Syllabus for Master of Science

in Chemistry
Under Choice Based Credit System

2015

Department of Chemistry
College of Basic Science & Humanities
Orissa University of Agriculture and Technology
Bhubaneswar - 751003

Content

Semester wise Course Outline and Credit Structure

1st Semester

Paper Code	Paper Title	Credits	Marks
CHE(C) 4101	Physical Chemistry – I	4	50
CHE(C) 4102	Inorganic Chemistry – I	4	50
CHE(C) 4103	Organic Chemistry – I	4	50
CHE(C) 4104	Spectroscopy – I	4	50
CHE(E) 4105	Nuclear and Photochemistry / Medicinal Chemistry*/ Chemistry of Natural Products*	4	50
CHE(P) 4106	Laboratory Course – I	4	100
Total		24	350

2nd Semester

Paper Code	Paper Title	Credits	Marks
CHE(C) 4207	Physical Chemistry – II	4	50
CHE(C) 4208	Inorganic Chemistry – II	4	50
CHE(C) 4209	Organic Chemistry – II	4	50
CHE(C) 4210	Spectroscopy – II	4	50
CHE(E) 4211	Organotransition Metal Chemistry / Chemistry of Materials*/ Physical Organic Chemistry*	4	50
CHE(P) 4212	Laboratory Course – II	4	100
Total		24	350

3rd Semester

Paper Code	Paper Title	Credits	Marks
CHE(C) 5313	Matter and Physical Transformation	4	50
CHE(C) 5314	Quantum Chemistry and Chemistry of Special Elements	4	50
CHE(C) 5315	Organic Synthesis	4	50
CHE(C) 5316	Application of Spectroscopy – I	4	50
CHE(E) 5317	Heterocyclic Chemistry / Polymers*/ Liquid State*	4	50
CHE(P) 5318	Laboratory Course – III	4	100
Total		24	350

4th Semester

Paper Code	Paper Title	Credits	Marks
CHE(C) 5419	Analytical and Environmental Chemistry	4	50
CHE(C) 5420	Application of Spectroscopy – II	4	50
CHE 5421	Dissertation	14	200
CHE 5422	Seminar	2	50
Total		24	350

The Paper Title marked (*) under Paper Code CHE 405, CHE 411 and CHE 517 are not offered at present.

First Year

1st Semester

Course Outline and Credit Structure

Paper Code	Paper Title	Credits	Marks
CHE(C) 4101	Physical Chemistry – I	4	50
CHE(C) 4102	Inorganic Chemistry – I	4	50
CHE(C) 4103	Organic Chemistry – I	4	50
CHE(C) 4104	Spectroscopy – I	4	50
CHE(E) 4105	Nuclear and Photochemistry	4	50
CHE(P) 4106	Laboratory Course – I	4	100
Total		24	24

Paper Code: CHE(C)4101 **Credit: 4**
Paper Title: Physical Chemistry – I **Full Mark: (External: 40 and Internal: 10)**
(Each unit carries equal mark)

UNIT – I

Classical Thermodynamics (16 Periods)

Brief resume of concepts of laws of thermodynamics, free energy, chemical potential and entropies, partial molar properties - partial molar free energy, partial molar volume and partial molar heat content and their significances. Determination of these quantities.Concept of fugacity and determination of fugacity. Non-ideal systems: Excess functions for non-ideal solutions.

UNIT – II

Statistical Thermodynamics – I (16 Periods)

Concept of distribution, thermodynamic probability and most probable distribution. Ensemble averaging, postulates of ensemble averaging. Canonical, grand canonical and microcanonical ensembles, corresponding distribution laws (using Lagrange's method of undetermined multipliers). Most probable distribution and Maxwell- Boltzmann distribution law of energy. Partition functions – translational, rotational, vibrational and electronic partition functions.

UNIT – III

Statistical Thermodynamics – II (16 Periods)

Calculation of thermodynamic properties in terms of partition functions. Application of partition functions, equilibrium constant in terms of partition functions, Maxwell- Boltzmann statistics, Femi-Dirac statistics, distribution law and applications to metal. Bose-Einstein statistic – distribution law and application to helium.

UNIT – IV

Surface Chemistry (10 Periods)

Surface tension, capillary action, pressure difference across curved surface (Laplace – Young equation), Vapour pressure of droplets (Kelvin equation), Gibbs adsorption isotherm, estimation of surface area using BET equation(derivation not required), Surface films on liquids (Electro-kinetic phenomenon), Catalytic activity at surfaces.

Micelles (6 Periods)

Surface active agents, classification of surface active agents, micellization, hydrophobic interaction, critical micellar concentration (CMC), factors affecting the CMC of surfactants, counter ion binding to micelles, thermodynamics of micellization, micro emulsion, reverse micelles.

Books Recommended

1 Physical Chemistry; P.W. Atkins; ELBS.
2 Physical Chemistry; W.J. Moore.
3 Physical Chemistry; Barrow.
4 Physical Chemistry; Snehi Hemant.
5 Advanced Physical Chemistry; Gurtoo & Gurtoo.
6 Physical Chemistry through problems; Dogra and Dogra.
7 Thermodynamics for Chemists; S. Glasstone.

Paper Code: CHE(C)4102 **Credit: 4**
Paper Title: Inorganic Chemistry – I **Full Mark: (External: 40 and Internal: 10)**
(Each unit carries equal mark)

UNIT – I

Geometry and Bonding of Main Group Compounds (12 Periods)
VSEPR Theory, Walsh diagrams (tri- and penta- atomic molecules), d_{π}–p_{π} bonding, bent rule and energetics of hybridization, some simple reactions of covalently bonded molecules.

Coordination Compounds –Bonding, Stereochemistry and Structure (8 Periods)
Crystal field theory, crystal field diagram, ligand field theory, spectrochemical series, nephelauxetic series, structural distortion and lowering of symmetry, electronic, steric and Jahn-Teller effect on energy levels, conformation of chelate ring, structural equilibrium, spectral and magnetic properties.

UNIT – II

Molecular Orbital Theory of Metal Complexes (16 Periods)
Limitations of crystal field theory, Introduction to molecular orbital theory: LCAO, Modes of overlap of atomic orbitals, Hybrid orbitals as LCAOs, Integrals and normalization constants, symmetry of MO, σ- bonding in octahedral complexes; Ligand group orbitals and formation of MO, Construction of MO energy level diagrams, HUMO and LUMO, π- bonding in octahedral complexes, σ- bonding and π- bonding in tetrahedral and square plannar complexes and their MO energy level diagrams.

UNIT – III.

Reaction Mechanism of Transition Metal Complexes (12 Periods)
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, acid hydrolysis, factors affecting acid hydrolysis, base hydrolysis, conjugate base mechanism, direct and indirect evidences in favour of conjugate mechanism, anation reactions, reactions without metal ligand bond cleavage, substitution reactions in square planar complexes, the trans effect, mechanism of the substitution reaction,

UNIT – IV

Redox reactions (4 Periods)
Redox reactions: Principle involved in extraction of metals, Electron transfer reactions, mechanism of one electron transfer reactions, outer sphere type reactions, inner sphere type reactions, Application to metal complex reactions.

Metal – Ligand Equilibria in Solution (8 Periods)
Stepwise and overall formation constants and their interaction, trends in stepwise constants, factors affecting the stability 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 spectrophotometric methods.

Books Recommended

1. Advanced Inorganic Chemistry; F. A. Cotton and Wilkinson; John Wiley.
2. Inorganic Chemistry; J. E. Huhey, Harpes & Row
3. Chemistry of the Elements; N. N. Greenwood and A. Earnshow; Pergamon
4. Inorganic Electronic Spectroscopy; A. B. P. Lever, Elsevier.
5. Magneto Chemistry; R. L. Carlin, Springer Verlag.
6. Comprehensive Coordination Chemistry ; G. Wilkinson, R. D. Gillars and J.A. McCleverty; Pergamon.
7. Modern Inorganic Chemistry; W.L.Jolly, TMH.
8. Introduction to Ligand Fields; B. N. Figgis.
9. Theoretical Inorganic Chemistry; M. C. Day and J. Selbin.
10. F. A. Cotton, Chemical Applications of Group Theory, 3rd Edn. (1999), John Wiley & Sons, New York
11. K. Veera Reddy, Symmetry and Spectroscopy of Molecules, (1999) New Age International Pvt. Ltd., New Delhi.

Paper Code: CHE(C)4103 **Credit: 4**
Paper Title: Organic Chemistry – I **Full Mark: (External: 40 and Internal: 10)**
(Each unit carries equal mark)

UNIT – I

Nature of Bonding in Organic Molecules (14 Periods)

Delocalized chemical bonding: conjugation, cross conjugation, resonance, hyperconjugation, tautomerism; Aromaticity in benzenoid and nonbenzenoid compounds, alternant and nonalternant hydrocarbons, Huckel's rule, energy level of π-molecular orbitals, annulenes, anti aromaticity, homo aromaticity. Bonds weaker than covalent: addition compounds, crown ether complexes and cryptands, inclusion compounds, cyclodextrins, catenanes and rotaxanes.

UNIT – II

Stereochemistry (15 Periods)

Conformational analysis of cycloalkanes, decalins, effect of conformation on reactivity, conformation of sugars, steric strain due to unavoidable crowding. Elements of symmetry, chirality, molecules with more than one chiral center, threo and erythro isomers, methods of resolution, optical purity, enantiotopic and diastereotopic atoms, groups and faces, stereospecific and stereoselective synthesis, asymmetric synthesis, optical activity in the absence of chiral carbon (biphenyls, allenes and spiranes), chirality due to helical shape, stereochemistry of the compounds containing nitrogen, sulphur and phosphorus.

UNIT – III

Reaction Mechanism: Structure and Reactivity (12 Periods)

Types of mechanisms, types of reactions, thermodynamic and kinetic requirements, kinetic and thermodynamic control, Hammond's postulate, Hammett – Curtain principle, Potential energy diagrams, transition states and intermediates, Methods of determining mechanisms-product identification, presence of intermediate, isotope labeling, crossover product; study on carbocations, carbanions, free radicals, carbenes and nitrenes – generation, structure, stability and reactivity.

UNIT – IV

Aliphatic Nucleophilic Substitution (13 Periods)

The S_N2, S_N1, mixed S_N1 and S_N2 and SET mechanism. The neighbouring group mechanism, neighbouring group participation by π and σ bonds, anchimeric assistance; Classical and nonclassical carbocation, phenonium ions, norbornyl system, common carbocation rearrangements, The S_Ni mechanism. Nucleophilic substitution at an allylic. aliphatic trigonal and a vinylic carbon. Reactivity effects of substrate structure, attacking nucleophile, leaving group and reaction medium, ambident nucleophile, regioselectivity.

Aromatic Nucleophilic Substitution (5 Periods)

The S_NAr, S_N1, benzyne and $S_{RN}1$ mechanisms, reactivity – effect of substrate structure, leaving group and attacking nucleophile, The Von Richter, Sommelet–Hauser, and Smiles rearrangements.

Books Recommended

1 Advanced Organic Chemistry – Reactions, Mechanism And Structure; Jerry March; John Wiley.
2 Advanced Organic Chemistry; F. A Carey and R.J. Sundberg; Springer
3 A Guide Book To Mechanism In Organic Chemistry; Peter Sykes; Longman.
4 Structure and Mechanism In Organic Chemistry; C. K. Ingold; Cornell University Press .
5 Organic Chemistry; R. T Morrison And R. N Boyd; Pearson .
6 Reaction Mechanism In Organic Chemistry; S. M. Mukherji and S. P. Singh; Macmillan.
7 Stereochemistry of Organic Compounds; D. Nasipuri; New Age International.
8 Stereochemistry of Organic Compounds; P. S. Kalsi; New Age International.
9 Stereochemistry of carbon compounds; E.L. Eliel ;Tata Mcgraw Hill .

Paper Code: CHE(C)4104 **Credit: 4**

Paper Title: Spectroscopy – I **Full Mark: (External: 40 and Internal: 10)**

(Each unit carries equal mark)

UNIT – I

Group Theory (15 Periods)

Molecular symmetry, elements of symmetry and symmetry operations, Products of operation, point group, classification of Molecules into point group, reducible and irreducible representation, the great Orthogonality theorem, character table, symmetry aspects of Molecular orbitals.

Unit-II

Unifying Principles (5 Periods)

Electromagnetic radiation, interaction of electromagnetic radiation with matter(general ideas only). Uncertainty relation and natural line width and natural line broadening, transition probability, transition moment, Selection rules, intensity of spectral lines, Born – Oppenheimer approximation, rotational, Vibrational and electronic energy levels.

Infrared and Raman Spectroscopy (9 Periods)]

Molecular vibrations, force constants, Molecular vibrations and absorption of Infrared radiations Raman Spectroscopy, polarized Raman lines, Use of symmetry considerations to determine the no. of lines in IR and Raman Spectra, Spectra of gases, applications of Raman and Infrared spectroscopy. Selection rule in Inorganic structure determinations, Hydrogen bonding and infrared spectra, metal ligand and related vibrations.

UNIT – III

Atomic Spectroscopy (6 Periods)

Energies of atomic orbitals, vector representation of momenta and vector coupling, spectra of hydrogen atom and alkali metal atoms.

Molecular Spectroscopy(7 Periods)

Energy levels, molecular orbitals, vibronic transitions, vibrational progressions and geometry of the excited states, Franck – Condon principle, electronic spectra of polyatomic molecules.Emission spectra.Charge transfer spectra.

Unit-IV

Microwave spectroscopy (6 Periods)

Basic concept, rotation spectra of simple inorganic compounds, Classification of molecules, rigid rotor model, effect of isotopic substitution on transition frequencies & intensities non rigid rotor, stark effect nuclear and electron spin interaction and effect of external field. Applications of Micro wave Spectroscopy

Photoelectron & Photo acoustic Spectroscopy (7 Periods)

Introduction, principle, Instrumentation and applications of following techniques photoacoustic Spectroscopy (PAS) photo electron Spectroscopy (PES),Koopman's theorm,ESCA and chemical informations obtained from it. Auger electron Spectroscopy (AES)

Books Recommended

1 Group theory and symmetry in Chemistry; Grudeep Raj, Ajay Kumar Bhagi, Vinod Kumar Jain; Krishna Prakashan Media PVT. Ltd.
2 Chemical Application Group Theory; F.A. Cotton; Wiley.
3 Group Theory; P K Bhattacharya ; Himalaya Publication.
4 Modern Spectroscopy; J.M.Hollas; John Wiley.
5 NMR, NQR, EPR and Mossbaur Spectroscopy in Inorganic Chemistry; R. V. Parish; Ellis Harwood.
6 Physical Methods in Chemistry; R. S. Drago; .
7 Introduction to Molecular Spectroscopy; G. M. Barrow; McGraw Hill.
8 Basic Principles of Spectroscopy; R. Chang; Mcgraw Hill.
9 Theory and Applications of UV Spectroscopy; H. H. Jaffe and M. Orchin; IBH – Oxford.
10 Introduction to Photoelectron Spectroscopy; P. K. Ghosh; John Wiley.
11 Analytical Chemistry; U.N. Dash.
12 Fundamentals of Molecular Spectroscopy; C. N. Banwell and E.M.McCash; McGraw Hill
13 Group theory and its applications to chemistry by K. V. Ramen , Tata McGrew Hill.
14 Molecular Structure and Molecular Spectra by G. Herzberg, Van Nostrand .
15 Molecular Spectroscopy by I. N. Levine , Willey interscience.
16 Molecular Spectroscopy by G. M. Barrow.

Paper Code: CHE(E)4105 **Credit: 4**

Paper Title: Nuclear & Photochemistry **Full Mark: (External: 40 and Internal: 10)**

(Each unit carries equal mark)

UNIT – I

Radioactive Decay Processes (7 Periods)

Radioactive decay and equilibrium, Nuclear reactions, Q value, cross sections,types of reaction,Chemical effect of nuclear transformation-Fission and Fusion,Fission products and fission yield.

Nuclear Energy (6 Periods)

Classification of reactors, Breeder reactor, Reactor safety, Fuel cycle, Nuclear waste management.

UNIT – II

Photochemistry of Transition Metal Complexes (14 Periods)

Photoreactions of complexes of Cr(III) – photo-aquation, photo-substitution and photo-racemization; Photo-substitution and photoredox reactions of Co(III) complexes; Ru(II) polypyridyl and dinuclear Rh(I) isocyanide complexes as sensitizers; supramolecular complexes as antenna. Applications of quenching and sensitization techniques in the identification of reactive state in coordination complexes

UNIT – III

Photochemical Reactions (6 Periods)

Interaction of electromagnetic radiation with matter, types of excitations, quantum yield, transfer of excitation energy,actinometry

Determination of Reaction Mechanism (8 Periods)

Classification, rate constants and life times of reactive energy states determination of rate constants of reactions. Effect of light intensity on the rate of photochemical reactions. Types of photochemical reactions, photo-dissociation, gas-phase photolysis

UNIT – IV

Photochemistry of Alkenes (4 Periods)

Intramolecular reactions of the olefinic bond- geometrical isomerism, cyclisation reactions, rearrangement of 1, 4- and 1, 5-dienes.

Photochemistry of Carbonyl Compounds (6Periods)

Intramolecular reactions of carbonyl compounds – saturated, cyclic and acylic β,γ-unsaturated and α,β-unsaturated compounds, cyclohexadienones. Intermolecular cycloaddition reactions – dimerisations and oxetane formation.

Photochemistry of Aromatic Compounds (2 Periods)

Isomerisations, additions and substitutions.

Books Recommended

1 Introductory Photochemistry; A. Cox and T. Camp, McGraw-Hill.
2 Fundamentals of Photochemistry; K. K. Rohtagi-Mukherji; Wiley Eastern.
3 Photochemistry; R. P. Kundall and A. Gilbert, Thomson Nelson.
4 Organic Photochemistry; J. Coxon and B. Halton, Cambridge University Press
5 B. G. Harvey, Introduction to Nuclear Physics and Chemistry, (1969) Prentice Hall, Inc.
6 H.J. Arnikar, Essentials of Nuclear Chemistry, 4th Edition (1995), Wiely-Eastern Ltd.,
7 G. Fridlander, J.W. Kennedy, E.S. Macias and J.M. Miller, Nuclear & Radiochemistry, 3rd Edition (1981) John-Wiley & Sons, New York. .
8 C.H. Depuy and O.L. Chapman, Molecular Reactions and Photochemistry, 2nd Edition (1988), Prentice-Hall of India (P) Ltd., New Delhi.
9 W.M. Horspool, Aspects of Organic Photochemistry, Academic Press, New York.
10 F.A. Carey and R.J. Sundberg, Photochemistry in Advanced Organic Chemistry, Chapter 13, Part A, 3rd Edition (1990), Plenum Press, New York.
11 N. J. Turro, Modern Molecular Photochemistry, (1991) University Science Books, Sausalito.
12 D. M. Roundhill, Photochemistry and Photophysics of Metal Complexes, (1994) Plenum Press, New York and London.
13 G. J. Ferraudi, Elements of Inorganic Photochemistry, (1988) John Wiley & Sons.
14 V. Balzani and V. Carassiti, Photochemistry of Coordination Compounds, (1970) Academic Press, London.
15 O. Horvath and K.L. Stevenson, Charge Transfer Photochemistry of Coordination Complexes, (1993) VCH Publishers Inc.

Paper Code: CHE(P)4106 **Credit: 4**
Paper Title: Laboratory Course – I **Full Mark: 100**

Qualitative Analysis **45 Marks**

Identification of the basic and acid radicals in a mixture of inorganic substances containing not less than six radicals with less common metal ions: Mo, W, Ti, V and U in cationic / anionic forms and Insoluble: oxides, sulphates and halides

Synthesis **25 Marks**

1. Dibenzal acetone from benzaldehyde (Aldol condensation)
2. Methyl orange.
3. Adipic acid by nitric acid oxidation of cyclohexanol (oxidation).
4. p-Bromo aniline (aromatic electrophilic substitutions) .
5. Sodium tetrathionate $Na_2S_4O_6$.
6. $[Ni(NH_3)_6]Cl_2$
7. Ni $(dmg)_2$
8. $K_3[Fe(C_2O_4)_3]$

Viva **20 Marks**
Record **10 Marks**

Books Recommended

1. Experiments and Techniques in Organic Chemistry; D. Pasto, C. Johnson & M. Miller; Prentice-Hall.
2. Systematic Qualitative Organic Analysis; H. Middleton, Adward Arnold.
3. Hand book of Organic Analysis-Qualitative & Quantitative; H. Clarke, Adward Arnold.
4. Vogel's Text Book of Practical Organic Chemistry; A.R. Tatchell; John Wiley.
5. Macroscale and Microscale Organic Experiments; K. I. Williamson, D. C. Heath.
6. A Text Book of Practical Organic Chemistry (Qualitative); I. Vogel.
7. Inorganic Experiments; J. Derck Woollins; VCH.
8. Qualitative Inorganic Analysis; I. Vogel
9. Microscale Inorganic Chemistry; Z. Szafran, R. M. Pike and M.M. Singh; Wiley.
10. Practical Inorganic Chemistry; G. Marr and B. W . Rocket; Van Nostrand.
11. J.A.C.S. 1953 (75). 5670.
12. J.Chem. Edue., 1982. (59).57.
13. Inorg. Synth. 1972. (13).184.
14. Inorg Synth. 1953.(4).119

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First Year

2nd Semester

Course Outline and Credit Structure

Paper Code	Paper Title	Credits	Marks
CHE(C) 4207	Physical Chemistry – II	4	50
CHE(C) 4208	Inorganic Chemistry – II	4	50
CHE(C) 4209	Organic Chemistry – II	4	50
CHE(C) 4210	Spectroscopy – II	4	50
CHE(E) 4211	Organotransition Metal Chemistry	4	50
CHE(P) 4212	Laboratory Course – II	4	100
Total		24	350

Paper Code: CHE(C)4207 **Credit : 4**
Paper Title: Physical Chemistry – II **Full Mark: (External: 40 and Internal: 10)**
(Each unit carries equal mark)

UNIT – I

Chemical Kinetics (8 Periods)

Methods of determining rate laws for second order reaction of the type: 2A → P, A+B → P and third order reactions of type: 3A → P, 2A+B → P and A+B+C → P). Determination of order of reactions, Arrhenius equation and determination of activation energy.

Theories of reaction rates (8 Periods)

Collision theory of bimolecular reactions, Failures of collision theory, Steric factor, Collision theory of unimolecular reactions- Lindemann's theory and its criticism, Rice – Ramsperger – Kassel – Marcus (RRKM) theories of unimolecular reactions. Activated complex theory-postulates and thermodynamic treatment. Comparison of Activated complex theory and Collision Theory.

UNIT – II

Homogeneous catalysis (6 Periods)

Kinetics of Homogeneous catalysis , Acid and Base catalysis, Generalisation of rate constant, Enzyme catalysis,Factors affecting enzyme catalysis, Kinetics of enzyme catalysis, Michaelis-Menten equation.

Kinetics of Photochemical Reaction (6 Periods)

Reaction kinetics of photochemical hydrogen-bromine reaction, hydrogen-chlorine reaction, Pyrolysis of acetaldehyde and decomposition of ethane. Oscillatory reactions (Belousov – Zhabotinsky reactions)

UNIT – III

Ionic Reactions (4 Periods)

Reaction between ions, influence of solvent, double sphere model, Kinetic salt effects-Primary and Secondary salt effects.

Kinetics of Fast Reactions (8 Periods)

General features of fast reactions. Study of fast reactions by flow method, relaxation method, flash photolysis and the nuclear magnetic resonance method. Dynamics of molecular motion and experimental technique of studying molecular motion dynamics.

UNIT – IV

Electrochemistry (12 Periods)

Debye – Huckel – Onsager treatment and its extension, ion solvent interactions. Debye–Huckel- Bjerrum mode. Thermodynamics of electrified interface equations. electro-capillarity,Lippmann equation (surface excess), Structure of electrified interfaces. Guoy – Chapman, Stern, Graham, Bockris, models. Over potentials, exchange current density, derivation of Butler – Volmer equation, Tafel plot. Hydrogen electrode. .Activity, activity coefficient, Debye-Huckel theory for activity coefficient of electrolytic solutions; determination of activity and activity coefficients; ionic strength.

Books Recommended

1 Physical Chemistry; P.W. Atkins; ELBS.
2 Chemical Kinetics; K. J. Laidler; Mc Graw Hill.
3 Modern Electrochemistry Vol. and Vol. II; J. O. M. Bockris and A .K. N. Reddy; Plenum.
4 Physical Chemistry; Barrow.
5 Physical Chemistry; Snehi Hemant.
6 Advanced physical Chemistry; Gurtoo & Gurtoo.
7 Electrochemistry ;Glasstone

Paper Code: CHE(C)4208 **Credit: 4**
Paper Title: Inorganic Chemistry – II **Full Mark: (External: 40 and Internal: 10)**
(Each unit carries equal mark)

UNIT – I

Metal π – Complexes (12 Periods)

Metal carbonyls, structure and bonding, vibrational spectra of metal carbonyls for bonding and structural elucidation, important reactions of metal carbonyls; preparation, bonding structure and important reactions of transition metal nitrosyl, dinitrogen and dioxygen complexes, tertiary phosphine as ligand.

UNIT – II

Electronic spectra and magnetic Properties of Transition Metal Complexes - I (12 Periods)

Spectroscopic ground states, correlation, Orgel and Tanabe – Sugano diagrams for transition metal complexes (d^1 – d^9 states), calculations of Dq, B and β-parameters, charge transfer spectra.

UNIT – III

Electronic spectra and magnetic Properties of Transition Metal Complexes - II (12 Periods)

Spectroscopic method of assignment of absolute configuration in optically active metal chelates and their stereochemical information, anomalous magnetic moments, magnetic exchange coupling and spin crossover.

UNIT – IV

Metal Clusters (10 Periods)

Higher boranes, carboranes, metalloboranes and metallocarboranes. Metal carbonyl and halide clusters, compound with metal – metal multiple bonds.

Books Recommended

1 Progress in Inorganic Chemistry; Vol. 18 and 38 ed.; J. J. Lippard; Wiley.
2 Advanced Inorganic Chemistry; F. A. Cotton and Wilkinson; John Wiley.
3 Inorganic Chemistry; J. E. Huheey, Harpes & Row
4 Introduction to Ligand Fields Theory; B. N. Figgis
5 Theoretical Inorganic Chemistry; M. C. Day and J. Selbin
6 Inorganic Chemistry; Shriver and Atkins; Oxford
7 Electronic spectra of transition metal complexes; R.K.Ray; NCBA

Paper Code: CHE(C)4209 **Credit: 4**
Paper Title: Organic Chemistry – II **Full Mark: (External: 40 and Internal: 10)**
(Each unit carries equal mark)

UNIT – I

Aliphatic Electrophilic Substitution (5 Periods)

Bimolecular mechanism- S_E2 and S_E1. The S_Ei mechanism, electrophilic substitution accompanied by double bond shifts. Effect of substrates, leaving group and solvent polarity on the reactivity.

Aromatic Electrophilic Substitution (7 Periods)

The arenium ion mechanism, orientation and reactivity, energy profile diagrams. The ortho/para ratio, ipso attack, orientation in other ring systems, quantitative treatment of reactivity in substrates and electrophiles, Diazonium coupling, Vilsmeir reaction, Gattermann–Koch reaction.

UNIT – II

Addition to Carbon –Carbon Multiple bonds (6 Periods)

Mechanistic and stereochemical aspects of addition reactions involving electrophiles, nucleophiles and free radicals, region- and chemoselectivity, orientation and reactivity. Addition to cyclopropane ring.Hydrogenation of double and triple bonds, hydrogenation of aromatic rings. Hydroboration. Michael reaction, Sharpless asymmetric epoxidation.

Addition to Carbon-Hetero Multiple Bonds (9 Periods)

Mechanism of metal hydride reduction of saturated and unsaturated carbonyl compounds, acids, esters and nitriles. Addition of Grignard reagents, organozinc and organolithium reagent to carbonyl and unsaturated carbonyl compounds. Wittig reaction. Mechanism of condensation reactions involving enolates – Aldol, Knoevenagel, Claisen, Mannich, Benzoin, Perkin and Stobbe reactions. Hydrolysis of esters and amides, ammonolysis of esters.

UNIT – III

Pericyclic Reactions (13 Periods)

Molecular orbital symmetry, Frontier orbitals of ethylene, 1,3 – butadiene, 1,3,5 – hexatriene and allyl system. Classification of pericyclic reactions. Woodward – Hoffmann corelation diagrams. FMO and PMO approach. Electrocyclic reactions – conrotatory and disrotatory motions, 4n, 4n+2 and allyl systems. Cycloadditions – antarafacial and suprafacial additions, 4n, 4n+2 systems, 2+2 addition of ketenes, 1,3 dipolar cycloadditions and cheleotropic reactions. Sigmatropic rearrangements – suprafacial and antarafacial shifts of H,sigmatropic shifts involving carbon moieties, 3,3– and 5,5- sigmatropic rearrangements. Claisen, Cope and aza – Cope rearrangements. fluxional tautomerism, ene reaction.

UNIT – IV

Free Radical Reactions (8 Periods)

Types of free radical reactions, free radical substitution mechanism, mechanism at an aromatic substrate, neighbouring group assistance, reactivity for aliphatic and aromatic substrates at a bridgehead, reactivity in the attacking radicals. The effect of solvents on reactivity. Allylic halogenation (NBS), oxidation of aldehydes to carboxylic acids, auto–oxidation, coupling of alkynes and arylation of aromatic compounds by diazonium salts, Sandmeyer reaction. Free radical rearrangement. Hunsdiecker reaction.

Elimination Reactions (5 Periods)

The E2, E1 and E1cB mechanism and their spectrum; Orientation of the double bond; Reactivity: effects of substrate structures, attacking base, the leaving group and the medium. Mechanism and orientation in pyrolytic elimination .

Books Recommended

1 Advanced Organic Chemistry – Reactions, Mechanism and Structure; Jerry March; John Wiley.
2 Advanced Organic Chemistry; F. A. Carey and R. J. Sunberg; Plenum.
3 A Guide Book to Mechanism In Organic Chemistry; Peter Sykes Pearson.
4 Structure and Mechanism In Organic Chemistry; C. K. Ingold, CBS Publication.
5 Organic Chemistry; R. T. Morrison And R. N. Boyd; Pearson
6 Principle of Organic Synthesis; R. O. C. Norman and J. M. Coxon ;CRC Press
7 Pericyclic Reactions; S. M. Mukherji; Macmillan, India.
8 Reaction Mechanism in Organic Chemistry; S. M. Mukherji and S. P. Singh; Macmillan.

Paper Code: CHE(C)4210 **Credit : 4**
Paper Title: Spectroscopy – II **Full Mark: (External: 40 and Internal: 10)**
(Each unit carries equal mark)

UNIT-I

Nuclear Magnetic Resonance Spectroscopy (10 Periods)
Principle Instrumentation of NMR, the chemical shift, mechanism of electron shielding and factors contributing to the magnitude of chemical shift. Local & remote effect, spinspin splitting, applications of spin coupling to structural determination, double Resonance techniques.

Nuclear Quadrupole Resonance Spectroscopy (4 Periods)
Quadrupole nuclei, quadrupole moments, electric field gradient, coupling constant, splittings. Applications

UNIT-II

Electron Spin Resonance Spectroscopy (9 Periods)
Basic principle, Hyperfine splittings (isotropic systems); the g-value and the factors affecting thereof; interactions affecting electron energies in paramagnetic complexes (Zero-field splitting and Kramer's degeneracy); Anisotropic effects (the g-value and the hyperfine couplings); The EPR of triplet states; Structural applications to transition metal complexes.

Optical Rotatory Dispersion and Circular Dichroism (3 Periods)
Definition, deduction of absolute configuration, octant rule for ketones

UNIT-III

X-ray Diffraction (12 Periods)
Bragg Condition, Miller Indices, Laue method, Bragg Method, Debye-Scherrer method of X- ray structural analysis of crystals, index reflections, identification of unit cells from systematic absences in diffraction pattern. Structure of simple lattices and X-ray intensities,structure factor and its relation to intensity and electron density, phase problem. Description of the procedure for an X-ray structure analysis, absolute configuration of molecules,

UNIT –IV

Electron Diffraction (3 Periods)

Scattering intensity vs scattering angle, Wierl equation, measurement techniques

Neutron Diffraction (3 Periods)

Scattering of neutrons by solids and liquids, magnetic scattering, measurement techniques

Books Recommended

1 E. A. V. Ebsworth, D. W. H. Rankin and S. Cradock, Structural Methods in Inorganic Chemistry, 1st Edn.(1987), Blackwell Scientific Publications, Oxford, London.
2 R. S. Drago, Physical Methods for Chemists, (1992), Saunders College Publishing, Philadelphia.
3 K. Nakamoto, Infrared and Raman Spectra of Inorganic and Coordination Compounds, 4th Edn. (1986), John Wiley & Sons, New York.
4 G. Aruldhas, Molecular Structure and spectroscopy, (2001) Prentice Hall of India Pvt. Ltd., New Delhi.
5 Elements of x-ray diffraction, B.DCullity, Addison Wisley, 1967.
6 Diffraction Method, Wormald, Oxford University, Press, 1973
7 Neutron Scattering in Chemistry, Baun, G.E. Butleworth, London, 1971.
8 Spectroscopy in Inorganic Compounds CNR Rao & Ferraro G.R., Academic Press,1970.
9 Carl Djerassi ; Optical rotatory dispersion.
10 P. Crabbe : Optical rotatory dispersion and C.D

Paper Code: CHE(E)4211 **Credit: 4**
Paper Title: Organotransition Metal Chemistry **Full Mark: (External: 40 and Internal: 10)**

(Each unit carries equal mark)

UNIT – I

Alkyls and aryls of transition metals (4 Periods)
Types, routes of synthesis, stability and decomposition pathways, agostic interactions ,

Compounds of transition metal – carbon multiple bonds (8 Periods)
Alkylidenes, alkylidynes, low valent carbines – synthesis, nature of bond, structural characteristics, nucleophilic and electrophilic reactions on the ligands, role in organic synthesis.

UNIT – II

Transition metal π - complexes (12 Periods)
Transition metal π - complexes with unsaturated organic molecules, alkenes, alkynes and allyl complexes, preparations, properties, nature of bonding and structural features, important reactions relating to nucleophilic and electrophilic attack on ligands

UNIT – III

Compounds of transition metal – hydrogen bonds (4 Periods)
Transition metal compounds with bonds to hydrogen

Fluxional organometallic compounds (8 Periods)
Fluxionality and dynamic equilibria in compounds such as η^2 – olefin, η^3 – allyl and dienyl complexes

UNIT – IV

Homogeneous catalysis (12 Periods)
Stoichiometric reactions for catalysts, homogeneous hydrogenation of unsaturated compounds, Zeigler – Natta polymerization of Ethylene and propylene, catalytic reactions involving carbon monoxide such as hydrocarbonulation of olefins (oxo reaction), reductive carbonylation of alcohols and other compounds ,Oxidation reactions like oxidative carbonylations,Palladium catalysed oxidation of Ethylene, Reduction of carbonmonoxide by hydrogen Fischer – Tropsch synthesis.

Books Recommended

1. Metallo- Organic Chemistry; A.J Pearson; Wiley
2. Organometallic chemistry; R.C Mehrotra, A. Singh; New Age Int
3. F. A. Cotton and G. Wilkinson, Advanced Inorganic Chemistry, 6th Edn., (1999), John-Wiley & Sons, New York.
4. James E. Huheey, Inorganic Chemistry, 4th Edn., (1993), Addison Wesley Pub. Co., New York
5. R.H. Crabtree, The Organometallic Chemistry of the Transition Metals, 1st Edn.(1988), John-Wiley & Sons, New York.
6. J. P. Collman, L. S. Hegedus, J. R. Norton and Richard G. Finke, Principles and Applications of Organotransition Metal Chemistry, 1st Edn.(1987), University Science Books, Mill Valley, California.

Paper Code: CHE(P)4212 **Credit: 4**
Paper Title: Laboratory Course – II **Full Mark: 100**

Physical Experiments **45 Marks**

1. Saponification of ethyl acetate with sodium hydroxide by chemical method.
2. Comparison of strength of acid by ester hydrolysis method.
3. Determination of energy of activation of acid catalyzed hydrolysis of methyl acetate.
4. Adsorption of oxalic acid on animal charcoal and verification of Freundlich isotherm.
5. Determination of critical solution temperature of phenol-water system
6. Determination of strength of strong and weak acid in a given mixture conductometrically.
7. Estimation of ferrous ion in ferrous ammonium sulphate potentiometrically
8. Determination of the strength of strong and weak acids in a given mixture using a potentiometer.
9. Determination of partial molar volume of solute (KCl) and solvents in a binary mixture.
10. Determination of the temperature dependence of the solubility of benzoic acid in water

Extraction of Organic compounds from natural sources **25 Marks**

1. Isolation of caffeine from tea leaves.
2. Isolation of casein from milk.
3. Isolation of lactose from milk.

Viva **20 Marks**
Record **10 Marks**

Books Recommended

1. Experiments In Physical Chemistry: R. C. Das And B. Behera; Tata Mc Graw Hall .
2. Findlay Practical Chemistry (Revised Ed.); B. P. Levitt; Longman.
3. Advanced Practical Physical Chemistry; J. B. Yadav; Goel Publishing House, Meerut.
4. Vogel's Text Book of Quantitative Chemical Analysis; J.Mendham, R. C Denney, J. D. Barnes, M. J. K. Thomas; Pearson Education Publishers, 6th Edition.

Second Year

3rd Semester

Course Outline and Credit Structure

Paper Code	Paper Title	Credits	Marks
CHE(C) 5313	Matter and Physical Transformation	4	50
CHE(C) 5314	Quantum Chemistry and Chemistry of Special Elements	4	50
CHE(C) 5315	Organic Synthesis	4	50
CHE(C) 5316	Application of Spectroscopy – I	4	50
CHE(E) 5317	Heterocyclic Chemistry	4	50
CHE(P) 5318	Laboratory course-III	4	100
Total		24	350

Paper Code: CHE(C)5313 **Credit: 4**
Paper Title: Matter and Physical Transformation **Full Mark: (External: 40 and Internal: 10)**
(Each unit carries equal mark)

UNIT – I

Properties of Real Gases (16 Periods)

Equation of state for real gases and their range of applicability, van der Waals equation of state, Redlich – Kwong equation of state, Beattie – Bridgeman equation of state, Virial equation of state, the compression factor, law of corresponding state, fugacity and equilibrium constant for real gases.

UNIT – II

Properties of Liquids (16 Periods)

Liquid as dense gases, liquids as disordered solids, internal pressure and its thermodynamic derivation; Introduction to liquid – vapour interface: surface tension, contact angle and wetting, spreading of one liquid on another, Antoff's rule, surface films and surface pressure, thermodynamics of surface layer.

UNIT – III

Electronic Properties and Band Theory (16 Periods)

Perfect and imperfect crystals, intrinsic and extrinsic defects – point defects, line defects and plane defects, Schottky defects and Frenkel defects. Thermodynamics of Schottky and Frenknel defect formation, colour centres, non – stoichiometric defects. Electronic structure of solids – band theory, band structure of metals, insulators and semiconductors. Intrinsic and extrinsic semiconductors, doping on semiconductors, p-n junctions, super conductors. Electrically conducting solids-organic metals, organic charge transfer complex- new superconductors Optical properties- Optical reflectance, photoconduction - photoelectric effects

UNIT – IV

Physical Transformation of Pure Substances (16 Periods)

Stability of phases, phase transitions, thermodynamic criteria of phase stability, phase boundaries, characteristic properties related to phase transitions, phase diagram of Helium, super critical fluids. Thermodynamic aspects of phase transition: temperature dependence of phase stability, the response of melting to applied pressure, the vapour pressure of a liquid subjected to pressure; The location of phase boundaries: the solid – liquid boundary, liquid – vapour boundary and solid – vapour boundary.

Books Recommended

1. Physical Chemistry by Atkins and Paula
2. Physical Chemistry by Engel and Reid
3. Physical Chemistry by Glasstone

1 Solid state chemistry and Its Applications; A. R. West, Plenum.
2 Principles of solid state; H. V. Keer, Wiley Eastern.
3 Solid state chemistry; N. B. Hannay.
4 Solid state chemistry; D. K. Chakrabarty; New Age International

Paper Code: CHE(C)5314
Paper Title: Quantum Chemistry and Chemistry of Special Elements
Credit : 4 **Full Mark: (External: 40 and Internal: 10)**
(Each unit carries equal mark)

UNIT – I

Introduction of Exact Quantum Mechanical Results (10 Periods)

Brief review of failure of classical mechanics The Schrodinger equation and interpretation of the wave function. Eigen function and Eigen values postulates of quantum mechanics Discussion of solutions of the Schrodinger equation to some model systems viz. particle in a box, the harmonic oscillator. classical & quantum mechanical treatment, Hermite's differential equation, the complete Eigenfunctions and the energy Eigenvalue of the rigid rotator, the hydrogen atom. Spherical co-ordinates, the r, θ ,Ø equation, solving radial equation,laguerre and associated laguerre polynomials, nature of n & L, Significance of n, l and m.

Angular Momentum (6 Periods)

Ordinary angular momentum, generalized angular momentum, eigen functions for angular momentum, eigenvalues of angular momentum, operator using ladder operators, addition of angular momenta, spin, anti symmetry and Pauli's exclusion principle.

UNIT – II

Approximate Methods (4 Periods)

The variation theorem, linear variation principles. Perturbation theory (first order and non-degenerate). Applications of variation method and perturbation theory to the helium atom.

Molecular Orbital Theory (5 Periods)

Huckel theory of conjugated systems, bond order and charge density calculations. Applications to ethylene, butadiene, cyclopropenyl radical, cyclobutadiene. Introduction to extended Huckel theory

Electronic Structure of Atoms (7 Periods)

Electronic configuration, Russell-Saunders terms and coupling schemes, Slater-Condon parameters, term separation energies of the p^n configuration, term separation energies for the d^n configuration, magnetic effects: spin-orbit coupling and Zeeman splitting

UNIT – III

Chemistry of Innertransition Elements (15 Periods)

Lanthanides: separation techniques (fractional crystalization, precipitation, ion-exchange, solvent-extraction and thermal decomposition, selective reduction and oxidation) - oxidation states -size relationships -lanthanide contraction -spectral and magnetic properties of lanthanides -uses of lanthanides and their compounds.
Actinides: Synthesis of elements -electronic configuration and oxidation states- spectral and magnetic properties -comparative account of lanthanides and actinides.

UNIT – IV

Chemistry of Some Important elements (15 Periods)

Silanes, silicates, silicones, silanols; germanium, tin and lead organyls; silenes, germenes and stannenes; phosphorous halides, acids and oxyacids of phosphorous, phosphazenes; oxo acids of sulpur.
Synthesis and reactivity: calixarines, cryptands and crown ethers in complexation chemistry.

Books Recommended

1. Inorganic Chemistry: principles of Structure and Reactivity; James E. huheey, Ellen E. Keiter, Richard L. Keiter; Pearson Education Asia
2. Concise Inorganic Chemistry; J. D. Lee; Blackwell Science Ltd.
3. Advanced Inorganic Chemistry; F. A. Cotton and G. Wilkinson; Wiley Interscience
4. Selected Topics in Inorganic Chemistry; Wahid U. Malik, G. D. Tuli, R. D. Madan; S Chand Company Ltd.
5. Introduction to Quantum Chemistry; A.K. Chandra; Tata McGraw Hill
6. Modern Quantum Chemistry; N.S.Ostlund and A. Szabo, McGraw Hill
7. P.W. Atkins and R.S. Friedman, Molecular Quantum Mechanics, 3rd edition (1997), Oxford University Press. Oxford.
8. H.Eyring,J.Walter and G.E. Kimball,Quantum Chemistry,(1944)John Wiley,New York.
9. I.N. Levine, Quantum Chemistry, 5th edition (2000), Pearson Educ., Inc., New Delhi.
10. R.K.Prasad Quantum chemistry, 4th edn., New Age International publishers
11. Frank L. Pilar, Elementary Quantum Chemistry, Mc Graw-Hill Book Com., New York.

Paper Code: CHE(C)5315 **Credit: 4**
Paper Title: Organic Synthesis **Full Mark: (External: 40 and Internal: 10)**
(Each unit carries equal mark)

UNIT – I

Oxidation (7 Periods)
Introduction, Different oxidative processes. Hydrocarbons: alkenes, aromatic rings, saturated C – H groups (activated and unactivated), alcohols, aldehydes, ketones, carboxylic acids and amines. Oxidations with ruthenium tetraoxide, iodobenzene diacetate and thallium.

Reduction (7 Periods)
Introduction, Different reductive processes. Hydrocarbons: alkenes, alkynes and aromatic rings, Carbonyl compounds: aldehydes, ketones, carboxylic acids, Nitro, azo and oxime. Hydrogenolysis

UNIT – II

Protecting Groups (4 Periods)
Principle of protection of alcohol, amine, carbonyl, and carboxyl groups.

Disconnection Approach (10 Periods)
An introduction to synthons and synthetic equivalents, disconnection approach, functional group inter-conversions, the importance of the order of events in organic synthesis, one group C-X and two group C-X disconnections, chemoselectivity, reversal of polarity. cyclisation reactions, amine synthesis

UNIT – III

One Group C-C Disconnections (7 Periods)
Alcohols and carbonyl compounds, regioselecitivity. Alkene sysnthesis, use of acetylenes and aliphatic nitro compounds in organic synthesis

Two Group C-C Disconnections (7 Periods)
Diel's – Alder reaction, 1,3- difunctionalised compounds, unsaturated carbonyl compounds, control in carbonyl condensations, 1,5-difunctionalised compounds, Michael addition and Robinson annellation

UNIT – IV

Synthesis of Some Complex Molecules (6 Periods)

Synthesis of following compounds: camphor and cortisone.

Organometallic Reagents (10 Periods)

Principles, preparation, properties and applications of the followings in organic synthesis with mechanistic details: Cd, Zn, Cu, Pd, Rh.

Books Recommended

1. Principle of Organic Synthesis; R. Norman And J. M. Coxon; Blackie Academic & Professional.
2. Organic Synthesis; Smith.
3. Designing Organic Synthesis; S. Warren; Wiley.
4. Organic Synthesis; Jagadamba Singh; Pragati Prakashan.
5. Organic Synthesis – Concept , Methods And Starting Materials; J. Fuhrhop And G. Penzilin; VCH.
6. Some Modern Methods of Organic Synthesis;W. Carruthers; Cambridge Univ. Press.
7. Disconnection Approach; Stuart Warren; Wiley and sons.
8. Advanced Organic Synthesis; F .A. Carey and Saunder (Part A & B); Plenum Press
9. Modern Organic Synthetic Reactions – H. O. House, W. A. Benjamin
10. Rodd's Chemistry of Carbon Compounds – Ed. S. Coffey, Elsevier

Paper Code: CHE(C)5316 **Credit: 4**

Paper Title: Application of Spectroscopy – I **Full Mark: (External: 40 and Internal: 10)**

(Each unit carries equal mark)

UNIT-I

Chemical Application of Group Theory (16 Periods)

Molecular orbitals for AB_n type molecules; the group theoretical approach to bonding in H_2O and NH_3. Ligand Field Theory - Splitting of levels and terms in a chemical environment, energy level diagrams, construction of energy level diagrams, estimation of orbital energies, Molecular Vibrations- The symmetry of normal vibrations, determining the symmetry types of the normal modes, selection rules for fundamental vibrational transitions (IR and Raman); illustrative examples

UNIT-II

Vibrational Spectroscopy (11 Periods)

Spectra of AB_2 AB_3, AB_4, AB_5 and AB_6, Mode of bonding of ambidentate ligands, ethylenediamine and diketonato complexes, application of resonance, Raman spectroscopy - active sites of metalloproteins.

Election Spin Resonance Spectroscopy (8 Periods)

Hyperfine coupling, spin polarization for atoms and transition metal irons, spin –orbit coupling and significance of g-tensors, application to transition metal complexes (having one unpaired electron) including biological systems.

UNIT-III

MössbauerSpectroscopy (8 Periods)

Basic principle, conditions for Mossbauer spectroscopy, Spectral parameters (Isomer shift, electric quadrupole interactions, magnetic interactions), temperature-dependent effects, structural deductions for iron and tin complexes, miscellaneous applications.

Nuclear Magnetic Resonance of Paramagnetic substances in Solution (7 Periods)

The contact and pseudo contact shifts, factors affecting nuclear relaxation, some applications including biochemical systems, an overview of NMR of metal nuclides with emphasis on ^{195}Pt and ^{119}Sn NMR

UNIT –IV

CMR Spectroscopy (8 Periods)

General considerations; chemical shift aliphatic; olefinic; alkyne; aromatic; heteroaromatic and carbonyl compounds; problems associated with 13C, FT-NMR, proton decoupled off resonance spectra.

Books Recommended

1. Physical methods for Chemistry; R. S. Drago; Saunders Company.
2. Inorganic Electornic Spectoscopy; A. P. B. Lever; Elsevier.
3. NMR, NQR, EPR and Mossbauer Spectroscopy in inorganic chemistry; R. V. Parish, Eills Horwood.
4. Introduction to NMR Spectroscopy; R.J. Abraham, J. Flsher and P. Lottus; Willey.
5. Spectroscopy; Donald .L Pavia; Cengage Learning
6. F. A. Cotton, Chemical Applications of Group Theory, 3rd Edn. (1999), John Wiley & Sons, New York.
7. G. L. Miessler and D. A. Tarr, Inorganic Chemistry, 2nd Edn. (1999), Prentice Hall International Inc., London.
8. K. Veera Reddy, Symmetry and Spectroscopy of Molecules, (1999) New Age International Pvt. Ltd., New Delhi.
9. Mossbaur Spectroscopy, Greenwood N.N., Gibbs T.C., Chapmann Hall, 1971.
10. Chemical Application of Mossbaur Spectroscopy, Goldanski V.I & Harber R.H., Academic Press 1968.

Paper Code: CHE(E)5317 **Credit: 4**

Paper Title: Heterocyclic Chemistry **Full Mark: (External: 40 and Internal: 10)**

(Each unit carries equal mark)

UNIT – I

Nomenclature of Heterocycles (4 Periods)

Hantzsch – Widman system for monocyclic heterocycles; fusion nomenclature system. Replacement nomenclature system for monocyclic, fused, spiro and bicyclic molecules.

Aromatic Heterocycles (5 Periods)

General chemical behaviour of aromatic heterocycles, the common structural type – five and six membered, benzo and other fused heterocycles; criteria of aromaticity – bond lengths, ring current and chemical shifts in ^{1}H NMR – spectra for five and six membered monocyclicheterocycles; heteroaromatic reactivity – basic principle, selectivity and reactivity in five and six membered heteroatomic rings.

Non-aromatic Heterocycles (5 Periods)

Introduction; strain – angle strain and bonding in small ring heterocycles and its consequences (IR & PMR spectra, conjugative effect, basicity) torsional strains about single bond in small ring heterocycles. Basic idea on stereoelectronic effects in saturated six membered heterocycles– anomeric effect, other related effects and attractive interactions through space.

UNIT – II

Principles of Heterocyclic Synthesis (4 Periods)

Basic Principles of nucleophile-electrophile cyclisation, 1,3-dipolar reaction [3+2→5] cycloaddition and hetero Diels Alder reaction [4+2→6] cycloaddition.

Three membered Heterocycles (4 Periods)

Aziridines: synthesis – Gabriel method, Hassner method, reactions – nucleophilic, electrophilic ring opening reaction, Friedel – Craft reaction.
Oxiranes: synthesis – peracid epoxidation of alkene, Darzen reaction, reaction–nucleophilic, electrophilic ring opening reaction, reaction with carbonyl compounds

Four membered Heterocycles (4 Periods)

Azetidines: synthesis – intramolecular cyclisation, cycloaddition reaction; reaction with H_2O_2, HCl, HCHO, CS_2.
Oxetanes: intramolecular cyclisation, photochemical cycloaddition, reaction – nucleophilic, electrophilic ring opening reaction.

UNIT – III

Five membered Heterocycles with one hetero atom (4 Periods)

Pyrrole: Orientation in electrophilic substitution reaction, reaction – Gattermannformylation, Friedel – Craft alkylation and acylation
Furan: photochemical cyclisation, reaction – with aldehydes and ketones, maleic anhydride
Thiophene: Reaction – Birch reduction, reaction with nitrenes.

Six-Membered Heterocycles with One Heteroatom (4 Periods)

Pyridine: Reaction – radical substitution; Pyrylium salts: synthesis from tert-butyl alcohol, reaction – nucleophilic substitution reaction

Six-Membered Heterocycles with Two Heteroatoms (4 Periods)

Synthesis of pyrimidines from urea and urea derivatives, synthesis of purines from pyrimidines, synthesis of 1,3-oxazininium cation derivative and its reaction with ammonia.

UNIT – IV

Benzo-Fused Five –membered Heterocycles (6 Periods)

Indole: Synthesis – Reissert synthesis, reaction – basicity, reaction with electrophile (general mechanism), nitrosation
Benzo[b]furan: synthesis – from ortho substituted phenol, reaction – reactivity and orientation, photosensitized cycloaddition
Benzo[c]furan: synthesis – Retro-Diels-Alder reaction, reaction – photopolymerisation

Meso – ionic Heterocycles (6 Periods)

Introduction, general classification, chemistry of type – A: 1,3-oxazolium-4-olates – synthesis from diazoketones, reaction – with carbonyls, 1,3-diazolium-4-aminides - synthesis from nitriles, reaction – cycloaddition reaction, chemistry of type – B: 1,2-diazolium-4-aminides – synthesis from amino pyrazole derivative, reaction – thermal isomerisation.

Books Recommended

1 Heterocyclic Chemistry Vol 1 – 3; R. R. Gupta, M. Kumar, Springer Verlag.
2 The Chemistry of Heterocycles; T. Eicher and S. Hauptmann, Thieme.
3 Heterocyclic Chemistry; J. A. Joule, K. Mills And G. F. Smith; Chapman And Hall.
4 Heterocyclic Chemistry; T. L. Gilchrist, Pearson Publication
5 An Introduction to Heterocyclic Compounds; R. M. Acheson; John Wiley.
6 Comprehensive Heterocyclic Chemistry; A. R. Katritzky And C. W. Rees; Pergamon Press.
7 Heterocyclic Chemistry; V.K Ahluwalia;Narosa

Paper Code: CHE(P)5318 **Credit: 4**
Paper Title: Laboratory course – III **Full Mark: 100**

Multi-step synthesis of organic compounds **45 Marks**

1. Benzene → Benzophenone → Benzpinacol → Benzpinacolone
2. Benzene → Benzophenone → Benzophenoneoxime → Benzanilide
3. Benzoin → Benzil →Benzilic acid
4. Nitrobenzene → m-dinitrobenzene → m-nitroaniline → m-nitrophenol
5. Phthalicacid → phthalic anhydride → phthalimide → Anthranilic acid

Analytical Experiments **25 Marks**

1. Determination of Na^+ ions by flame photometry.
2. Determination of K^+ ions by flame photometry.
3. Determination of dissolved oxygen (DO) in water sample.
4. Determination of chemical oxygen demand (COD) in water samples.
5. Determination of biological oxygen demand (BOD) in water samples.
6. Measurement of pH of soil by pH meter.
7. Verification of Beer-Lambert's law by colorimetry.
8. Determination of ultrasonic velocity in water and glucose mixture.
9. Determination of ascorbic acid in vitamin C tablets.
10. Analysis of fat in a butter sample

Viva **20 Marks**

Record **10 Marks**

Books Recommended

1. Experimental Physical Chemistry; D. P Shoemaker, C. W. Garland and J. W. Niber; McGraw Hill interscience.
2. Findlay's Practical Physical Chemistry; B. P. Levitt; Longman.
3. Experiments in Physical Chemistry; J. C. Ghosh; Bharati Bhavan.
4. Inorginic Experiments; J. Derek Woollins.
5. Microscale Inorganic Chemistry; Z. Szafran, R. M Pike and M. M. Singh; Wiley.
6. Practical Inorganic Chemistry, G. Marr and B. W. Rockett; Van Nostrand.
7. Experimental Organic Chemistry; M. P. Doyle and W. S Mungall.
8. Small Scale Organic preparations; P. J. Hill

Second Year
4th Semester
Course Outline and Credit Structure

Paper Code	Paper Title	Credits	Marks
CHE(C) 5419	Analytical and Environmental Chemistry	4	50
CHE(C) 5420	Application of Spectroscopy – II	4	50
CHE 5421	Dissertation	14	200
CHE 5422	Seminar	2	50
Total		24	350

Paper Code: CHE(C)5419 **Credit: 4**
Paper Title: Environmental & Analytical Chemistry **Full Mark: (External: 40 and Internal: 10)**
(Each unit carries equal mark)

UNIT – I

Atmosphere (6 Periods)

Chemical composition of atmosphere – particles, ions and radicals and their formation. Chemical and photochemical reactions in atmosphere, smog formation, oxides of N,C, S, O and their effect, pollution by chlorfluorohydrocarbons. Green house effect, acid rain, air pollution, controls and their chemistry. Analytical methods for measuring air pollutants.

Hydrosphere (8 Periods)

Chemical composition of water bodies-lakes, streams, rivers and wet lands etc.Hydrological cycle. Aquatic pollution – inorganic, pesticide, agricultural, industrial and sewage, detergents. Water quality parameters – dissolved oxygen, biochemical oxygen demand, solids, metals, content of chloride, sulphate, phosphate, nitrate and micro-organisms, water quality standards. Analytical methods for measuring BOD, DO, COD, F, metals (As, Cd, Hg, etc.). Purification and treatment of water.

UNIT – II

Soils (06 Periods)

Composition, micro and macro nutrients, pollution – fertilizers, pesticides, plastics and metals, waste treatment. Analysis of moisture, P^H, total nitrogen, phosphorus,. Lime, magnesia, sulphur and alkali salts.

Industrial Pollution (6 Periods)

Cement, sugar, distillery, drug, paper and pulp, thermal power plants, nuclear power plants, metallurgy.polymers, drugs etc. Radionuclide analysis. Disposal of wastes and their management

UNIT – III

Environmental Toxicology (12 Periods)

Toxic chemicals in the environments, Impact of toxic chemicals on enzymes, Biochemical effects of arsenic, cadmium, lead, mercury, carbon monooxide, nitrogen oxides, sulphur oxides, ozone, PAN, cyanide, pesticides, insecticides and carcinogens

UNIT – IV

Errors and Evaluation (8 Periods)

Definition of terms in mean and median, Precision – standard deviation, relative standard deviation. Accuracy-absolute error, relative error. Types of error in experimental data – determinate (systematic), indeterminate (or random) and gross. Sources of errors and the effects upon the analytical results. Statistical evaluation of data-indeterminate errors.

Fuel analysis (6 Periods)
Solid, liquid and gaseous fuels. Calorific value of fuel and its determination. grading of coal, analysis of coal- proximate and ultimate analysis. Liquid fuels- flash point, aniline point, octane number and carbon residue. Gaseous fuels- producer gas and water gas.

Books Recommended

1 Environmental Chemistry; Sharma & Kaur; Krishna Publishers.
2 Environmental Chemistry; A. K. De; New age publishers
3 Environmental Pollution Analysis; S. M. Khopkar; Wiley Eastern.
4 Analytical Chemistry – Principles and Techniques; L. G. Hargis; Prentice Hall.
5 Quantitative Analysis; R. A. Day Jr. and A. L. Underwood; Prentice Hall.
6 Basic Concepts of Analytical Chemistry; S. M. Khopkar; Wiley Eastern.

Paper Code: CHE(C)5420 **Credit: 4**
Paper Title: Application of Spectroscopy – II **Full Mark: (External: 40 and Internal: 10)**
(Each unit carries equal mark)

UNIT-I

Ultraviolet Spectroscopy (6 Periods)
Woodward- Fisher rules for conjugated dienes and carbonyl compounds; Calculation of λmax.Ultraviolet spectra of aromatic and heterocyclic compounds.Steric effect in biphenyls.

IR Spectroscopy (9 Periods)
Characteristic vibrational frequencies of alkanes; alkenes; alkynes; aromatic compounds; alcohols; ethers; phenols and amines. Detailed study of vibrational frequencies of carbonyl compounds: ketones, aldehydes, esters, amides, acids, anhydrides, lactones, lactams and conjugated carbonyl compounds. Effect of hydrogen bonding and solvent effect on vibrational frequencies; overtones, combination bands and Fermi resonance. FT–IR of gaseous, solids and polymeric materials.

UNIT-II

Mass Spectrometry (15 Periods)
Introduction, ion production- EI, CI, FD and FAB, factors affecting fragmentation, ion analysis, ion abundance. Mass spectral fragmentation of organic compounds, common functional groups, molecular ion peak, metastable peak, Mc Lafferty rearrangement, nitrogen rule. High-resolution mass spectrometry.Examples of mass spectral fragmentation of organic compounds with respect to their structure determination.

UNIT-III

NMR Spectroscopy (15 Periods)
General introduction and definition; chemical shift; spin –spin interaction; shielding mechanism of measurement; chemical shift values and correlation for protons bonded to carbons [aliphatic; olefinic; aldehydic and aromatic] and other nuclei [alcohols; phenols; enols; acids; ammines; amides and mercapto]; chemical exchange; effect of deuteration; complex spin-spin interaction between two; three; four; and five nuclei [first order spectra]; virtual coupling. Stereochemistry; hindered rotation; Karplus curve variation of coupling constant with dihedral angle. Simplification of complex spectra; nuclear magnetic double resonance; shift reagent; solvent effect. Fourier transform technique; nuclear overhauser effect [NOE] .

UNIT –IV

Carbon-13 NMR Spectroscopy (6 Periods)
General considerations, chemical shift, coupling constants. Nuclear Overhauser effect.Spin-spin, spin-lattice relexations.Off resonance decoupling. DEPT. Interpretation of simple CMR spectra. 2 DNMR: COSY, NOESY and HETCOR

Structure elucidation using spectral data (6 Periods)
Structural problems based on combined spectroscopic techniques.

Books Recommended

1 J.R. Dyer, Application of Absorption Spectroscopy of Organic Compounds, Prentice Hall, New Delhi (1978).

2 R.M. Silverstein and F.X. Webster, Spectroscopic Identification of Organic Compounds, 6th Edition (2003) John Wiley, New York.

3 D.H. Williams and I.F. Fleming, Spectroscopic Methods in Organic Chemistry, 4th Edition (1988), Tata-McGraw Hill, New Delhi.

Paper Code: CHE – 5421 **Credit: 14**
Paper Title: Dissertation **Full Mark: 200**

The Topic for Dissertation will be assigned to the students at the beginning of the 3rd Semester.

Paper Code: CHE – 5422 **Credit: 2**
Paper Title: Seminar **Full Mark: 50**

The seminar talk delivered by the student and will be properly assessed by the faculty members of the Department under the chairmanship of the Head of the Department.