MASTER OF SCIENCES

CHEMISTRY

SYLLABUS & REGULATIONS
WITH EFFECT FROM 2025-2026

M.Sc. CHEMISTRY
P.G. Degree Programme(CBCS) Regulations-2016
Amended as per NEP-2020

CENTRE FOR DISTANCE AND ONLINE EDUCATION (CDOE)
SRI VENKATESWARA UNIVERSITY
Accredited by "NAAC" with A+ Grade
Tirupati, Andhra Pradesh - 517502

CENTRE FOR DISTANCE AND ONLINE EDUCATION (CDOE)
SRI VENKATESWARA UNIVERSITY::TIRUPATI
S.V.U.COLLEGE OF SCIENCES
DEPARTMENT OF CHEMISTRY

M.Sc., CHEMISTRY (ORGANIC CHEMISTRY)

Semester-I

Sl. no	Code	Title of the course	Hrs/ week	No. of Credits	IA	Semester end exam	Total Marks
1.	CHE-101	Inorganic Chemistry	6	4	30	70	100
2.	CHE-102	Organic Chemistry	6	4	30	70	100
3.	CHE-103	Physical Chemistry	6	4	30	70	100
4.	CHE-104	Spectroscopy	6	4	30	70	100
5.	CHE-105	Practical - I	6	4	-	-	100
6.	CHE-106	Practical - II	6	4	-	-	100
		TOTAL	36	24	--	--	600

Semester-II

Sl. no	Code	Title of the course	Hrs/ week	No. of Credits	IA	Semester end exam	Total Marks
1.	CHE-201	Quantitative Data, Analytical, Electro Chemical and Separation Techniques	6	4	30	70	100
2.	CHE-202	Organic Spectroscopy, Drug Design, Conformational Analysis, & Heterocyclic Compounds	6	4	30	70	100
3.	CHE-203	Organic Photochemistry, Pericyclic Reactions & Organic Synthesis	6	4	30	70	100
4.	CHE-204	Advanced Natural Products	6	4	30	70	100
5.	CHE-205	Practical - I	6	4	-	-	100
6.	CHE-206	Practical - II	6	4	-	-	100
		TOTAL	36	24	--	--	600

SEMESTER-III

Sl. No	Course Code	Components of Study	Title of the Course	Credit Hrs/ Week	No. of Credits	IA Marks	SEM End Exam Marks	Total
1	CHE-OC-301	Core-Theory	Organic Chemistry-III	6	4	30	70	100
2	CHE-OC -302	Core-Theory	Organic Spectroscopy	6	4	30	70	100
3	CHE-OC-303	* Generic Elective	(a) Inorganic Spectroscopy & Thermal Methods of analysis	6	4	30	70	100
			(b) Physical Chemistry III					
4	CHE-OC-304	Core & Gen. Practicals	Organic Estimations	6	4	-	-	100
5	CHE –OC- 305 A	Skill Oriented Course (theory)	Chemotherapy and drug analysis	3	2	10	40	50
	CHE –OC- 305 B	Skill Oriented Course (Practicals)	Multistep preparations	3	2	-	-	50
6	CHE- 306	Open Elective (For other departments)	(a) Spectral Techniques (b) Chromatographic Techniques	6	4	30	70	100
		Total		36	24			600

*Among the Generic Elective a student shall choose any one.

SEMESTER-IV

Sl. No	Course Code	Components of Study	Title of the Course	Credit Hrs/ Week	No. of Credits	IA Marks	SEM End Exam Marks	Total
1	CHE-OC-401	Core-Theory	Organic Synthesis - I	6	4	30	70	100
2	CHE-OC-402	Core-Theory	Organic Synthesis - II	6	4	30	70	100
3	CHE-OC-403	Generic Elective*	(a) Heterocycles and natural Products	6	4	30	70	100
			(b) Bioinorganic, Bioorganic & Biophysical Chemistry					
4	CHE-OC-404	Core & Gen. Practicals	Spectral Identification	6	4	-	-	100
5	CHE-OC-405	Multi disciplinary Course / Project work	Project work	6	4	-	-	100
6	CHE-406	Open Elective (For other departments)	(a)Drug Chemistry (b) Electro analytical Techniques	6	4	30	70	100
		Total		36	24			600

*Among the Generic Elective a student shall choose any one.

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SRI VENKATESWARA UNIVERSITY::TIRUPATI
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DEPARTMENT OF CHEMISTRY
M. Sc. ORGANIC CHEMISTRY – 1st YEAR / I Semester

CHE 101: INORGANIC CHEMISTRY

Unit – 1: METAL – LIGAND BOND: THEORIES and STEREOCHEMISTRY

Crystal Field Theory (CFT) for bonding in transition metal complexes, crystal field splitting of 'd' – orbitals in octahedral, tetrahedral, tetragonal and square planar fields. Crystal Field Stabilization energy (CFSE). Factors affecting the magnitude of Δo in octahedral complexes, Jahn-Teller effect and its consequences, Limitations of crystal field theory, Symmetry of atomic and molecular orbitals; concept of ligand group orbitals; construction of molecular orbital energy level diagrams for Octahedral, tetrahedral and square planar complexes with sigma bonding only; nature of metal-ligand π-bonding; classification of π-ligand; effect of π-bonding on CFSE of octahedral complexes; π-bonding and spectrochemical series; construction of MO diagrams for octahedral complexes with π-bonding; Experimental evidence for π-bonding – Crystallography, Infra red spectroscopy; Photoelectron spectroscopy.

Unit – 2: MAGNETIC AND SPECTRAL BEHAVIOUR OF METAL COMPLEXES

Types of magnetic behavior, Temperature independent paramagnetism. Magnetic susceptibility and its determination by Gouy's and Faraday methods. Calculation of magnetic moment from magnetic susceptibility, spin-only formula, Orbital contribution to magnetic moment (Oh and Td Complexes)
Free Ion Terms; and Energy Levels: Configurations, Terms, States and Microstates. Calculation of Microstates for P^2 and d^2 configuration, L-S (Russel-Saunders) Coupling Schemes, J-J Coupling scheme, derivation of terms for P^2 and d^2 configuration. Hole Formulation, Energy ordering of terms (Hund's Rules), Selection rules: Laporte orbital selection rule, spin selection rules. Splitting of energy levels and spectroscopic states, Orgel diagrams of d^1 to d^9 metal complexes. Interpretation of electronic spectra of aquo complexes of ti(III), Cr(III), Mn(II), Fe(II), Fe(III), Co(II), Ni(II) and Cu(II). Calculation of inter electronic and spectral parameters for d^8 metal complexes. Charges transfer ($L \rightarrow M$ and $M \rightarrow L$) spectral of metal complexes.

Unit – 3: REACTION MECHANISM OF TRANSITION METAL COMPLEXES

Reactivity of metal complexes. Inert and Labile complexes. Nucleophilic and electrophilic substitution reactions, dissociative (D) and Dissociative interchange Mechanism (ID) & Associative (A) and Associative interchange Mechaism (Ia). Ligand substitution reactions of octahedral complexes. Acid hydrolysis. Factors affecting acid hydrolysis, Base hydrolysis. Dissociative conjugate base mechanism (D-CB). Nucleophilic substitution reactions in square planar complexes. Trans influencing ligands. Complementary and non-complimentary reactions. Electron transfer reactions of complexes. Bridged or inner sphere Mechanism. Tunneling or outer sphere Mechanisms.

SYNTHETIC COORDIANTION CHEMISTRY

Ligands, variety, classification, design and synthesis of d and f block coordination compounds; illustrative examples; Reaction types – simple addition, substitution, etc., synthesis of air sensitive complexes, trans effect, Isomerization reactions, Optically active complexes and resolution of enantiomers, novel ligands and novel complexes, Polynuclear complexes.

Stability and instability constants. Step-wise and overall formation constants and their relationship. Trends in step-wise constants, Factors influencing stability constants – ligand effects and metal ion effect.

Unit – 4: METAL CARBONYLS and CARBONYL CLUSTERS

Meal Carbonyls: Synthesis of metal carbonyls, Structures of metal carbonyls of the types $M(CO)_n$ (M = Cr, Fe, Ni; n = 4-6), $M_2(CO)_n$ (M – Co, Fe, Mn; n = 8-10), $M_3(CO)_{12}$ (M = Ru and Os) $M_4(CO)_{12}$ (M = Co Rh and Ir). IR Spectra of metal carbonyls – (i) Detection of bridging CO ligand, (ii) Determination of molecular symmetry. Synergistic effect. EAN and 18-electron rules as applied to metal carbonyls, Electron counting methods – (i) Oxidation State method and (ii) Neutral Atom method, Applications of Metal Carbonyls. Metal carbonyl clusters – [Low Nuclearity Carbonyl Clusters (LNCCs) – triatomic and tetra atomic clusters]; Iso – electronic and Isolobal relationships; High Nuclearity Carbonyl clusters (HNCCs) – Electron counting schemes for HNCCs; HNCCs of Fe, Ru and Os group; HNCCs of Co, Rh and Ir group; HNCCs of Ni, Pd and Pt group. Metal atom clusters with metal-metal multiple bonds, Edge sharing, face-sharing, tetragonal prismatic and trigonal antiprismatic structures; Quadruple bond.

Reference Books

1. Inorganic Chemistry by J.E. Huheey., E.A. Keiter and R.A. Keiter, 4th edition, Harper; Collins, 1993.
2. Advanced Inorganic Chemistry by F.A. Cotton, G. Wilkinson, C.A. Murillo and M. Bochmann, 6th edition, Wiley-Interscience N.Y. 1999.
3. Coordination Chemistry by F. Basalo and R. Johnson (WA Benjamin Inc). 1964
4. Inorganic Chemistry, Principles and Applications by I.S. Butler and I.F. Harper, Benjamin Cummings, Redwood City, CA, 1989.
5. Chemistry of Coomplex Equillibria, M.T. Beck, Von nostrand Reinhold, London, 1990.
6. Metal Complexes in Aqueous solutions. A.E. Martell and R.D. Hancock, Plenum Press, New York., 1996.
7. Mechanism of Inorganic Reactions by F. Basalo and R.G. Pearson, 2nd Edn.,
8. Concise Inorganic chemistry by J.D. Lee, 5th edition, Balckwell science Ltd., 1996.
9. Inorganic Reaction Mechanisms, M.L. Toba and John Burgess, Addision Wesley, Longman, 1999.
10. Mechanism of Reactions in transition metal sites, Richard A. Henderson, Oxford Science Publications, London, 1993.
11. Kinetics and Mechanisms of Reactions of Transition metal complexes, R.G. Wilkins, 2nd Ed., V.C.H. Publications, 1991.
12. Inorganic Electronic Spectroscopy by A.B.P. Lever, Elsevier.
13. Synthesis and characterization of Inorganic Compounds by William L. Jolly Prentice Hall 1970.

CHE 102: ORGANIC CHEMISTRY

UIT – 1: AROMATICITY AND DETERMINATION REACTION MECHANISM

Aromaticity – Huckel's rule, aromaticity in benzenoid and non-benzenoid compounds, anti-aromaticity and homo-aromaticity. Criag's rule
Determination of reaction mechanism: Types of reactions and reagents – Energy profiles of addition and elimination reactions, transition states, product isolation and structure of intermediates, use of isotopes, chemical trapping, cross over experiments. Use of IR and NMR in the investigation of reaction mechanism.

UNIT – 2: STEREOCHEMISTRY

Chiral point group classifications of stereosomers based on symmetry and energy considerations-Dissymmetric and asymmetric molecules.
Molecules with a tetra-co-ordinate chiral centre (quarternary ammonium salts, N-oxide, silane derivatives, phosphines and sulfones). Molecules with a tri coordinate chiral centre (tertiary amines, carbanions, phosphines and sulfoxides). Concept of dynamic enantiomerism. Molecules with two or more chiral centres. Constitutionally unsymmetrical molecular (with dissimilar chiral carbons) and constitutionally symmetrical molecular (with similar chiral carbons).
Principles of axial chirality. Stereochemistry of allenes, spiranes and biphenyls.
Geometrical isomerism in molecular having C = C, C = N, N = N and in cyclopropane, cyclobutane & cyclopentane, E.Z nomenclature. Physical, spectral and chemical methods of determining E, Z configuration.

UNIT – 3: REACTION MECHANISM – I

Aliphatic Nucleophilic Substituiton: Nucleophilic substitution as a saturated carbon - S_N^1, S_N^2, S_N^i mechanisms. Factors affecting nucleophilic substitution – effect of structure of the substrate, effect of solvent, effect of leaving group and effect of nature of the nucleophilic reagent.

Aromatic nucleophilic substitution: S_N^1 (Ar), S_N^2 (Ar) and benzyne mechanisms. Evidence for the structure of benzyne.
Ambident nucleophiles: Definition and types.
Neighbouring group participation: Definition – neighboring group participation involving halogens, oxygen, sulphur, nitrogen aryl, cycloalkyl groups, σ and π bonds. Introduction to non-classical carbocations.

UNIT – 4: REACTION MECHANISM – II

(a) Addition to carbon-carbon multiple bonds: Addition involving symmetrical and unsymmetrical reagents-addition of halogens to alkenes-evidence for halonium iion intermediacy – stereo selectivity and specificity. Syn addition of reagents like $KMnO_4$, OsO_4. Anti addition – epoxidation followed by ring opening.
(b) Elimination reactions: E_2, E_1, CB mechanisms. Orientation and stereo selectivity in elimination reactions. Pyrolytic syn elimination and α - elimination.

INTRODUCTION TO REACTIVE INTERMEDIATES AND MOLECULAR REARRANGEMENTS

Reactive intermediates – Generation, structure and stability of (i0 Carbocations (ii) Carbanions, (iii) Carbenes, (iv) Nitrenes and (v) Free radicals.
Molecular rearrangements: Definition and classification. Molecular rearrangements involving (i) electron deficient carbon: Wagner – Meerwein, Pinacol – Pinacolone rearrangements. (ii) Electron deficient nitrogen: Hoffmann, Lossen, Curtius and Beckmann rearrangements. (iii) Electron deficient oxygen: Baeyer-villiger oxidation.
Base catalyzed rearrangements: Benzilic acid rearrangement, Favorskii rearrangement.

Recommended Books

1. A guide book to mechanism in organic chemistry by Peter Sykes.
2. Advanced organic chemistry: Reactions, Mechanisms and Structure by Jerry March.
3. Reactive intermediates by Isaac.
4. Mechanism and structure in organic chemistry by S. Mukherjee.
5. Organic synthesis by O. House.
6. Stereochemistry of carbon compounds by Ernest L. Eliel.
7. Stereochemistry by V.M. Potapov
8. Stereochemistry of organic compounds – Principles and Applications by D. Nasipuri.
9. Stereochemistry, Conformation and Mechanism by P.S. Kalsi
10. The third dimension in organic chemistry by Alan Bassindale.
11. Organic chemistry by T.J. Solomons.
12. Organic chemistry by Robert T Morrison and Robert N Boyd.

CHE 103: PHYSICAL CHEMISTRY

UNIT – 1: THERMODYNAMICS

Brief review of concepts of I & II Laws of thermodynamics, Concepts of entropy as state function, entropy changes in ideal gas, Entropy changes of mixing of ideal gases. Entropy and disorder. Free energy and work function, free energy work function relationships, Gibbs Hemoltz partial relations, Partial molal free energy – Chemical potential (Gibbs – Duhem Equation), Thermodynamic temperature scale and absolute zero of temperature, Third law of thermodynamics, Determination of entropies of solids, liquids and gases using heat capacity data, lowering of temperature by Adiabatic demagnetization.

Thermodynamic derivation of phase rule. Applications of phase rule to two component systems – azeotropes. Three component systems – Phase equilibrium diagrams of systems with two salts and water. Roozeboon Plots, Determination to clausius – clapeyron equation – Differential and integral forms. Free energy change and equilibrium constant – Van't Hoff reaction isotherm.

UNIT – 2: ELECTROCHEMISTRY

Thermodynamic and kinetic derivation of Nernst equation, Chemical cells and concentration cells with and without transference, Liquid junction potential, Derivation of the expression for liquid junction potential Elimination, Applications of emf measurement from (i) solubility product, (ii) pH determination and (iii) potentiometric titration. Theory of electrolytic coneductance, calculation of solubitliy of sparingly soluble salt from conductance measurements, conductometric titrations.

Concept of activity and activity coefficient of an electrolyte – Forms of activity and activity coefficient – The mean ionic activity coefficient – calculation of mean ionic activity coefficient (i) from solubility (ii) from emf measurements. Debye Huckel limitingt law and its verification.

Standard Electrode Potential. IUPAC definition and sign convention for the Elctrode potential, Standard Reduction potential, Electrochemical or Galvanic series, Gibbs – Helmholtz equation for electrochemical systems and derivation of thermodynamic parameters (Free energy, entropy and enthalpy) from the electrode potentials, Electrochemical cells. Electrolytic cells, Batteries, Carbon – Zinc Dry cell, Alkaline dry cell, Lead acid battery and Lithium ion battery – Applications.

UNIT – 3: QUANTUM C HEMISTRY

Brief review of the following: Photoelectric effect – Black – Body radiation, Plank's concept of quantization, Plank's equation, Wave particle duality and uncertainity principle, Significance of these microscopic entities. Hydrogen emission spectrum, Bohr's model of the atom (without derivation). Emergence of quantum mechanics. Operators – Operator algebra, Commutation of Operators, Linear operators, Complex functions, Hermitian operators, Operators del and del^2, Eigen values and Eigne functions of an operator, Well behaved functions, Normalized and orthogonal functions.

Postulates of quantum mechanics: Physical Interpretation of wave function, Observables and operators, Measurability of operators, Average values of observables. The time dependant Schrodinger equation, Separation of variables and the time independent Schrodinger equation.

Particle in a box-One dimensional and the dimensional. Plots of ψ and ψ^2 discussions. Schrodinger equation for the hydrogen atom-Separation of Varible. Quantum numbers, n, l, and m and their significance. Hydrogenlike wave functions. Molecular orbital and valence bond theories of diatomic molecular. The molecular orbital theory (LCAO approximation). The hydrogen molecule ion. The hydrogen molecule (MO method).

CHEMICAL KINETICS

Theories of reaction rates, Collision theory, steric factor, Theory of absolute reaction rates, Thermodynamic formulation of reaction rates Unimolecular reactions – Lindemann's theory and its drawbacks, Complex reactions, rate expressions for opposing, parallel and consecutive reactions (all first order type) Chain reactions – General characteristics, steady state treatment of H_2 – Br_2 – Cl_2 reactions, Comparison of hydrogen – halogen reactions.,

Acid Base catalysis: specific acid catalysis – Skrabal diagrams. Protolytic and prototropic mechanism. Free details in chemical reactions – Hydrogen – Oxygen reaction. Upper and lower explosion limits (electronic theories of chemisorptions and heterogeneous catalysis) Reactions on surfaces and in solid state-absorption and adsorption isotherms – Langmuir adsorption isotherm. Chemical reactions on surfaces, mechanism of surface reactions, unimolecular surface reactions – inhibition. Catalysts and promoters in chemical reactions industrial applications.

UNIT – 4: X-RAY CRYSTALLOGRAPHY

A. Crystal lattice. Unit cell. Crystal planes.miller indices. Distance between lattice planes (cubic). Bragg's law of diffraction. Powder method. Debye – Scherer method. Powder diffractometer. Indexing of planes. Systematic absence. Structure of KCI and NaCl.
B. Structure of solids: Close packing. Octahedral and tetrahedral voids. Raidus ratio rule. Structure of ionic crystals. Ionic crystals with stoichiometry MX and MX_2. Spine structure. Perovskite structure.
C. Point defects. Types of point defects. Vacancy. Misplaced atom. Interstitial, Frenkel and Schotky defects. Impurity defects. Electronic defects. Effective charge. Writing of defect equations. Specific defect structures. Defect spinel structures. Normal spinel, random spinel and inverse spinel with incomplete lattice. Other examples of fluorite structures.

Reference Books

General:

1. Physical Chemistry by Peter Atkins, Julio de Paula, 8th / or 9th Edition, Oxford University Press
2. Free on the course materials from MIT open course ware: http://ocw.mit.edu/courses/chemistry;

CHE 104: SPECTROSCOPY

UNIT – 1: SYMMETRY AND GROUP THEORY IN CHEMISTRY

Symmetry elements and symmetry operations; Point groups: Mathematical requirements for a point group schoenflies notations point groups; Systematic assignment of molecules to point groups, Sub-groups; Classes; Matrix representation of symmetry elements; Matrix representation of C_{2v}, C_{3v} and C_{4v} point groups; Reducible and Irreducible Representations; Properties of Irreducible representations; Construction of character tables (C_{2v}, and C_{3v} point group); Mulliken symbolysim rules for IPS; The standard reduction formula; The Direct product; Symmetry criteria for Optional activity; Symmetry restrictions on Dipole moments; Symmetry and Stereo-isomerism; Prediction of IR and Raman spectral activity of H_2O molecule.

Reference Books

1. Introduction of symmetry and Group theory for chemists, by Arthur M. Lesk
2. Physical Chemistry by G.W. Castellan, Narosa Publishers.

UNIT -2: UNIFYING PRINCIPLES & MICROWAVE SPECTROSCOPY

Unifying Principles: Electromagnetic radiation – Interaction of electromagnetic radiation with matter – Absorption and Emission. Quantization of energy – Regions of the electromagnetic spectrum and the mode of interactions with molecular. Representation of spectra. Basic components of a spectrometer. Signal to noise ratio. Intensity and width of spectral lines.

Microwave spectroscopy: Classification of rotating molecules – Diatomic molecules – rigid rotor model calculation of bond lengths in diatomic molecules. Intensity of spectral lines. Effect of isotopic substitution on transition frequencies, non rigid rotor. Selection rules. Techniques and Instrumentation. Nuclear and Electron spin interactions and effect of External field: Stark Effect. Applications in quality control.

UNIT – 3: VIBRATIONAL SPECTROSCOPY

(a) Infrared Spectroscopy

Introduction, Linear harmonic oscillator, an-harmonic oscillator Vibrational energy level of Diatomic molecular, Selection Rule, Fundamental band, overtones, hot band, zero point energy, vibrational rotational spectra – carbon monoxide molecule. Vibrational Spectral of Polyatomic molecular, Normal modes of vibration, Concept of group frequencies, Characteristics Vibrational frequencies of functional groups, Applications of IR Spectroscopy – Calculation of Force constant, Hydrogen Bonding, Investigation of Bond Isomerism, C is – Trans isomerism and back bonding in Co-ordination compounds, Tautomerism in Organic compounds, IR Spectrophotometer – Instrumentation. Application as characterizing tool.

(b) Raman Spectroscopy

Introduction, Raman & IR spectra comparative treatment, Mechanism of Raman Effect (Classical and Quantum theory), Selection Rules. Mutual Exclusion Principle;

Instrumentation, Applications:- Structural determination of XY_2 (CO_2, CS_2), XY_3(NO_3^-, NO_3-, CIF_3). Characterization tool for carbon nanotubes and grapheme. Applications in quality control and pharmaceutical products.

UV & VISIBLE SPECTROSCOPY

Electronic spectra of diatomic molecules. The Born – oppenheimer approximation. Vibrational coarse structure: Intensity of Vibrational – electronic spectra. The Franck – Condon Principle. Rotational fine structure of electronic vibration transitions. Electronic structure of diatomic molecules.

Types of transitions, Chromophores, Conjugated dienes, trienes and polyenes, unsaturated carbonyl compounds – Woodward – Fieser rules.

Electronic of transitions, Chromophores, Conjugated dienes, trienes and polyenes, unsaturated carbonyl compounds – Woodward – Fieser rules.

Electronic spectra of polyatomic molecules. Chemical analysis by Electronic Spectroscopy – Beer – Lambert's Law. Deviation from Beer's law. Quantitative determination of metal ions (Mn^{+2}, Fe^{+2}, NO_2^-, Pb^{+2})

UNIT – 4: NUCLEAR MAGNETIC RESONANCE SPECTROSCOPY

Nuclear spin, Principles of NMR – Classical and Quantum Mechanical methods, Magnetic moment and Spin angular momentum. Larmour Frequency. Instrumentation. Relaxation – spin – spin & spin lattice relaxation. Shielding constants, Chemical shifts, Shielding and Deshielding mechanism – Factors influencing Chemical shift. Spin-Spin interactiosn – AX, AX_2 and AB types. Vicinal, Geminal and Long range coupling – Factors

Influencing coupling constant. Spin decoupling, Spin tickling, Deuterium exchange, Chemical shift reagents and Nuclear overhauser effect. Applications in Medical diagnostics, Reaction kinetics.

Reference Books

1. Introduction to Molecular Spectroscopy, by Gordon, M. Barrow
2. Molecular Spectroscopy, by John M. Brown, Oxford University press
3. Fundamentals of Molecular Spectroscopy, Banwell, Mc Graw Hill

PRACTICAL – 1. INORGANIC CHEMISTRY
Practical Syllabus

I. Preparation of Metal Complexes:
- (i) Tetraammine copper (II) sulphate
- (ii) Mercury (II) tetrathiacyanato cobaltate (II)
- (iii) Hexaammine Nickel (II) chloride
- (iv) Tris (acetylacetonato) Manganese (III)
- (v) Tris (ethylene diamine) Nickel (II) thiosulphate

II. Analysis of Materials of general interest:
- (i) Estimation of free chlorine in bleaching powder
- (ii) Estimation of dissolved oxygen in water
- (iii) Estimation of Calcium in milk

III. Analysis of two component mixtures:
- (i) Determination of Al (III) and Fe (III)
- (ii) Determination of Cu (II) and Zn (II)
- (iii) Determination of Ca (II) and Mg (II)
- (iv) Determination of Cu (II) and Ni (II)
- (v) Determination of Ferrocyanide and Ferricyanide

PRACTICAL II: ORGNAIC CHEMISTRY
PRACTICAL SYLLABUS

I. Identification of organic compounds:

Identification of the organic compounds by a systematic study of the physical characteristics (mp/bp), extra elements (nitrogen, halogens and sulfur), solubility, functional groups, preparation of crystalline derivatives and identification by referring to literature.

II. Preparation:

Preparation of Aspirin (acetylation), Benzil (oxidation), Dibenzylidene acetone (condensation), m-dinitorbenzene (nitration), p-bromoacetanilide (bromination), Benzoic acid (cannizzaro reaction).

Recommended Books

1. A textbook of practical organic chemistry by A.I. Vogel, Vol. I and II.
2. Unitized experiments in organic chemistry by R.Q. Brewster and others.
3. Practical Organic Chemistry by Mann and Saunders.
4. Laboratory Manual of Organic Chemistry by B.B. Dey and M.V. Sitaraman Revised by T.R. Govindachari.

M. Sc ORGANIC CHEMISTRY – 2nd YEAR II Semester SYLLABUS
CHE 201: QUANTITATIVE DATA, ANALYTICAL ELECTRO CHEMCIAL AND SEPARATION TECHNIQUES

Unit – 1: STATISTICAL TREATMENT OF DATA

Definition of error and uncertainty; Types of errors; Distribution of random errors; Precision and Accuracy; Standard deviation, Relative standard deviation; confidential limit; Statistical treatment of data – F test, T test and Q test; Method of least squares; Significant figures, uncertainity evaluation, use of spread sheets in analytical chemistry and reporting data.

Reference Books

1. Statistical Analysis Methods for Chemists, William P Gardiner, RSC Publishing (e-book available)
2. Modern Analytical Chemistry David Harvey. Mc Graw Hill (e-book available)
3. Principles of Analytical Chemistry, Skoog, West, Holler and Crouch 8th Ed. India ed, Brooks/Cole, 2004.

SOLVENT EXTRACTION AND ION EXCHANGE

A. **Solvent extraction** – General introduction – factors favouring solvent extraction. Quantitative.
treatment of solvent extraction – Extraction reagents. Applications

B. **Ion exchange chromatography**
General introduction. Action in ion exchange resins. Ion exchange chromatography. Ion exchange equilibria. Ion exchange capacity and its determination. Applications:
   (1) Determination of the total cation concentration in water.
   (2) Separation of the fluoride with the aid of cation exchanger.
   (3) Separation of Cl^- and Br^- using anion exchanger.

Reference Books

1. Analytical Chemistry by Skoog, West and Holler, Harcourt College Publishers, 1996.
2. vogel's Text Book of Quantitative Inorganic analysis by J. basett *et. al.,* Elbs, Longman 1978.

UNIT 2: CHROMATOGRAPHIC METHODS

Introduction, Definitions, Classifications in Chromatography.

A. Adsorption column chromatography:

Types of columns, Experimental requirements, Development of column, Factors affecting column efficiency, Applications and experiments, Separation of (1) Methylene Blue and malachite green; (2) Metal ions and (3) Chlorophylls and carotenoids.

B. Paper Chromatography.

Theory, Principles and techniques. Development of chromatogram (Ascending and Descending), Two dimensional and Multi dimensional paper Chromatography, Measurement

of R_f values, Applications and experiments, Separation of: (1) Amino acids (2) Cations and (3) Complexes.

C. Thin layer Chromatography:
Preparation and development of plates. Advantages of TLC, Applications and Experiments – Separation of : (1) Ink Pigments (2) Dyes and (3) Amino acids. High Performance, Thin Layer Chromatography (HPTLC), Features and Applications.

D. Gas Chromatography:

Principles and theory, Instrumentation – Columns and detectors, Types of chromatograms. Analysis of elution peaks, applications in qualitative and quantitative analysis

E. High Performance Liquid Chromatography:
Introduction, characteristic features of HPLC, comparison of super critical fluid, fluid chromatography with HPLC and GLC; Principle of HPLC, Instrumentation; Components, Types of detactors. Applications HPLC on the separation of inorganic, Organic and Pharmaceutical compounds

Reference Books:

1. Chromatography by B.K. Sharma, Goel Publishing House, Meerut 2001.
2. An Introduction to Chromatography by H. Kaur, Pragathi Prakasam.
3. Analytical Chemistry by Skoog, West and Holler, Harcourt College Publishers, 1996.
4. Vogel's Text Book of Quantitative Inorganic analysis by J. Basett *et. al.,* Elbs, Longman 1978.

UNIT – 3: ELECTRO ANALYTICAL TECHNIQUES

A. **Polarography:** Principles, Advantages of Dropping Mercury Elctrode, Diffusion current, migration current,half wave potential, ilkovic equation, reversible and irreversible polarographic processes, Quantitative polarographic analysis.
B. **Amperometric titration:** Principle – Determination of lead using oxalic acid titration curves, Determination of nickel using dimethylglyoxime
C. **Cyclic Voltammetry:** Principle, Randles-Sevcik equation (only statement and no derivation), Criteria for the cyclic volatmograms for reversible, irreverisble, quasi-reversible waves, Identification of intermediates in organic reactions using cyclic voltammetry.

Reference Books

1. Laboratory Techniques in Electroanalytical Chemistry, Second Edition, Revised and Expanded, Peter Kissinger, William R. Heineman, Marcel Dekker Inc. 1996.
2. Electrochemical Methods – Fundamental and Applications, A.J. Bard and L.R. Faulkner, John Wiley & Sons
3. Polarography (Article), Resonance Journal, pp: 51-51 September 2004 (Available in www.ias.ac.in/resonance/Sept 2004/pdf/Setp2004 p 51-61.pdf)
4. Analytical Electrochemistry, Joseph Wang (John Wiley and Sons)

UNIT – 4: ANALYTICAL SPECTROSCOPY

(a) Spectrophotometry: Beer – Lambert law, Method of analysis and applications – examples

(b) Spectrofluorimetry: Basics of the Method and Applications – Examples

(c) Flame photometry and Flame Emission Spectroscopy, Principles and experimental technique, Interferences: chemical reactions in flames. Dissociation equilibria, ionization in flames, use of organic solvents. Applications, advantages & disadvantages, limitations – Example of Water analysis

(d) Atomic Absorption Spectroscopy, Introduction, Principles, relation between flame emission and atomic absorption. Instrumentation, Interferences, background correction.

Reference Books

1. Spectrophotometry and Spectrofluorimetry – A Practical approach, Michael G.Gore, Oxford University Press
2. Modern Analytical Chemistry, David Harvey, McGRaw Hill (e-bool available)
3. Principles of Instrumental analysis, Douglas A. Skoog, F. James Holler, Timothy A. Nieman, Holt Sounders Instrumental Edition, 5th ed., 1998. Philadelphia.

CHE 202: ORGANIC SPECTROSCOPY, DRUG DESIGN, CONFIRMATIONAL ANALYSIS, & HETEROCYCLIC COMPOUNDS

UNIT – 1: ^{13}C – NMR SPECTROSCOPY

^{13}CNMR – Spectroscopy – CW and PFT techniques. Types of CMR spectra – undecoupled proton decoupled. Off – resonance decoupled (SFORD): ^{13}C – chemical shifts, factors affecting the chemical shifts Hononuclear (^{13}C - ^{13}CJ), and heteronuclear (^{13}C – ^{1}H, ^{13}C – ^{2}HJ) couplings. Applications of ^{13}C – NMR Spectroscopoy in confirmation of structure and stereochemistry of organic molecules and in determining the reaction mechanism and dynamic processes of organic reactions – examples. Multipulse, techniques: HOMO and HETERO – 2D – J – resolved spectra. Explanation of the principle, application to structure elucidation of simple organic molecules.

UNIT – 2: APPLICATIONS OF MASS SPECTROMETRY AND OPTICAL ROTATORY DISPERSION

MASS SPECTROSCOPY: Basic principles – instrumentation – magnetic sector instruments. Ion production electron impact ionization – chemical ionization. Mass spectra – Molecular ion – types of ions in mass spectra. Effect of isotopes on mass spectra. Mc Lafferty rearrangement. Ortho effect – Meta stable ions. Nitrogen rule. General fragmentation modes. Mass spectral fragmentation of some classes of organic compounds.

OPTICAL ROTATORY DESPERSION: Basic rotation. Circular birefringence, circular dichroism and cotton effect. Plain curves and anomalous curves and their applications. Axialhalo keto rule and octant rule. Applications to the study of configuration and conformations of organic molecules.

DRUG DESIGN

Introduction to drug discovery. Drug discovery without lead – serendipity – Pencillins as example. Lead discovery – random and non-random screening of natural products – medical folklore, synthetic banks. Existing drugs from natural ligand or modular combinational synthesis. Computer aided designing (introductory treatment only).

Drug metabolism studies – Phase I and Phase II metabolism. Clinical observations. Phase – I, Phase – II, Phase – III and Phase – IV trials (introductory treatment only).
Principles of drug design against agonist, antagonist drugs.

UNIT – 3: CONFORMATIONAL ANALYSIS

Introduction to conformational isomerism and the concept of dynamic stereochemistry. Study of confirmations in ethane and 1, 2 – disubstituted ethane derivatives like butane, dihalobutanes, halohydrin, ethylene glycol, butane – 2, 3 – iol, amino alcohols and 1,1,2,2-tetrahaobutanes. Klyne-Prelog terminology for conformers and torsion angles. Conformations of unsaturated acyclic compounds (1.butene, propionaldehyde and butanone). Conformational diastereoisomers and conformational enantiomers. Factors affecting the conformational stability and conformational equilibrium – attractive and repulsive interactions. Use of physical and spectral methods in conformational analysis.

Conformation effects on the stability and reactivity of acyclic diastereoisomers – steric and stereo electronic factors – examples. Conformation and reactivity: The Winstein – Holness equation and the Curtin – Hammett principle.
Conformations of cyclohexanes, mono and di substituted cyclohexanes. Stereochemistry of decalins. Factors governing the reactivity of axial and equatorial substituents in cyclohexanes. Stereochemistry of addition to the carbonyl group of rigid cyclohexane ring.

UNIT – 4: HETEROCYCLIC COMPOUNDS

Importance of heterocyclic compounds as drugs. Nomenclature of heterocyclic systems based on ring size, number and nature of hetero atoms. Synthesis and reactivity of Pyridine, Quinoline, Isoquinoline, Indole, benzofuran, Benzothiophene, Pyrazole, Thiazole, Oxazole and Pyrimidine.

Recommended Books

1. Spectroscopic identification of Organic Compounds by R.M. Silverstein G.C. Bassier and T.E. Morrill.
2. Spectroscopic Identification of Organic Compounds by R.M. Silversten and Webster.
3. Organic Spectroscopy by Willam Kemp
4. NMR in Chemistry – A Multinuclear introduction by William Kemp
5. Spectroscopic Identification of Organic Compounds by P.S. Kalsi
6. ^{13}C NMR for Organic Chemistry by G.C. Levy and G. L. Nelson
7. Optical rotatory dispersion by C. Djerassi.
8. Optical rotatory dispersion circular dichroism by P. Crabbe.
9. Sterechemistry of Organic Compounds – Principles & Applications by D. Nasipuri.
10. Stereochemistry confirmation and mechanism by P.S. Kalsi.
11. Stereochemistry of Organic Compounds by Eliel.
12. Heterocyclic Chemistry by J.A. Joule and Smith.
13. Heterocyclic Chemistry by T.L. Gilchrist.
14. Heterocyclic Chemistry by J.A. Joule and K. Mills.
15. An Introduction to the Chemistry of Heterocyclic compounds, R.M. Acheson.
16. Principles of Modern Heterocyclic Chemistry, A. Paquette.
17. Handbook of Heterocyclic Chemistry, A.R. Katritzky.
18. burger's Medicinal Chemistry and drugs discovery by Manfred E. Wolf.

CHE 203: ORGANIC PHOTOCHEMISTRY, PERICYCLIC REACTIONS AND ORGANIC SYNTHESIS

UNIT – I: ORGNAIC PHOTOCHEMISTRY

Organic photochemistry: Molecular orbitals, carbonyl chromophore – triplet states, Jablonski diagram, inter-system crossing. Energy transfer. Energies properties and reaction of singlet and triplet states of and transitions.

Photochemical reactions; Phtoreduction, Paterno-Buchi reaction, Norrisch type I cleavage and NOrrisch type II cleavage, Photo Fries rearrangement. Photochemistry of unsaturated systems – Olefins, cis-trans isomerisation and dimerazation. Photochemistry of 1,2-butadienes.

UNIT – II: PERICYCLIC REACTIONS

Characteristics – Types of pericyclic reactions-Electrocyclic, cycloaddition – cycloreversion and sigmatropic reactions – examples. 4n and 4n+2 electron type-stereospecificity.

Theories involved in understanding pericylic reactions –

(a) Frontier Molecular Orbital theory concept-Woodward-Hoffmann selection rules for electrocyclic, cycloaddition – cycloreversion and sigmatropic reactions based on FMO approach.
(b) Conservation of Molecular Orbital theory concept-Framing of Woodward-Hoffmann selection rules for electrocyclic, cycloaddition and cycloreversions based on conservation of Molecular Orbital approach.
(c) Aromatic Transition state theory-concept- Woodward-Hoffmann selection rules for electrocyclic reactions cycloaddition – cycloreversions and sigmatropic reactions based on ATS aromatic transition state (Huckel-Mobius) approach.

UNIT – III: SYNTHETIC STRATEGIES AND PROTECTING GROUPS

Introduction to organic synthesis. Disconnection approach – examples – Terminology – Definition of target molecule, functional group intercoversion (FGI), disconnection product, disconnection, synthons, reagents and retrosynthesis. Linear and convergent synthesis. Importance of order of events in organic synthesis – examples. Synthesis of Benzocaine, paracetamol, (+) – disparlure.

Principles of Protection of alcohols, carboxylic acides, amines and carbonyl groups

REAGENTS OF SYNTHETCI IMPORTANCE (OXIDATIONS AND REDUCTIONS)

(a) Oxidations: (i) Alcohols to carbonyls: Cr(VI) oxidants, Swern oxidation, Silver Carbonate, (ii) Prevost and Woodward Oxidation, (iii) Oxidations of allylic and benzylic C – H bonds: DDQ and SeO_2.
(b) Reductions: (i) Catalytic hydrogenation, (ii) Homogeneous hydrogenation – Use of Wilkinsosn catalyst (iii) Dissolving metal reductions including Birch reduction. (iv) Nucleophilic metal hydrides: $LiAlH_4$, $NaBH_4$. Electrophilic metal hydrides: BH_3, AlH_3. (v) Hydrogenolysis – use of tri-n-butyltin hydride.
(c) Organometallic reagents: Preparation and application of the following in organic synthesis: (a) Grignard reagnts, Organo Lithium and Organo copper reagents.

UNIT - IV: ASYMMETRIC SYNTHESIS

Introduction and terminology: Topocity in moleculaes Homotpic, stereoheterotopic (enantiotopic and diastereotopic) groups and faces – symmetry, substitution and addition criteria. Prochirality nomenclature: Pro-R Pro-S, Re and Si.

Methodology or asymmetric synthesis –

Substrte controlled asymmetric synthesis: Nucleophilic addition to chiral carbonyl compounds. 1,2-asymmetric induction, Cram's rule and Felkin – anh Model.

Chiral auxiliary controlled asymmetric synthesis: Use of chiral auxiliaries in Diels – Alder.

Chiral reagent controlled asymmetric synthesis: Asymmetric reduction using BINAL-H. asymmetric hydroboration using IPC_2 BH and $IPCBH_2$.

Chiral catalyst controlled asymmetric synthesis: Sharpless and Jacobsen epoxidations.

Asymmetric aldol reaction, Diastereoselective aldol reaction and its explanation by Zimmerman – Traxel model

Recommended Books

Molecular reactions and Photochemistry by Charles Dupey and O.L. Chapman.

Molecular Photochemistry by Turru.

Importance of antibonding orbitals by Jaffe and Orchin.

Text Book of Organic Chemistry by Cram., Hammand and Henrickson.

Some modern methods of organic synthesis by W. Caruthers.

Guide Book to Organic Synthesis by R.K. Meckie, D.M. Smith and R.A. Atken.

Organic Synthesis by O. House.

Organic synthesis by Michael B. Smith.

Organic Chemistry Claydon and others 2005.

Name Reactions by Jie Jack Li

Reagents in Organic Synthesis by B.P. Mundy and others.

Tandem Organic Reactions by Tse – Lok Ho.

Organic synthesis by Robert E. Ireland.

Organic synthesis: the disconnection approach by Stuant Warren.

Guide Book to Organic synthesis by R.K. Hackie, D.M. Smith and R.A. Atken.

Asymmetric synthesis by Nagradi.

Stereochemistry of organic compounds – Principles and applications by D. Nasipuri.

Asymmetric Organic reactions by J.D. Morrison and H.S. Moschee.

Stereo Diffractionating reactions by Izumi

Organic Chemistry by Vol. 1 and 2, I.L. Finar

Organic Synthesis by C. Willis and M. Willis.

CHE 204: ADVANCED NATURAL PRODUCTS

UNIT – I: CARBOHYDRATES AND PROTEINS

Carbohydrates: Occurrence, importance and synthesis of monosaccharides containing functional groups such as amino, halo and sulphur. Structure elucidation and synthesis of sucrose. Conformational structures of D(+) ribose, 2-deoxy D-ribose, sucrose, lactose, maltose and cellobiose. Structural features of starch cellulose and chitin (structure elucidation not expected).

Proteins: Acid and enzymatic hydrolysis of proteins. Determination of amino acid sequence in polypeptides by end group analysis. Chemical synthesis of di and tri peptides.

UNIT – II: TERPENOIDS

Classification – isoprene and special isoprene rules. Occurrence, isolation, structure elucidation, stereochemistry and total synthesis of (i) santonin (ii) abeitic acid and (iii) β - carotene, Biosynthesis of mono and diterpenoids.

UNIT – III: ALKOLOIDS

Definition, medicinal importance occurrence and classification of alkaloids. General methods used for structural determination of alkaloids. Isolation, structural elucidation, stereochemistry and total synthesis of (i0 Quinine (ii) Morphine (iii) reserpine, Biosynthesis of morphine.

STERIODS, HARMONES AND PROSTAGLANDINS

Occurrence, isolation, structure determination, stereo chemistry and total synthesis of (i) cholesterol (ii) androsterone (iii) testosterone (iv) estrone and (v) progesterone. Biosynthesis of cholesterol.

UNIT – IV: NUCLEIC ACIDS AND ENZYMES

Nucleic acids: Primary, secondary and tertiary structure of DNA, Types of RNA – mRNA, tRNA and rRBA. Replication, transcription and translation. Genetic code. Protein biosynthesis.

Enzymes: Definition, Classification based on mode of action. Mechanism of enzyme catalysis. Lock and Key mode and Induced – Fit model. Factors affecting enzyme catalysis. Enzyme inhibition – reversible and irreversible inhibition. Enzymes in organic synthesis.

Recommended Books

1. Comprehensive Organic Chemistry by D.r. Barton and W.D Ollis.
2. Standard methods in plant analysis by Reach and Tracey
3. natural production by Kalsi
4. Text book of Organic Chemistry Vol. II by I.L. Finar.
5. An introduction to the chemistry of terpenoids and Steroids by Wiliam templetion.
6. Systematic identification of flavonoid compounds by Mabry & Markhan.

PRACTICAL SYLLABUS

PRACTICAL – I: Separation and identification of organic compounds

Separation of two component mixtures by chemical methods and their identification by chemical reactions – separation by using solvent ether, 5% aq.. hydrochloric acid, 5% aq. Sodium bicarbonate and 5% sodium hydroxide solutions. Identification of the compounds by a systematic study of the physical characteristics (mp/bp), extra elements (nitrogen, halogens and sulfur), solubility, functional groups, preparation of crystalline derivatives and identification by referring to literature.

PRACTICAL – II: Estimation and Two state preparations.

Estimations: Glucose (using Fehling solution), Phenol, Aniline (by bromination), Methyl Ketone (by Iodinatioin).

Preparations:

1. Preparations of Benzil and Benzilic acid (Benzilic acid rearrangements).
2. Preparations of Benzohenone oxime and Benzanilide (Beckmann rearrangement).
3. Preparations of p-bromo acetanilide and p-bromo aniline (hydrolysis)
4. Preparations of Benzil and Phenytoin (Pinacol – Pinacolone rearrangement)