SYLLABUS FOR POST GRADUATE (PG) COURSE IN CHEMISTRY UNDER

CHOICE BASED CREDIT SYSTEM

KHALLIKOTE AUTONOMOUS COLLEGE, BERHAMPUR

2018-2020

First Semester

Organic Chemistry (Theory)

CC 101 Marks: 100(80+20)
Duration: 3 hours

Unit-1
Reaction Mechanism :

Unit-I 20 Marks

Types of mechanisms, thermodynamic and Kinetic requirements, Kinetic and Thermodynamic control, Hammond's Postulates, Curtin-Hammett Principle, Potential energy diagrams, Transition states and intermediates, Isotope effects, Hammett equation and liner free energy relationship, Substituent and reaction constants, Taft equation.

Unit II 20 Marks

Stereochemistry:

Conformational analysis of alkanes, substituted alkanes, cycloalkanes and decalines, effect of conformation on reactivity, optical activity in the absence of chiral carbon (biphenyls, allenes and spiranes), Chirality due to helical shape, Asymmetric synthesis.

Unit-III 20 Marks

Photochemistry :

Photophysical processes: Jablonsky diagram, energy pooling, exciplexes, excimers, photosensitization, quantum yield, solvent effects, Stern-Volmer plot, delayed fluorescence.

Photochemistry of alkenes: Cis-trans isomerism, non-vertical energy transfer, photochemical addition, reactions of 1,3-,1,4-,1,5-dienes, dimerizations.

Photochemistry of carbonyl compounds: Norish type I & II reactions (cyclic & acyclic),α, β-unsaturated ketones, β,γ- unsaturated ketones, cyclohexenones (conjugated), cyclohexadienones (cross conjugated & conjugated), Paterno-Buchi reactions, photoreductions.

Photochemistry of aromatic compounds: Isomerizations, skeletal isomerizations, Dewar & Prismanes in isomerization, singlet oxygen reaction, photo Fries rearrangement of ethers & anilides, Barton reaction, Hoffman-Loefller-Freytag reaction.

Unit IV ` 20 Marks

Pericyclic Reaction:

Molecular Orbital Symmetry, Froniter Orbitals of ethylene,1,3- butadiene, 1, 3, 5 – hexa triene and allyl systems, Classification of pericyclic reactions – Woodward-Hoffmann Correlation diagram, FMO and FMO approach, Electrocyclic reactions – Conrotatory and Disrotatory motions, 4n and 4n+2 and allyl systems. Cycloadditions – Antarafacial and Suprafacial additions, 4n and 4n+2 systems, 2+2 addition of ketenes, 1, 3 dipolar cycloadditions and cheleotropic reactions.

Sigmatropic rearrangements – Suprafacial and Antrafacial shifts of hydrogen, Sigmatropic shifts involving carbon moieties, 3, 3- and 5, 5-sigmatropic rearrangements,

Claisen and Cope rearrangements, Ene reaction.

Internal Assessment - **20 marks**
20 Marks

CC 102 **Organic Chemistry (Theory)** Marks: 100(80+20)
Duration: 3 hours

Unit-I **20 Marks**

Aliphatic Nucleophilic Substitution :
SN^1, SN^2 Mechanisms, Neighboring group participation by α and π bonds, anchimeric assistance, classical and non classical carbonations, Phenonium ions, norbornyl system, the SNi mechanism, Nucleophilic substitution at an allylic, aliphatic trigonal and vinyilic carbon, Reactivity effects of substrate structure, attacking nucleophile, leaving group and reaction medium, ambident nucleophile, leaving group and reaction medium, ambient nucleophile, Regioselectivity.

Aliphatic Electrophilic Substitution :
Biomolecular mechanism – SE2, SE1, The SEi mechanism, electrophilic substitution accompanied by double bond shifts, effect of substrates,leaving group and the solvent polarity on reactivity.

Unit-II **20 Marks**

i. **Aromatic Nucleophilic Substitution:**
The SNAr,SN1, benzyne and SRN1 mechanism.Reactivity – effect of substrate structure, leaving group and attacking nucleophile. The Von-Richter, Sommelet – Hauser and Smile's rearrangement.

ii. **Aromatic Electrophilic Substitution.**

The Arenium ion mechanism, Orientation and reactivity, the ortho and para ratio, Ipso attack, quantitative reactivity in substrates and electrophile, Diazonium coupling, Vilsmeyer reaction, Gatterman-Koch reaction, Bischier-Napieralski reaction, Houben- Hoesch reaction, Fries rearrangement, Pechmann reaction.

Unit – III **20 Marks**

Free Radical Reactions :
Free radical reaction, Free radical mechanism, free radical substitution reactions, halogenation at alkyl carbon, halogenation of allylic carbon, neighbouring group assistance, oxidation of aldehydes, autooxidation, formation of cyclic ethers, coupling of alkynes, arylation of aromatic compounds, Hunsdiecker reaction, Reed reaction, rearrangement reaction, free radical quenching

Unit-IV **20 Marks**

Methods of Preparation & Synthetic Uses of the following reagents :

N-bromosuccinamide (NBS), meta-chloroperoxy acid, azo-bis-isobutyronitrile (ABIN), N-butyl lithium,N-chlorosuccinamide,DDQ(2,3-Dichloro-5,6-dicyano-1,4-benzoquinone)
, DCC (dicyclohexylcarbodiimide), Lithium
Diisopropyl amide (LDA), dithianes , SeO_2 , perbenzoic acid, Boron trichlorideetherate, Wilkinsons catalyst (Rhodium chloride triphenyl phosphate), Ziegler-Natta catalyst, (Triethylaluminium & $TiCl_4$

Internal Assessment - **20 marks**

CC 103 **INORGANIC CHEMISTRY**

Marks: 100(80+20)
Duration: 3 hour

Unit-1 20 Marks

Quantum Chemistry :

Matter waves, the uncertainty principle, Schrodinger wave equation, (Time dependent and Time independent), Postulates of quantum mechanics, Operator Concept, Particle in one and three dimensional boxes Partial in circular ring, Wave mechanical picture of hydrogen atom, Harmonic Oscillator, rigid rotator.

Unit- II 20 Marks

i. Electronic Structure of Atom:

Qualitative treatment for many-election atoms, the self-consistent field theory, the variation principle, angular momentum, LS and JJ coupling, spectral terms: $p^1 – p^6$ and $d^1 – d^{10}$ metal ions.

ii. Molecular Orbital Theory:

Huckel molecular theory for conjugated pi electron system, Application to ethylene, butadiene, cycloproppane, cyclobutadiene, benzene, bond order charge density.

Unit- III 20 Marks

VSEPR Theory:

Directional characteristics of covalent bond, hybridization and hybid orbitals – SP, SP^2, SP^3 (with wave mechanical model), dsp^2, dsp^3 and d^2sp^3 (qualitative idea). VSEPR theory, shapes of simple molecules like N_2O, F_2O, ICI_2, ICI_3, ClF_3, IF_5, IF_7, $TeCl_4$, $XeOF_4$, XeF_6.

Unit – IV 20 Marks

i. Nuclear chemistry: Radioactive decay – General characteristics, decay kinetics, parent –daughter decay growth relationships, determination of half-lives, Nuclear stability –packing fraction, binding energy, Nuclear reactions – Bethe's notation, types of nuclear reactions – specific nuclear reactions, photonuclear reactions,

ii. Radioisotopes as tracers: use of isotopic tracers in the elucidation of reaction mechanism, structure determination and solubility of sparingly soluble substances. 14C dating, medical applications of isotopic tracers. Hazards in radiochemical work and radiation protection.

Internal Assessment - 20 marks

CC 104 **INORGANIC CHEMISTRY**

Marks: 100(80+20)
Duration: 3 hours

Unit-I 20 Marks

Solid State Chemistry:
Crystal defects and Non-stoichiometry: Perfect and imperfect crystals, intrinsic and extrinsic defects. Points defects, line and plane defects, Schottky defects and Frenkel defect formation, colour centres, non-stoichiometry and defects.

Unit- II 20 Marks

Electronic properties and band theory in solids:
Metals, insulators and semiconductors, Electronic structure of solids – band theory, band structure of metals, insulators and semiconductors. Intrinsic and extrinsic semiconductors, doping semiconductors, p-n junctions.

Solid state Reactions: General principles, experimental procedures, co-precipitation as a precursor to solid state reactions, Kinetics of solid state reactions.

Unit – III 20 Marks

Metal – Ligand Equilibria in solution:
Step-wise and overall formation constants and their relation. Factors affecting the stability of metal complexes with reference to the nature of metal complexes with reference to the nature of metal ion and ligand, Chelate effect and its thermodynamic origin, determination of binary formation constants by pH-metry and spectrophotometry.

Unit- IV 20 Marks

Coordination Chemistry:
Bonding in coordination compounds, Valence bond theory – its strength and shortcomings, Crystal field theory and crystal field effects, spin types, CFSE, measurements of 10Dq, tetrahedral, tetragonally distorted, square pyramindal and square planner fields. ACFT / LFT, Molecular diagrams, Sigma and pi-bonding and their importance in coordination complexes.

Internal Assessment- 20 Marks

CC 105

ORGANIC CHEMISTRY (PRACTICAL)

Marks: 100
Duration: 6hours

1. Identification of organic compounds having at least two functional groups.

2. Estimation of (a)Acetyl group, (b) Phenol group,(c) Keto group,(d)Nitrogen by (Kjeldahl's) method,(e) Sulphur.

3. Synthesis of Organic Compound: Preparation of
   a. P-nitroacetanilide,
   b. P-nitroaniline,
   c. m-dinitrobenzene
   d. Methyl orange,
   e. Sulphanilic acid,
   f. Ethyl benzoate,
   g. P-iodotoluene,
   h. P-bromoacetanilide,
   i. P-bromoaniline,
   j. m-nitroaniline.

4. Synthesis of simple dyes and check the purity by paper chromatography and extinction coefficient measurements.

CC 201

SECOND SEMESTER
ORGANIC CHEMISTRY

Marks: 100(80+20)
Duration: 3 hours

Unit – I 20 Marks

Addition to Carbon – Carbon Multiple Bonds:
Mechanistic and stereochemical aspects of addition reactions involving electrophiles, nucleophiles and free redicals, region and chemosectivity, orientation and reactivity, Hydrogenation of double and triple bonds, Hydrogenation of aromatic rings, hydroboration, Michael reaction, Sharpless asymmetric epoxidation.

Unit – II 20 Marks

Addition to Carbon- Hetero Multiple Bonds:
Mechanism of metal hydride reduction of saturated and unsaturated carbonyl compounds, acids, esters and nitriles. Addition of Grignard regents to carbonyl compounds, Witing reaction, Mechanism of condensation reactions involving enolates – Aldol, Knoevenagel, Claisen, Mannich, Benzoin, Perkin and Stobbe reactions, Hydrolysis of esters and amides.

Unit – III 20 Marks

Application of Organo – metallics in Organic synthesis:
Introduction: Metal ion/atom functionality in organo metallic reactions, carbanionic behavior, carbonium ion behavior, free radical intermediate, Synthetic applications of organo zinc, organo cadmium, organo aluminium, organo copper, organo mercury and organo silicon compounds, Rearrangements catalysed by metal ions and complexes.

Unit – IV 20 Marks

Mechanism of Molecular Rearrangements:
A detailed study of the following rearrangements:
Pinacol – Pinacolone, Wagner – Meerwein, Tiffenev – Demjanov, Dienone – Phenol, Benzil- Benzilic acid, Favorskiii, Wolff, Neber, Curtius, Schmidt, Beckmann, Baeyer-Villiger, Hofmann and Shapiro reaction.

Internal Assessment - 20 marks

ORGANIC CHEMISTRY

CC 202

Marks: 100(80+20)
Duration: 3 hours

Unit – I 20 Marks

Oxidation:
Introduction: Different oxidative processes, Hydrocarbons, alkenes, aromatic rings, saturated C-H groups, alcohols, diols, aldehydes, ketones and carboxylic acids, amnies, Oxidation with Ruthenium letroxide, lodobenzene diacetate, Thallium (III) nitrate.

Unit – II 20 Marks

i. Reduction:
Introduction: Different reductive process, Hydrocarbon: alkenes and aromatic rings, carbonyl compounds – aldehydes, ketones, acids and their derivatives, hydrogenolysis.

ii. Catalysis:
Catalysed synthetic processes including heterogeneous catalyst, a brief descripition of phase transfer catalyst, micellar catalyst, polymer supported reangents and biocatalyst in organic synthesis.

Unit – III 20 Marks

Nucleophilic And Electrophilic Reactivity:
Sructure and electronic effects of SN1 and SN2 reactivity: Solvent effect, kinetic isotope effects, intramolecular assistance, Electron transfer nature of SN2 reaction, Nucleophilicity and SN2 reactivity based on curve – crossing model, Relationship between polar and electron transfer reaction, SRN1 mechanism, Electrophilic reactivity, general mechanism, kinetics of SE2 – Ar reaction, Structural effects on rates and selectivity, Curve – crossing approach to electrophilic reactivity.

Unit – IV 20 Marks

i. Reaction of Electron Deficient Intermediates:
Carbene structure and reactivity, addition reaction, insertion action, rearrangement reactions, related reactions, Nitrenes – Rearrangement of electro deficient nitrogen atom, Rearrangement of carbonium ion intermediates, carbon-carbon bond formation involving carbonium ions, Fragmentation reactions.

ii. Reaction of Carbon Nucleophiles with Carbonyl Group:
Aldol condensation, amines – catalysed aldol condensation reactions, Mannich reaction, Acylation of carbonions, Claisen, Dieckmann and related carbonyl clefination reaction, sulphur yields and related species as nucleophile.

Internal Assessment- 20 Marks

CC 203 **INORGANIC CHEMISTRY** **Marks: 100 (80+20**
Duration : 3 Hours)

Unit – I 20 Marks

i. Elementary idea about magnetochemistry of metal complexes, diamagnetism, paramagnetism, and temperature independent paramagnetism, magnetic susceptibility and its measurements. Types of paramagnetism as applied to metal complexes. Elementary idea about ferromagnetism, ferrimagnetism, and antiferromagnetism.

ii. Elementary idea about electronic spectral properties of some simple metal complexes. Electronic spectra and Orgel diagram of simple complexes of ions in octahedral and tetrahedral fields.

Unit – II 20 Marks

Reaction Mechanism of Transition metal complexes:
Energy profile of a reaction, reactivity of metal complexes, inert and labile complexes, kinetic application of valence bond and crystal field theories, Kinetics of octahedral substitution, general mechanism (D, Id, ia and A) acid hydrolysis, conjugate base mechanism, Direct and indirect evidences in favor of conjugate mechanism of the substitution reactions.

Unit – III 20 Marks

Structure and reactivity in redox reactions of coordinate compounds. Electron transfer vs atom transfer, Complementary and noncomplementry redox reaction. One electron and two electron transfer reaction. Mechanisms of electron transfer – outer sphere mechanism and Marcus theory, Inner sphere mechanism.

Unit – IV 20 Marks

Chemistry of metal carbonyls:
Constitution of metal carbonyls of mononuclear, polynuclear and clusters with terminal and bridging carbon monoxide ligand units, carbonylate anion, carbonyl hydrides and carbonyl halides. Metal nitrosyls and other types of metal nitric-oxide complexes, cyanonitrosyl complexes of metals, the brown – ring compounds.

Internal Assessment - **20 Marks**

CC 204 **INORGANIC CHEMISTRY**

Marks: 100(80+20)
Duration: 3 hours

Unit – I 20 Marks

Bio – inorganic Chemistry:
Elementary study of bio-inorganic chemistry, role of metal ions and other inorganic elements in biological systems, active transport system, Daniel-Davisson model of cell, molecular mechanism of alkali ion (Na & K) transport, antibiotic – valinomycin, lonophores, transport by anionic carriers, sodium, potassium pump.

Unit – II 20 Marks

Metalloporphyrins:
Iron porphyrins, the iron and dioxygen transport system. Haemoglobin and Myoglobin, O_2 affinity. Cooperativity and Bohr's effect. Non-heme proteins: Ferredoxins, nitrogenase, structure and function of nitrogenase in relation to bioinorganic aspects of nitrogen fixation. Structure and biological role of vitamin B_{12}.

Unit – III 20 Marks

Organometallic Compounds:
Classification, nomenclature and characteristics of organometallic compounds – Introduction, classification based on the polarity of M-C bond, general chacteristics of different types of organometallic compounds. Few transition metal organo metallics as catalytic and synthetic agents.

Unit – IV 20 Marks

Chemistry of metallocenes:
Synthesis and reactions of ferrocene – Bonding and structure of metallocenes with special reference to ferrocene – the eighteen electron rule, MO picture (Qualitative & Quantitative).

Internal Assessment- 20 Marks

CC 205

INORGANIC CHEMISTRY (Practical)

Marks: 100
Duration: 6hours

1. Qualitative analysis of mixtures containing not less than six radicals (organic acid radicals should be excluded). Any one of the following rare metal ions may be included (a) Vanadium, (b) Molybdenum, (c) Tungsten, (d) Titanium.

2. Quantitative analysis:

    1. Use of EDTA as volumetric regent
        a. Standardization of EDTA
        b. Determination of Ca^{2+} and Mg^{2+}
        c. Determination of Tin and Lead in Type metal
        d. Determination of Nickel in stainless steel

    2. A complete analysis of following:
        a. Brass,
        b. Cement,
        c. Chrome iron ore

3. Preparation and characterization (including spectroscopic methods) of the following inorganic complexes.

    a. Hexaammine cobalt (III) Chloride
    b. Tris (oxalate) Chromate (III)

4. Chromatography Separation of Cation and Anion
    a. Paper chromatography
    b. Thin layer chromatography
    c. Column chromatography

THIRD SEMESTER

CC 301

PHYSICAL CHEMISTRY

Marks: 100(80+20)
Duration: 3 hours

Unit – I – Classical Thermodynamics: 20 Marks

i. Brief resume of the concept of enthalpies, entropy, free energy, and laws of thermodynamics, Partial molar properties. Partial molar free energy, partial molar volume and partial molar heat content and their significance. Determination of partial molar properties by (i) direct method, (ii) from apparent molar properties, (iii) method of intercepts.

Unit-II 20 Marks

i Thermodynamics of ideal and real gases and gas mixtures. Fugacity of gases and their determination by (i) graphical method, (ii) from equation of state, (iii) approximate method.

ii. Nernst heat theorem, application to solids, third law of thermodynamics, experimental determination of entropy by third law.

Unit-III 20 Marks

Statistical Thermodynamics:

Thermodynamic probability and entropy, Maxwell Boltzmann statistics, partition function (translational, vibrational, rotational) for diatomic molecules. Calculation of thermodynamic functions and equilibrium constant from molecular properties.

Unit-IV 20 Marks

Activity and activity coefficient of electrolytes, ionic-strength, Debey–Huckel limiting law and its verification. Determination of activity coefficient by freezing point, vapour pressure and solubility measurements, Ion–Association, fraction of association, Association constant, Determination of dissociation constant of electrolytes.

Internal Assessment- **20 Marks**

CC 302

PHYSICAL CHEMISTRY

Marks: 100(80+20)
Duration: 3 hours

Unit – I Ion Solvent Interactions **20 Marks**

Nonstructural treatment of ion – solvent interaction. Quantitative measure of ion solvent interaction. Born model, electrostatic potential at the surface of a charged sphere. The Born expression for the free energy of ion solvent interaction, the interaction of single ionic species with the solvents. Experimental evaluation of the heat of interaction of a salt and solvent, limitation of Born theory.\

Unit-II **20 Marks**

Structural treatment of ion – solvent interaction. Structure of water near an Ion. Ion – dipole model of ion solvent interaction. Ion–Dipole model approach to the heat of solvation, water molecule as electrical quadrupole, ion- quadrupole model of ion – solvent interaction. Ion induced dipole interaction in the primary solvation sheath. Limitation of ion – quadrupole theory of solvation..

Unit – III **20 Marks**

Kinetics of complex (consecutive, concurrent and reversible) reactions. Arrhenius equations, Collision theory of bimolecular reactions, test for the validity of the collision theory, interpretation of frequency tests, study of kinetics of $H_2 + l_2$ 2HI in terms of collision theory. Steady state treatment, theory of absolute reaction rate.

Unit-IV **20 Marks**

Catalysis – Acid–base catalysis,enzyme catalysis,.Photochemical equilibrium,Kinetics of photochemical reaction, photolysis of acetaldehyde, Flash photolysis, Stopped flow method.

Internal Assessment- **20 Marks**

CE 303 ANALYTICAL CHEMISTRY

Marks: 100 (80 + 20)
Duration: 3 hours

Unit-I **20 Marks**

Application of UV spectroscopy:

Basic principles, Ultraviolet bands for carbonyl compounds, unsaturated carbonyl compounds, dienes, conjugated polynes, Fieser – Woodward rules for conjugated dienes and carbonyl compounds ultraviolet spectra of aromatic compounds, steric effect in biphenyls.

Unit-II **20 Marks**

Applications of IR spectroscopy:

Theory of molecular vibrations, vibrational frequency finger print region, characteristic vibrational frequency of alkanes, alkenes, alkynes, aromatic hydrocarbons, alcohols and phenols, detailed study of IR spectra of carbonyl compounds (aldehydes, ketones, acids, esters, amides), amines, nitro compounds and nitriles, effect of hydrogen bounding and solvent effect on vibrational frequencies overtones.

Unit-III **20 Marks**

NMR spectroscopy and Applications:

Chemical shift, spin – spin interaction, shielding mechanism, chemical shift values and correction for protons bonded to carbon (aliphatic, olefinic, aldehydic and aromatic), chemical exechange, effect of deuteration, hindered rotation, contact shift reagents, NMR spectra of simple molecules like n-propanol, 1-3-dichloropane, benzaldehyde, 2,3 dibromo propene and cis and trans – stilbene.

Unit-IV **20 Marks**

NQR: Quadrupole nuclei, Quadrupole moment, Electric field gradient and coupling constant, Theory of NQR, Splitting in NQR spectra, Zeeman effect in NQR spectra, Instrumentation, Interpretation of NQR data, Structural information of the following: PCl_5, $TeCl_4$, $Na^+GaCl_4^-$, BrCN, HIO_3 and Hexahalometallates

Internal Assessment- **20 Marks**

AE 304 **BIO CHEMISTRY**

Marks: 100 (80 + 20)
Duration: 3 hours

Unit – I 20 Marks

i. **Multistep Synthetic Strategy:**
Concept of protective groups, principles of protection of hydroxy, amino, carbonyl and carboxyl groups, synthetic equa – equivalent groups, concept of umpolong, synthetic strategy in the retro synthesis of Juviborne and Longifolene.

ii. **Alkaloids:**
Total synthesis of the following alkaloids will be studied. Quinine, Strychnine, Reserpine and Lycopodine.

Unit – II 20 Marks

i. **Terpenes:** Synthesis of the following terpenes will be studied:
Camphor, Santonin, Abietic acid and Squalene.

ii. **Steroids:** Synthesis of the following steroids will be studied. Cholesterol, Bile, Androsterone and Estrone.

Unit – III 20 Marks

Studies on Biosynthetic Pathways of Natural Products:
The acetate hypothesis, poly-betaketo acids & their aldol type cyclisation and meta orientation of hydroxyl groups in naturally occurring phenols, biogenesis of mascon, isoprene rule, mechanism of formation of mevalonic acid from acetylcoenzyme – A, Biogenetic isoprene rule, pyrophosphates and their conversion into alphapinene, thujine and burneol. Farnesyl and geranyl pyrophosphates & their conversion into cardinanes and abietic acid.

Unit – IV 20 Marks

i. **Drugs:** A general study of the following type of drugs: Histamines and antihistaminic agents, analgesic and antiviral agents, antifertility agents, anti-inflammatory agents, Diuretics and cardiac agents.

ii. **Antibiotics:** Structure determination and synthesis of the following antibiotics: Penicillin, Streptomycin, Tetracyclin and chloramphenicol.

Internal Assessment- 20 Marks

CC 305 **ANALYTICAL PRACTICAL**

Marks: 100
Duration: 6 hours

I. Separation Techniques

Chromatography:

(a) Separation of mixtures

(i) Paper chromatographic separation of Co^{2+} and Ni^{2+}

(ii)Separation and identification of the amino acids present in the given mixture by paper chromatography. Reporting the Rf values.

II. Solvent Extractions:

(i) To separate a mixture of Ni 2+ & Fe 2+
by complexation with DMG and extracting the Ni 2+ - DMG complex in chloroform, and determine its concentration by spectrophotometry.

Analysis of soil:

(i) Determination of pH of soil.
(ii) Total soluble salt
(iii) Estimation of calcium, magnesium
(iv) Qualitative detection of nitrate, phosphate

Ion exchange:

(i) Determination of exchange capacity of cation exchange resins and anion exchange resins.
(ii) Separation of amino acids from organic acids by ion exchange chromatography.

III Spectrophotometry

Verification of Lambert-Beer's law and determination of concentration of a coloured species (CuSO 4 , KMnO 4)

Reference Books:

• Vogel, Arthur I: A Text book of Quantitative Inorganic Analysis (Rev. by G.H. Jeffery and others) 5
th
Ed. The English Language Book Society of Longman .
• Willard, Hobart H. et al.: Instrumental Methods of Analysis, 7th Ed. Wardsworth Publishing Company, Belmont, California, USA, 1988.
• Christian, Gary D; Analytical Chemistry, 6th Ed. John Wiley & Sons, New York, 2004.
• Harris, Daniel C: Exploring Chemical Analysis, Ed. New York, W.H. Freeman, 2001.

• Khopkar, S.M. Basic Concepts of Analytical Chemistry. New Age, International Publisher, 2009.
• Skoog, D.A. Holler F.J. and Nieman, T.A. Principles of Instrumental Analysis, Thomson Asia Pvt. Ltd. Singapore, 1998.
• Mikes, O. & Chalmers, R.A. Laboratory Hand Book of Chromatographic & Allied Methods, Elles Horwood Ltd. London.
• Dilts, R.V. Analytical Chemistry – Methods of separation Van Nostrand 1974

FOURTH SEMESTER
PHYSICAL CHEMISTRY

CC 401 Marks: 100(80+20)
Duration: 3 hours

Unit – I

Symmetry and group theory: 20 marks

Symmerty elements and symmetry operations, definition of group, subgroup, relation between orders of a finite group and its subgroup. Conjugacy relation and classes, point symmetry group, schonflies symbols, representation of groups by matrices (representation for the Cn, Cnv, Cnh, Dnh, etc. groups to be worked out explicity), character of a representation. The great orthogonality theorem (without proof) and its importance. Character tables and their use.

Unit-II Macromolecules:

Concept of molecular mass, number and mass average molecular mass. Determination of molecular mass by (Osmometry, Viscometry, diffusion and light scattering methods), Sedimentation, chain configuration of macromolecules, calculation of average dimensions of various chain structures.

Unit -III 20 Marks

Surface Chemistry:

Freundlich adsorption, Langmuir adsorption, Gibbs adsorption isotherm, BET equation, application of BET equation for determination of surface area, catalytic activity at surfaces.

Unit –IV 20 Marks

Photoelectron Spectroscopy: Basic Principle, photoelectric effect, photoelectron spectra of simple molecules like N_2, CO, ESCA, Chemical information from ESCA

Internal Assessment- **20 Marks**

PHYSICAL CHEMISTRY

CC-402 **Marks:100(80+20)**

Unit-I **20 Marks**

Molecular Spectroscopy:

Rotational Spectra of diatomic molecule – rigid rotator, intensity of spectral lines, effect of isotopic Substitution, non rigid rotator and its spectrum, Calculation of internuclear distances.

Unit – II 20 Marks

Vibrational Spectroscopy:

The vibrating diatomic molecule, linear harmonic oscillator, unharmonic vibration, vibration – rotation fine structure. P, Q, R branch, Parallel vibrations and perpendicular vibrations in symmetric top molecules. Elementary idea about FTIR spectroscopy. Application for IR Spectroscopy to different functional groups, finger print region.

Unit-III

Raman Spectroscopy:

Classical and quantum theory of Raman effect, pure rotational Raman spectra, Vibrational Raman Spectra, Polarisation of light and Raman effect, Structure determination by Raman and IR spectroscopy.

Unit – IV 20 Marks

i. **ESR Spectroscopy:**
Basic principle, hyperfine splitting in some simple system – Hydrogen atom, Deuterium methyl radical, Factors affecting the 'g' values, zero field splitting and Kramer's degeneracy, applications of E.S.R. spectra.

ii. **Mossbauer Spectroscopy:**
Principle of Mossbauer Spectroscopy, experimental technique, Hyperfine interactions in Mossbauer Spectroscopy. Application in determining nature of bond and structure of compounds.

Internal Assessment- **20 Marks**

CE 403 **ANALYTICAL CHEMISTRY**

Marks: 100(80+20)

UNIT – I **Duration: 3 hours**

Flame photometry and Atomic absorption spectrometry: Energy level diagrams - atomic absorption spectra. Flame characteristics. Flame atomizers and electrothermal atomization. Comparison of spectral interferences, chemical and physical interferences in FP and AAS. Use of organic solvents. Quantitative techniques - calibration curve procedure and the standard addition technique. Typical commercial instruments for FP and AAS, applications. Qualitative analysis and quantitative evaluations. Relative detectabilities of atomic absorption and flame emission spectrometry.

UNIT – II

Molecular luminescence spectrometry: Theoretical basis for fluorescence and phosphorescence. Singlet and triplet excited states. Variables affecting luminescence - quantum efficiency, transition types, structure and structural rigidity, temperature and solvent effects, effect of *p*H, dissolved oxygen and concentration effect. Excitation spectra *vs* emission spectra. Fluorescence instrumentation - fluorometers and spectrofluorometers. Sensitivity and selectivity. Modification necessary to measure phosphorescence. General scope of applications of luminescence. Chemiluminescence spectrometry-Principles, instrumentations and applications

UNIT – III

Thermal method of analysis: Introduction,

(i)**Thermogravimetricanalysis (TGA):** types of thermogravimetric analysis,principles.

Factors affecting the results - heating rate, furnace, instrument control/data handling.

Applications - purity and thermal stability, evaluation of correct drying temperature, analysis of complex mixture and determination of kinetic parameters of thermal degradation.

i. **Differential thermal analysis (DTA):** Theory - variables affecting the DTA curves. Differences between TGA and DTA. General principles. Instrumentation. Applications - analysis of the physical mixtures and thermal behaviour study. Determination of melting point, boiling point and decomposition point.

ii. **Differential scanning calorimetry (DSC):** Basic principle. Differences between DTA and DSC. Instrumentation - power compensated DSC, Heat flux DSC. Applications - testing the purity of the samples.

UNIT – IV

i. **Gas chromatography (GC):** Principles, instrumentation **-** mobile phase, chromatographic columns, stationary phases, sample introduction, temperature control, and detectors for gas chromatography. Quantitative and qualitative applications.

ii. **High performance liquid chromatography (HPLC):** Principles, instrumentation - columns (analytical and guard columns), stationary phases, mobile phases, choosing a mobile phase, isocratic *vs* gradient elution, HPLC plumbing, sample introduction. Detectors for HPLC - spectroscopic, electrochemical and other quantitative applications.

Internal Assessment- **20 Marks**

CC 404 **PHYSICAL CHEMISTRY (PRACTICAL)**

Marks: 100
Time: 6 Hours

1. Kinetic study of hydrolysis of an ester (Acid and Alkaline hydrolysis) and Comparison of strength of acids.
2. Determination of the velocity constant of hydrolysis of an ester in micellar medium.

3. Determination of activation energy for the acid hydrolysis of an ester.
4. Study the critical solution temperature effect of impurities.

5. To determine the triple point from the phase diagram of three component partially miscible liquid system.
6. To determine the partition coefficient for distribution of iodine between CCl 4 and water.
7. Study the distribution of benzoic acid between benzene and water.

8. Determine the percentage of glycerol water mixture and radius of the glycerol molecule from viscosity measurements.
9. Surface tension of liquid and liquid mixtures by drop weight method.

10. Determination of heat of solution of sparingly soluble salt from solubility measurement.
11. Determination of molecular weight by Victor mayer method.

12. Determination of C M C of sodium dodecyl sulphate by Spectro photometry / conductometry / surface tension measurements.
13. Study of inversion of sucrose by polarimetry – comparison of strength of acids.

14. Absorption isotherm (Freundlich) verification and preparation of sols.
15. Transport number of Cu +2 by Hittorf's method.

16. Conductometric titrations – Neutralisation and precipitation of sols.
17. Determination of hydrolysis constant of aniline hydrochloride by conductometry.

18. Determination of thermodynamic dissociation constant of a weak acid by potentiometry and conductometry.
19. Determination of the strength of strong and weak acids in a given mixture using a potentiometer / pH meter.

20. Determination of thermodynamic constants, *G, *S and *H for the reaction by e.m.f. method.
Zn + H 2 SO 4 → ZnSO 4 + 2H
21. Determination of compostion of a metal complex by Job's method spectrophotometry.

CE 405 PROJECT WORK Marks: 100

Students are assigned with one project work each. They are required to do either field work or
laboratory work and submit a synopsis which is to be examined by internal and external
examiners.

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Books for reference:

1. Advanced Organic Chemistry- Reaction mechanism and structure – Jerry March, John
Wiley
2. Advanced organic chemistry – F.A. Caray & R.J. Scandberg, Skyes, Longmann
3. Organic chemistry – R.T. Morrison & R.N. Bose, Prentice Hall
4. Modern organic reaction – H.O, House, Benjamin
5. Pericyclic reaction – S.M. Mukherjee, Macmillan, India
6. Stereochemistry of organic compounds – P.S. Kalsi, New Age International
7. Organic chemistry of natural products-V-1 & V-2, Gurudeep R. Chatwal, Himalaya
Publishing House
8. StereoChemistry of organic compounds – D.Nasipuri, New Age International
9. Organic reaction & their mechanism – P.S. Kalsi, New Age International
10. Synthetic Organic Chemistry – Indu Sekhar Jha, Himalaya Publishing House
11. Advanced Inorganic Chemistry – F.A. Cotton, Willikinson, John Wiley
12. Inorganic Chemistry- J.D. Lee
13. Magneto Chemistry – R.I. Carlin, Springer Verlag
14. Introduction to Quantum Chemistry – A.K. Ca, Tata Mc Grew Hill
15. Chemical Kinetics – K.J. Laidler, Tata Mc Grew Hill
16. Modern Electrochemistry Vol-1 & 2 – J.O.M. Bokris & A.K.N. Reddy
17. Physical chemistry – P.W. Atkins
18. Physical Method in chemistry- R.S. Drago, Sanders College
19. Clinical application of group theory – F.A. Cotton
20. Introduction to Polymer Science, V.R. Gowarikar, N.V. Vishwanathan & J. Sridhar,
Wiley Publication
21. Modern spectroscopy-J.M Holla, John Wiley Publication
22. Introduction to Molecular spectroscopy – G.M. Barrow, Tata Mc Grew Hill
23. Introduction to Photoelectron spectroscopy – P.K.Ghosh, John Wiley
24. Fundamental of photochemistry – K.K. Rastogi, Mukherjee, Wiley – Eastern
25. Molecular Photochemistry – N.J. Turro, W.A. Benzamin
26. Organic Photochemistry, J.Cox & B.Halter, Cambridge University Press

27. Solid state Chemistry & its application- A.R.West, Plenum
28. Solid state chemistry- D.K.Chakraborty, New age publisher
29. Principle of solid state, H.B. Keer, Wiley Eastern
30. Principle of Bio-inorganic Chemistry-S.J.Lipaard & J.M. Berg, Universty Science Book
31. Bioinorganic-Berini, H.B Grey, Science Book
32. Inorganic biochemistry Vol 1 & 2, G.L.Bichhiom, Elsevier

33. Biorganic & Bioinorganic as Supramolecular Chemistry, P.S.Kalsi & J.P. Kalsi, New age
publisher
34. Solid State Chemistry, 3rd Edition by D.K.Chakravarty, New age publisher
35. A Text Book of Physical Chemistry, 2nd Edition by A.S. Negi & S.C. Anand, New age
publisher
36. Symmetry & Spectroscopy of Molecules, 2nd Edition by K. Veera Reddy, New age
publisher
37. Basic Concepts of Analytical Chemistry, 3rd Edition by S.M.Khopkar, New age
publisher
38. Atomic & Molecular Spectroscopy by M.C.Gupta, New age publisher
39. Vibrational Spectroscopy Theory & Applications by
D.N.Sathyanarayana, New age
publisher
40. Spectrometric Identification of Organic Compounds by Robert M. Silverstein and Francis
X. Webster
Organic Chemistry Practical
41. Experiment & Technique in organic Chemistry – D. Pasto, C.Johnson, M. Miller,
Prentice Hall
42. A text book of practical organic chemistry (Qualitative)- I. Vogel
43. Hand book of organic analysis qualitative & quantitative-M.T. Clarke, Edward Arnold
(publisher)
Inorganic Chemistry Practical
44. Inorganic experiment – J. Perck Woolins, Vett
45. Microscale inorganic chemistry – Z.Szafram, R.M. Pike & M.M. Singh, Wiley India
46. Practical inorganic chemistry – G. Marr & B.W. Rockett, Van Nostrand
47. Quantitative Analysis – I. Vogel
Physical Chemistry Practical
48. Findley Practical Chemistry – B.D. Lecith, Longmann
49. Experimental physical chemistry – R.C. Das & B. Behera, Tata McGrew Hill
50. Practical physical chemistry – A.M. James & Prichand, Longmann

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