry-Adam, Johnson & Wicon(McMillan, London), 1979.
5. Experimental Organic Chemistry- H.D.Durst & G.E.Goke(McGraw-Hill)1980.

CH 557: PHYSICAL CHEMISTRY PRACTICALS-IV

A. Kinetics and Catalysis (Any Five Experiments are to be carried out)

Determination of reaction order and activation parameters, study of acidity/salt/solvent/catalytic effects on reaction rates of any FIVE of the reactions listed below.

1. Acid catalyzed hydrolysis of methyl acetate.
2. Saponification of ethyl acetate by conductivity method.
3. Decomposition of benzenediazonium chloride.
4. Reaction betweem potassium persulphate and potassium iodide (including the study of salt effect and catalysis by Ag^{+}, Fe^{2+} and Cu^{2+}ions).
5. Decomposition of diacetone alcohol by NaOH & Hydrolysis of t-butylchloride.
6. (i) Reaction between iodine and acetone and (ii) iodination of aniline.
7. Reaction between hydrogen peroxide and HI.
8. Decomposition of H_2O_2 (including the study of catalytic effect).
9. Reaction between Chromic acid and oxalic acid. 11. Iodine clock reactions.
10. Reduction of aqueous solution of ferric chloride by stannous chloride.
11. Determination of the mechanism of the oxidation of an organic compound from kinetic data.
12. Determination of catalytic constant of an acid.
13. Determination of effect of surface area of catalyst &T on the kinetics of Metal-acid reaction.
14. Determination of dissociation of trichloroacetic acid-Kinetic method.

B. Polymer Chemistry (Any Two experiments are to be carried out)

1. Determination of molecular weight and size parameters of polymers by viscometry.
2. Determination of sequences in polyvinylalcohol by viscometry.
3. Determination of molecular weight of a polymer by turbidimetry.
4. Preparation of Polymethylmethacrylate by suspension polymerization / polystyrene by free radical polymerization / Nylon by interfacial polymerization / Polyacrylamide by solution polymerisation method / polyvinylalcohol from polyvinylacetate / Phenol formaldehyde/ urea formaldehyde resins.

C. Thermodynamics Experiments (Any Five experiments to be carried out)

1. Determination of activities of an electrolyte and non-electrolyte by cryoscopy.
2. Determination of partial molar volumes of (a) Salts-water and (b) alcohol-water (methanol & ethanol) systems by density method.
3. Study of complex formation between mercury and potassium halides by cryoscopy.
4. Determination of specific heat of liquids and solutions by calorimetry.
5. Determination of stepwise neutralisation of acids.
6. Study of phase diagram of a ternary aqueous system of potassium chloride, sodium chloride and water.
7. Study of phase diagram of a ternary system of benzene-acetic acid-water or DMSO- water-benzene or ethanol-benzene-water etc.
8. Determination of heat of solution of KNO_3 in water, integral heat of dilution of H_2SO_4 and heat of ionization of acetic acid and ammonium hydroxide calorimetrically.
9. Cryoscopic and ebullioscopic analysis of the given mixture of urea and glucose.
10. Determination of vant Hoff's factor for benzoic and acetic acid mixtures in benzene.
11. Determination cryoscopically the pH value of 0.5 M malonic acid in water.
12. Determination of heat of neutralisation of two acids and hence their relative strength.

D.Computer related Practicals: Solution of some selected chemical engineering problems to develop skill for computer applications,

1. Programme writing and numerical analysis.
2. Use of commercial software packages such as Mathcad, Matlab, Aspan Plus, Design II,
3. Use of Chem draw and Chem sketch for construction of molecules. Use of Window excel for drawing graphs estimation of slope intercept.

References:

1. Findlay's Practical Physical Chemistry- B. P. Levitt (Longman, London).
2. Experiments in Physical Chemistry–James and Prichard.
3. Experimental Physical Chemistry - Daniels et al.
4. Experimental Physical Chemistry-Das & Behera(Tata McGraw Hill, New Delhi)1983.
5. Advanced Practical Physical Chemistry–Yadav (1989).
6. Experiments in Physical Chemistry–J. C. Ghosh(Bharathi Bhavan)1974.
7. Computers and their applications to Chemistry, Ramesh Kumari, Narosa
8. Theory and Problems of Programming with Basic, Mc graw Hill, NY, 1987.
9. Computer programming in Fortran IV, V, Rajaraman, Prentice Hall of India, 1987.
10. Computers in Chemistry & Instrumentation,Vol.1-5 Mattson, Marcel Dekker, NY,1974.