DETAILED SYLLABUS FOR DISTANCE EDUCATION POST GRADUATE DEGREE PROGRAM
MASTER OF SCIENCE - CHEMISTRY (M.sc - chem)

(YEARLY SYSTEM)
MATER OF SCIENCE IN CHEMISTRY

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1ST - SEMESTER
Paper – 1
MSCH/S/110
ORGANIC CHEMISTRY – I

UNIT – I

UNIT – II

UNIT – III
Aromaticity: Hukel’s rule and MO approach to aromaticity in various carbocyclic systems and charged species – non-aromatic and anti-aromatic systems – absorption spectra and induced ring current.

UNIT – IV

Conformational Analysis:
Conformation in open chain system energy consideration – conformation of cyclohexane and its mono, disubstituted derivatives. Effect of conformation on reactivity in acyclic compounds and cyclohexane derivatives.

UNIT – V

Text Books and References:
3. Pelletier (Ed.) Chemistry of Carbohydrates.
5. P.J. Garrat, Aromaticity.
UNIT – I


UNIT – II

Schrodinger equation for hydrogenation, separation of variables, phi-equation, theta equation and radial equation, total wave function, quantum numbers and their significance, shapes of atomic orbitals, Electron spin and Pauli exclusion principle, poly electronic atoms, Inter electron repulsion and its consequences. Energy levels in poly electronic atoms, R-S coupling, spin-orbit coupling, J-J coupling, Microstates and their classification, Term symbols.

UNIT – III

Nature of covalent bond, valence bond Method, concept of resonance and hybridization and bond angles, application to simple molecules, molecular orbital theory, Geometrics of the orbitals, symmetry and anti-symmetry of molecular orbitals, construction of molecular orbitals in diatomic molecules molecular orbitals in polar molecules. Ionic bonding, Lattice energy, Born equation and its derivation radius ratio rules, structures of some ionic crystals (Sodium Chloride, Cesium Chloride, Rutile, Wurtzite, Flourite)., hydrogen bonding.

UNIT – IV


UNIT – V


Text Book and Eeference :

MSCH/S/130
PRACTICALS

ORGANIC CHEMISTRY – I

1. Preparation of p-Bromoacetanilide
2. Preparation of p-Bromoaniline
3. Preparation of Benzoin
4. Preparation of Nenzil
5. Preparation of S-Benzyl-iso-Thiruonium chloride
6. Preparation of Benzpinacol

Organic Mixture Analysis

Analysis if organic mixture contain two components including separation.
1. Qualitative Analysis
   Qualitative Analysis involves the analysis of a mixture containing four cations.

2. Colorimetric estimations.
   b. Estimation of Nickel
   c. Estimation of Copper.
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2ND - SEMESTER
Paper – 1
UNIT – I
Thermodynamics: Calculation of adiabatic flame temperature, Maxwell’s relations, thermodynamic equations of state, thermodynamics of open systems, partial molal quantities, chemical potential, Gibb’s – Duham equation, variation of chemical potential with temperature and pressure, third law of thermodynamics. Nernst heat theorem, Chemical equilibrium Van’t Hoff reaction isotherm, standard free energy change of reactions, variation of equilibrium constant with temperature and pressure.

UNIT – II

UNIT – III
Group Theory: symmetry operations point groups, identification of point group, reducible and irreducible representation, orthogonability theorem. Construction of \( C_2V \) and \( C_3V \) character tables, symmetry selection rules for I.R. and Raman spectra, procedure for determining symmetry of normal modes of vibration hybrid orbitals in non-linear molecules \( BF_3, PCl_5, CH_4, NH_6 \).

UNIT – IV

UNIT – V

Text Book and Reference:

**Text Book and Reference** :

**Paper – 2**

**MSCH/S/220 POLYMER CHEMISTRY**

**UNIT – I**

**UNIT – II**

**UNIT – III**
Molecular weight and properties of polymers : Polydispersion – average molecular weight concept, number, weight and viscosity average molecular weights. Measurement of molecular weights. Gel permeation chromatography, viscosity, light scattering, osmotic and ultracentrifugation methods. Polynet structure and physical properties – crystalline melting point $T_m$. The glass transition temperature. Determination of $T_g$. Relationship between $T_m$ and $T_g$.

**UNIT – IV**
Polymer Processing : Plastics, elastomers and fibers. Compounding processing techniques : calendaring, die casting, rotational casting, film casting, injection moulding extrusion moulding, thermoforming, foaming, reinforcing and fibre spinning.
UNIT – V
Properties of Commercial Polymers: Polyethylene, polyvinyl chlorides, polyesters, phenolic resins, epoxy resins and silicone polymers. Functional polymers – Fire retarding polymers and electrically conducting polymers. Biomedical polymers – contact lens, dental polymers, artificial heart, kidney, skin and blood cells.
UNIT – I

UNIT – II
$^1$H NMR Spectra : Nuclear spin – magnetic moments of a nucleus – nuclear spin energy levels in the presence of magnetic fields, basic principles of NMR experiments – CW and FT NMR – $^1$H NMR chemical shift and coupling constants – factors influencing proton chemical shifts and vicinal proton – proton coupling constants.

UNIT – III
$^{13}$C NMR and Two dimensional NMR Spectroscopy : $^{13}$C NMR – proton decoupled and off-resonance – $^{13}$C NMR spectra – factors affecting $^{13}$C chemical shifts – $^{13}$C NMR spectra of simple organic molecules – use of INEPT and DEPT methods in assigning $^{13}$C signals. Basic principles of two dimensional NMR spectroscopy – HOMOCOSY, HETCOSY, NOESY.

UNIT – IV

UNIT – V
Identification of organic compounds using UV, IR, NMR spectroscopy and mass spectrometry – problems.
Partition of Co-efficient

1. Determination of partition coefficient of iodine between carbon tetrachloride and water.

2. Determination of equilibrium constant for the reaction $I_2 + I^3 \rightarrow$.

3. Estimation of I ions from a knowledge of the equilibrium constant of the above reaction.

Conductivity Measurements

4. Determination of cell constant of a conductivity cell.

5. A study of variation of equivalent conductance of a strong electrolyte with concentration.

6. Determination of dissociation constant of a weak acid.

7. Conductometric Titrations:
   a. Mixture of HCL and acetic acid Vs NaOH.
   b. Ammonium chloride Vs NaOH.
   c. A solution containing $Ba^{2+}$ ions Vs a solution containing $SO_4^{2-}$.

Phase Rule

8. Construction of phase diagram for diphenyl-naphthalene system.

9. Determination of composition of a mixture of diphenyl and naphthalene.

Determination Of Molecular weights

10. Determination of molecular weight by cryoscopic method using benzene as solvent.

11. Determination of molecular weight by cryoscopic method using water as solvent.

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3RD - SEMESTER
Paper – 1

MSCH/S/310  ORGANIC CHEMISTRY – II

UNIT – I
ADDITIO
N TO CARBON-CARBON MULTIPLE BONDS

Electrophilic and nucleophilic additions, addition to conjugated systems, orientation and reactivity, addition of halogen and nitrosyl chloride to olefins, hydration of olefins and acetylenes, hydroboration, hydroxylation epoxydation, Michael addition, 1,3 diploar addition, carbenes and their additions, Diels-alder reactions.

UNIT – II
ADDITIO
N TO CARBON-HETRO ATOM MULTIPLE BONDS


UNIT – III
ELIMINATION REACTIONS

E1, E2, E1cB mechanisms, Orientation of the double bond, Hofmann and Saytzeff rule, competition between elimination and substitution, dehydration and dehydrohalogeneration reactions, stereochemistry of E2 eliminations in cyclohexane ring systems, mechanism of pyrolytic eliminations. Chugaev reaction and Cope elimination.

UNIT – IV
MOLECULAR REARRANGEMENTS

A detailed study of the mechanism of the following rearrangements : Nucleophilic, Electrophilic and Freeradical rearrangements – memory effects, Migratory aptitudes, Pinacol-Pinacolone, Wagner-Meerwin, Demyanov, Dienone-phenol, Favorski, Baeyer-Villiger, Wolff, Stevens and Von-richter (a few examples in each rearrangement are to be studied), rearrangements involving nitrenes – Hofmann, Curtius, Lossen, and Beckmann.

UNIT – V
IXIDATION AND REDUCTION
Study of the following oxidation reactions with mechanism: Oxidation of alcohols by CrO$_3$, DMSO alone, DMSO in combination with DC; acetic anhydride and oxaly chloride, oxidation of arylmethane, oxidation of methylene alpha to carbonyl, allylic oxidation of olefins, oxidative cleavage of glycols, oxidative cleavage of double by ozonolysis.

Study of the following reduction reactions with mechanism: Reduction of carbonyl compounds by hydrides, selectivity in reduction of 4-ter-butyl cyclohexanone using selectrides, Clemmensen and Wolff Kishner reductions, Birch reduction, MPV reduction.

**Text Books:**


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**MSCH/S/320 INORGANIC CHEMISTRY – II**

**UNIT – I**

**CO-ORDINATION CHMISTRY**

Crystal field theory, splitting of d-orbitals under various geometries, Factors affecting splitting, CFSE and evidences for CFSE (Structural and thermodynamic effects). Spectrochemical series, Jahn,Teller distortion, site preferences, limitations of CFT. Evidence for metal-ligand overlap. M.O. theory and energy level diagrams, concept of weak and strong fields, sigma and pi bonding in complex, nephelauxetic effect, magnetic properties of complexes.

**UNIT – II**

**ELECTRONIC SPECTRA OF COMPLEXES**

Term symbols for dn ions, characteristics of d-d transitions and selection rules, weak and strong field limits, Energy level diagrams. Orgal and Tanabe-Sugano diagrams, effect of distortion and spin orbital coupling on spectra. Evaluation of Dq and B value for octahedral complexes of Nickel, Charge transfer spectra.
UNIT – III
SOLID STATE CHEMISTRY
Structure of Solids, comparison of x-ray, neutron and electron diffraction, Structure of NiAs, Cdl2, pervoskite, spinels and inverse spinels, defects in solids, point defects, line effects and surface defects, non-stoichiometric compounds, Use of x-ray powder data in identifying inorganic crystalline solids, details for cubic systems.

UNIT – IV
PROPERTIES OF SOLIDS

UNIT – V
ANALYTIC TECHNIQUES
Chromatography : Gas, liquid chromatography, principle, retention volumes, carrier gas, columns, preparations, stationary phase, detectors, thermal conductivity, ionization, electron capture applications of GLC.
High performance liquid chromatography : scope, column efficiency, instrumentation, pumping systems, columns, column packing detectors, applications.

Text Books :

Reference:
3. Treatise on Analytical Chemistry, Klthoff and Goning (all series)
MSCH/S/330 ORGANIC CHEMISTRY PRACTICAL – II

1. Identification of components in a two component mixture and preparation of their derivatives. Determination of boiling point/melting point for components and melting point for their derivatives.

II. Preparation :
   1. Beta naphtyl methl ether form beta naphthol
   2. S- Benzyl isothiuronium chloride from benzyclhroide
   3. Beta glucose penta acetate from glucose
   4. Ortho-Benzoyl benzoic acid from phthalic anhydride
   5. Resacetophenone from resorcinol
   6. Para-Nitrobenzoic acid from para nitrotolune
   7. Meta-Nitroaniline from meta dinitrobenzene
   8. Methyl orange from sulphanillic acid
   9. Anthraquinone from antracene
  10. Benzyhydrol from benophenone

Part – I
Semimicro qualitative analysis of mixtures containing two common and two rae cations. The following are the care to be included: W, TI, Mo, Tc, Sc, Cc, Th, Be, Zr, V, U and Li.

Part – II
b. Preparation of the following:
   i. Potassium trioxalatoaluminate (III) trihydrate
   ii. Trithioureacopper (I) chloride
   iii. Potassium trioxalatochromate (III) trihydrate
   iv. Sodium bis (thiosulphato) cuprate (I)
   v. Tetramminecopper (II) sulphate
   vi. Potassium Tetrachlorocuprate (II)
c. Separation of mixture of two metal ions by paper chromatography.
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<td>Chemistry Of Natural Products, Biomolecules And Biotechnology</td>
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4TH - SEMESTER
Paper – 1

MSCH/S/410 PHYSICAL CHEMISTRY – II

UNIT –I
CHEMICAL KINTEICS – II
1.1 Catalysis by enzymes, kinetics of single substrate enzyme catalyzed reactions, effect of substrate concentration. pH and temperature of enzyme catalyzed reactions, inhibition of enzyme catalyzed reactions.

1.2 Kinetics of complex reactions, reversible reactions, consecutive reactions, parallel reactions chain reactions, general treatment of chain reaction, chain length, Rice Herzfeld mechanism, explosion limits.

UNIT – II

2.1 STUDY OF KINETICS OF SURFACE REACTIONS
Physical and Chemical absorption, adsorption, isotherms, types of adsorption isotherms, Longmuir adsorption isotherm. BET theory for multilayer adsorption, application of transition state theory to adsorption, measurement of surface area, catalysis by metals and semiconductor oxides. Mechanisms of heterogeneous catalytic reactions, the adsorption coefficient and its significance

2.2 Study of fast reactions
Relaxation methods, temperature and pressure jump methods, stopped flow and flash photolysis methods.

UNIT – III

THERMODYNAMICS – II

3.2 Partition function, evaluation of translational vibrational and rotational partition functions for mono, diatomic and polyatomic ideal gases, thermodynamic functions in terms of partition functions, calculation of equilibrium constants from partition functions (isotope exchange and dissociation of diatomic molecules), application of
partition functions to heat capacities of ideal gases, heat capacity of solids (Einstein and debye models).

UNIT – IV

Experiment results of black body radiation – photo effect, Compton effect, quantum mechanical postulates, the schrodinger equation – the particle in a box (one, two and three dimensional systems), the harmonic oscillator.

UNIT – V

Wave particle duality – de Brogile equation, uncertainty principle. Schrodinger equation for the rigid rotator, the hydrogen atom – setting up the Schrodinger, arriving solution for energy and wave functions. The origin of quantum numbers and their physical significance.

Text Books :


Reference:

Natural products and biomolecules:
Classification of natural products: classification based on chemical structure, physiological activity, taxonomy and biogenesis.


Vitamins: definition, occurrence, structural formulae and physiological functions of Vit. A1, A2, B1, B2, B6, nicotinic acid, Vit. C, D, and vitamin K.

Alkaloids: quinine, morphine, thiophene, codeine, nicotine, reserpine. Anthocyanins, flavones and isoflavones, examples in each family.

Terpenoids: monoterpenes, synthesis of geraniol, citral, menthola and me

Heterocyclics and synthetic drugs:
Methods of synthesis, physical and chemical properties and aromatic character of pyrazole, imidazole, oxazole, thiazole, pyridazine, pyrimidine and pyrazine. Coumarine and chromones. Synthesis of pyrimidine and purine bases – uric acid, caffeine, theobromine and theophylline.

Synthetic drugs: chemotherapy, classification of drugs, synthesis of – benadryl (anti allergic), beta methasone (anti inflammatory steroid), diazeom (tranquilizer), ibuprofen, piroxicam and indomethacin (non steroidal anti inflammatory), 5-fluorouracil and 2-deoxyriboonuciside (anti cancer), micanzole (anti fungal). Chloroquine and pyrethrine (anti malarials).

Concepts in biotechnology:
Bioprocess technology, microbial growth dynamic, bioreactor concepts, immobilization of cells and enzymes, enzyme technology and applications, principles of DNA technology, monoclonal antibodies, and concepts in agricultural and other industrial biotechnology.
Combinatorial chemistry:
Introduction to the combinatorial chemistry, parallel synthesis, mixture of synthesis, Mix and Split method, combinatorial libraries.

PAPER-III

MSCH/S/430

DRUGS

Principles of Drug Discovery and Drug design
Introduction: Drug discovery -- Folklore drugs
Design of agonist and antagonist drugs; drug receptor interactions
Use of physico - chemical properties in drug design, lipo-philic barrier to drugs, pKa, pH partition theory of drugs
Structure pruning technique in drug design (eg. Morphine, pharmacophore)
Lead structure discovery and development of lead, (eg; cimetidene and captopril discovery). Biosterism principle in lead structure modification.
Structure-activity relationship (SAR) in drug design: SAR of sulfa drugs, hypnotic, sedative, barbiturates, benzodiazepine, taxol analogs.
Quantitative structure activity relationships (QSAR) in drug design - Hammett electron substituent parameter, Hansch - Fujita lipophility parameter, Hansch Analysis (QSAR), Topliss method (OSAR).
Prodrug design and application. Molecular graphics based drug design.

Chiral Drugs & Drug Analysis
Chiral Drugs
Introduction: Chiral drugs, eutomers—distomers, three point contact model, Pfeiffer's rule, Eudesmic ratio.
Industrial synthesis of the following chiral drugs;
i) (S)-alpha Aryl propionic and anti-inflammatory drugs (NSAIDS)
ii) (S)-beta Blockers
iii) Calcium antagonist (2S, 3S)- Diltizen
iv) ACE inhibitor (R)-Carnitine
v) Intermediates for the semi synthesis of taxol,(2’R,3’R)--phenylisoserine,
Drugs and drug intermediates from fermentation process. Racemate drug resolution.
Analysis of drugs
Use of isotopes in the bioanalysis of drugs in the drug design/drug discovery program. Qualitative and quantitative analysis of drugs: Use of IR, UV, GLC and HPLC methods. Quality control methods in drug manufacture and drug formulations.

**DRUGS - MACROMOLECULAR TARGETS**

**Introduction**: The concepts of macromolecular targets, Drugs acting on metabolic processes, cell walls and genetic material.


**Drugs acting on cell walls**: Structural features of penicillins and cephalosporins. Common biosynthetic route for penicillins and cephalosporin. Cell wall structure and mechanism of activity of beta lactam groups of antibiotics.

**Natural Penicillins** and their commercial preparations (outline only) Development of semi-synthetic and orally active penicillins, long acting penicillins. Beta lactam inhibitors. Clavulanic acid betalactamovercoming the development of resistance to penicillins.

**Cephalosporins**: semi synthetic and orally active Cephalosporins. Synthesis of cephalosporin--C and cephaline.

**Drug acting on genetic** material: Classification into different types viz HA intercalating, DNA binding and nicking. DNA enzyme interfering, ribosomal RNA interfering and transcribing agent inhibiting drug.

**Drug interfering replication**
DNA binding and nicking agents - Synthesis of tinidazole and dimatridazole.

**Inhibitors of Transcribing** enzymes - Structure of rifamycin and rifampicin.
Drugs interfering with Translations - Structures of Tetracyclines, Aminoglycosides, macrolide antibiotics (erythrooxygen)-Synthesis of chlcramphenicol.
Antifungal agents: Structures of Griseofluvin and cyloseirine
Antiviral Agents; Synthesis of AZT and acyclovir. Brief note on Interferon.

**Drugs - Agonists, antagonists, neurotransmitters and Receptors**

**Introduction:** Definition and examples of agonists, antagonists, neurotransmitters and receptors.

- Alpha-Adrenergic receptor agonists: Synthesis of Norepinephrine, Epinephrine and methyl DOPA
- Alpha-Adrenergic receptor antagonists: Structural formulae of APC and Benektramine.
- Beta-Adrenergic receptor agonists: Synthesis of Salbutamol.
- Beta-Adrenergic receptor antagonists: Synthesis of Atenolol, propranalol and metaprolol
- Dopamine receptor agonists: Synthesis of L-dopa
- Dopamine receptor antagonists: Synthesis of Chlorpromazine
- H1 and H2 (Histamine) receptor agonists: Synthesis of Histamine.
- H1 receptor antagonists: synthesis of Chlorophenaramine.
- H2 receptor antagonists: Synthesis of Cimetidine and Ranitidine.
- Cholinergic receptor agonists: Synthesis of Acetylcholine
- Cholinergic receptor antagonists: Synthesis of succinylcholine and structural formula of Tubocurarine
- GHT receptor agonists: Synthesis of serotonin.
- SHT receptor antagonists: Synthesis of metaclopramide.

**Drugs - Ion Channels, Immune systems and Enzyme Inhibitors**

**Introduction** to Ion Channels and membranes, Immune systems and enzyme inhibitors.

- Drug acting on ion channels and membranes: Synthesis and mode of action of Nifedipine,
- Diltiazem,
- Immuno suppressing agents: Structural formulae and mechanism of action of cyclosporin.
- Glucosidase inhibitors: Synthesis and mechanism of action of Swainsonine.
- Angiotensin converting enzyme (ACE) inhibitors; synthesis and mode of action of (S, R)-Captopril, and (S, S, S)-Enalapril.
- H+, K+ - AT-phase Inhibitors: Synthesis and mechanism at action of Omeprazole
Experiments in chemical kinetics, phase rule, chemical equilibrium and Conductivity measurements:

DETAILED OF EXPERIMENTS:

Typical list of possible experiments are given. Experiments of similar nature and other experiments may also be given. The list given is only a guideline. A minimum of 15 experiments have to be performed in a year.

1. Study the kinetics of acid hydrolysis of an ester, determination of the temperature coefficient of the reaction and determination of the activation energy of the hydrolysis of ethylacetate.
2. Study the kinetics of the reaction between acetone and iodine in acidic medium by half life method and determine the order with respect to iodine and acetone.
3. Study of the saponification of ethylacetate by sodium hydroxide conductometrically and determine the order of the reaction.
4. Determination of dissociation of ethylacetate by sodium hydroxide conductometrically and determine the order the reaction.
5. Study the phase diagram for m-toluidine and glycerin system.
6. Construction of phase diagram for a simple binary system (naphthalene-phenanthrene and benzophenone-diphenylamine).
7. Construction of the phase diagram of the three component of partially immiscible liquid systems (DMSO-Water-Benzene; Water-Benzene-Acetic acid; Ethyl alcohol-Benzene-Water; Acetone-Chloroform-Water; Chloroform-Acetic acid-Water).
8. Determination of the equilibrium constant of the reaction between iodine and partition method.
9. Determination of equivalent conductance of a weak acid at different concentrations and verify Ostwald’s dilution law and calculation of the dissociation constant of the acid.
10. Determination of equivalent conductivity of a strong electrolyte at different concentrations and examine the validity of the Onsagar’s theory as limiting law at high dilutions.

11. Conductometric titrations of a mixture of HCL and CH₃COOH against Sodium hydroxide.

12. Compare the relative strength of acetic acid and monochloroacetic acid by conductivity method.