

# **Department of Chemistry**

**PROGRAMME M.Sc.** (Chemistry)

(Session: 2024-2025 Onwards)

- **➤** Programme Structure
- ➤ Programme Outcomes (POs)
- **➤ Course Outcomes (COs)**
- **➤** Detailed Syllabus (Course Contents)

#### **COURSE STRUCTURE WITH CREDITS DISTRIBUTION**

(Subject: M.Sc. Chemistry) (2024-2025 onwards) UG SEMESTER-VII/PG SEMESTER-I

Course Code		Course Name	Maximum Credits (20)	CIE	ЕТЕ
B020701T	Core	Inorganic Chemistry-I	3 Credits	25	75
B020702P	Core	Chemistry Laboratory -I	1 Credits	25	75
B020703T	Core	Organic Chemistry -I	3 Credits	25	75
B020704P	Core	Chemistry Laboratory -II	1 Credits	25	75
B020705T	Core	Research Methodology	4 Credits	25	75
B020706T	Discipline Centric	Physical Chemistry	4 Credits	25	75
В020707Т	Elective (Select any one)	Polymer Chemistry			
B020708T	Discipline Centric	Techniques of Chemistry -I	4 Credits		
В020709Т	Elective (Select any one)	Medicinal Chemistry		25	75

# Prof. Rajendra Singh (Rajju Bhaiya) University, Prayagraj

# UG SEMESTER-VIII (for Four Year Undergraduate Programme who obtained above 75% Marks)/ PG SEMESTER- II (for Two Year Post Graduate Programme- lateral entry)

С	ourse Code	Course Name	Maximum Credits (20)	CIE	ЕТЕ
B020801T	Core	Inorganic Chemistry-II	03 Credits	25	75
B020802P	Core	Chemistry Laboratory -III	01 Credits	25	75
B020803T	Core	Organic Chemistry -II	03 Credits	25	75
B020804P	Core	Chemistry Laboratory -IV	01 Credits	25	75
B020805R	Research Project	Research Project	12 Credits		100

#### OR

# UG SEMESTER-VIII (for Four Year Undergraduate Programme who obtained below 75% Marks)/PG SEMESTER- II (for Two Year Post Graduate Programme-lateral entry)

	Course Code	Course Name	Maximum Credits (20)	CIE	ЕТЕ
B020801T	Core	Inorganic Chemistry-II	3 Credits	25	75
B020802P	Core	Chemistry Laboratory -III	1 Credits	25	75
B020803T	Core	Organic Chemistry -II	3 Credits	25	75
B020804P	Core	Chemistry Laboratory -IV	1 Credits	25	75
B020805T	Discipline Centric Elective	Chemistry of Natural Products		25	75
B020806T	(select any one)	Techniques of Chemistry -I I	4 Credits		
B020807T	Discipline Centric Elective (select any one)	Supra-molecular Chemistry and Strategy in Chemical Synthesis	4 Credits	25	75
B020808T		Heterocyclic Chemistry			
B020809T B020810T	Ability Enhancement Course (select any one)	Reagents in Organic Synthesis  Analytical Chemistry	4 Credits	25	75

Note: The Core Course will be same in the both of UG Semester-VIII and PG Semester-II.

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PG SEM	ESTER-III/PG SEN	MESTER-I (One Year	PG Program	mme-L	ateral
		Entry)			
Course Code		Course Name	Maximum Credits (20)	CIE	ЕТЕ
B020901T	Core	Organic Spectroscopy	3 Credits	25	75
B020902P	Core	Chemistry Laboratory -V	1 Credits	25	75
B020903T	Core	Organometallic Chemistry	3 Credits	25	75
B020904P	Core	Chemistry Laboratory - VI	1 Credits	25	75
B020905T	Discipline Centric	Inorganic Spectroscopy		25	75
B020906T	Elective (select any one)	Nano Materials & Solid State Chemistry	4 Credits		
B020907T	Discipline Centric	Photochemistry	4 C dit	25	75
B020908T	Elective (select any one)	Quantum Chemistry	4 Credits		
B020909T	Ability Enhancement Course	Name reactions & Rearrangements in Organic Synthesis	4 Credits	25	75
B020910T	(select any one)	Molecular Spectroscopy			

# PG SEMESTER-IV/PG SEMESTER-II (One Year PG Programme)

Course Code		Course Name	Maximum Credits (20)
B021001D	MRP	MASTER DISSERTATION	20 Credits

**Instrumental Methods of Analysis** 

Paper Name: Inorganic Chemistry -I (Paper-I)

**Paper CODE: B020701T**Marks: 100 (ETE 75 & CIE 25)

## I. Stereochemistry and Bonding in main group compounds:

VSEPR, Walsh diagrams (tri-and penta-atomic molecules),  $d\pi$ -p $\pi$  bonds, Bent rule and energetics of hybridization, some simple reactions of covalently bonded molecules.

# II. Metal-Ligand Bonding in Transition Metal Complexes

Limitation of crystal field theory, molecular orbital theory, octahedral, tetrahedral and square planar complexes,  $\pi$ -bonding and molecular orbital theory and Jahn-Teller distortion.

#### III. Molecular symmetry and character tables

Symmetry elements and symmetry operations, symmetry groups, defining properties of a group, character tables and its applications.

Symmetry considerations in simple inorganic and coordination compounds.

#### IV. Chemistry of f-Block Elements

Comparative study of lanthanides and actinides. Electronic configuration, Oxidation state, Ionic radii (lanthanide contraction), complex formation, Structure of complexes, spectral properties and magnetic properties. General chemistry of actinides including E.M.F. diagrams, Extraction and metallurgy of thorium and uranium. Separation of transamericium elements.

## V. Metal ligand equilibria in solution:

Stepwise and overall formation constant, trends in stepwise constant, factors affecting the stability of metal complex with reference to the nature of metal ion and ligand, chelate effect and its thermodynamic origin.

## M.Sc. Chemistry (Practical)-Semester-I

Paper Name: Chemistry Laboratory -I

**Paper CODE: B020702P**Marks: 100 (ETE 75 & CIE 25)

#### Inorganic:

#### a) Qualitative Analysis:

Qualitative mixture analysis for seven radicals including two rare elements (Mo, W, Ti, Zr, Th, Ce, V) in cationic and anionic forms.

- Quantitative separation and determination of the following pairs of metal ions using gravimetric & volumetric methods.
- (i) Ni<sup>++</sup> and Cu<sup>++</sup>
- (ii) Cu<sup>++</sup> and Zn<sup>++</sup>
- (iii) Ag+ and Cu++
- (iv) Ag+ and Ca++

#### Organic

- Separation and identification of organic compounds using chemical methods from binary mixture.
- b) Isolation of
- (i) Caffeine from tea leaves
- (ii) Eugenol from cloves
- (iii) Casein from milk
- (iv) Lycopene from Tomatoes

Paper Name: Organic Chemistry -I (Paper-II)

**Paper CODE: B020703T**Marks: 100 (ETE 75 & CIE 25)

#### I- Nature pf bonding in organic molecules:

Delocalised chemical bonding-conjugation, crossonjugation, resonance, hyper-conjugation, Aromaticity in benzenoid and non-benzenoid compounds, alternant and non-alternant hydrocarbons, Huckel's rule, energy of pi-molecular orbitals, annulenes, anti-aromaticity, homo-aromaticity. Bonding in fullerenes.

# II - Reaction Mechanism: Structure and Reactivity:

Generation, structure stability and fate of reaction intermediates: carbocation(including nonclassical carbocation, phenonium ion, and norbornyl system), carbanion (including enolate ions), carbene, nitrenes, free radicals(allylic halogenation) and arynes. Hammond's postulate, Curtin-Hammett principle. Potential energy diagrams, transition states and intermediates. Methods of determining mechanism-isotope effects, product analysis, Kinetic and stereochemical studies.

#### III. Stereochemistry

Conformational analysis of cycloakanes-disubstituted cyclohexanes, decalins, effect of conformation on reactivity.

Elements of symmetry, chirality, molecules with more than one chiral centre, threo and erythro isomers, optical purity, enantiotopic and diastereotopic atoms, group and faces, regiospecific, stereospecific and stereoslective synthesis, Asymmetric synthesis. Optical activity in the absence of chiral carbon (biphenyls, allenes and spiranes), chirality due to helical shape. R/S nomenclature, chiral centres and chiral molecules.

#### IV Aliphatic Nucleophilic Substitution

The S<sub>N</sub><sup>1</sup>, S<sub>N</sub><sup>2</sup>, mixed S<sub>N</sub>1', S<sub>N</sub>2', S<sub>N</sub><sup>1</sup> and SET mechanisms.

neighbouring group participation by pi and sigma bonds, anchimeric assistance. Nucleophilic substitution at allylic, aliphatic trigonal and vinylic carbon. Effects of substrate structure, attacking nucleophile, leaving group and reaction medium on reactivity. Phase transfer catalysis, ambident nucleophile and regioselectivity. Stereochemistry of S<sub>N</sub><sup>1</sup> and S<sub>N</sub><sup>2</sup> reactions.

#### V. Aromatic Electrophilic Substitution

The arenium ion mechanism, orientation and reactivity, energy-profile diagrams. The ortho/para ratio, ipso attack. Diazonium coupling, Vilsmeier reaction, Gatterman-Koch reaction...

## VI. Aromatic Nucleophile Substitution

The ArSN<sup>1</sup>, ArSN<sup>2</sup>& ArSN<sup>1</sup> via benzyne mechanisms. Effect of substrate structure, leaving group and attacking nucleophile on reactivity. The Von Richter, Sommelet-Hauser and Smiles rearrangements.

#### M.Sc. Chemistry (Practical)-Semester-I

Paper Name: Chemistry Laboratory -II

**Paper CODE: B020704P**Marks: 100 (ETE 75 & CIE 25)

#### Physical

#### Chemical Kinetics:

- Kinetic studies of a reaction between acetone and iodine catalyzed by H<sup>+</sup> ions.
- Kinetics of oxidation of reducing sugars by potassium ferricyanide in presence of ammonium hydroxide or sodium hydroxide.
- Determination of rate constant and order of reaction between H<sub>2</sub>O<sub>2</sub> and HI
- Determination of velocity constant of hydrolysis of an ester/ionic reaction in miceller media.
- Determination of the effect of a) change of temperature, b) ionic strength of media, c)
  change of concentration of reactants and catalysts on the velocity constant of hydrolysis
  of an ester/ionic reaction.

#### Thermodynamics

- Determination of partial molar volume of solute (e.g. KCl) and solvent in a binary mixture.
- Determination of the temperature dependence of the solubility of a compound in two solvents having similar inter molecular interactions and to calculate the partial molar heat of solution.

Paper Name: RESEARCH METHODOLOGY

Paper CODE: B020705T

Marks: 100 (ETE 75 & CIE 25)

**Research Methodology** 

An Introduction, Meaning of Research, objective of research, motivation in research, types of

research, research approaches, importance of knowing how research is done. Research

processes - scientific research, formation of the topic, hypothesis, conceptual definitions,

operational definition, gathering of data, analysis of data, revising of hypothesis, Conclusion.

Literature survey - Journals, books and resources. Presentation and publication of research

output.

**Defining the research problems** 

What is the research problems, selecting the problems, necessity of defining the problem,

technique involved in defining the problems, bring clarity and focus to your research problem,

procedure for reviewing the literature existing literature. search for

Method of data collection

Collection of primary data, observation method, interview method, collection of data through

questionnaires, collection of data through schedules, some other method of data collection,

study design based on the nature of the investigation - experimental study, theoretical

study, comparison.

The computer-its role in research

Introduction, the computer and computer technology, the computer system. General awareness

of computer hardware, CPU, input and output devices, memory, other peripheral devices,

auxiliary storage devices. Basic knowledge of computer systems, softwares - System softwares

and application software's Programming languages: machine language, assembly language and

Interpreter and compiler. Flow charts and Algorithms. General high-level languages.

awareness of operating systems: Disk operating system, Windows, Macintosh, Linux.

Applications and uses of common softwares in chemistry, Origin, Chemsketch, Chemdraw.

Basic ideas on the use of Internet in Chemistry education.

#### **Paper Name: Physical Chemistry**

**Paper CODE: B020706T**Marks: 100 (ETE 75 & CIE 25)

# Partial Molar Properties, Nernst Heat Theorem (NHT) and Third Law of Thermodynamics:

Partial molar properties, Chemical potential and other thermodynamic functions, Fugacity of real gases, Nernst Heat Theorem and its application to non-condensed systems. Statement of the third law of thermodynamics. Derivation of unattainability of absolute zero. The relationship between entropy constant and Nernst chemical constant. Determination of entropy from the Third Law using the correction due to gas imperfections.

- Chemical Kinetics: Thermodynamic formulation of rate constant. Comparison of collision and absolute reaction rate theories. Calculation of transmission coefficient. Transition State theory in solution. Primary and secondary salt effects in the light of mechanistic tests. The theory of Absolute reaction rates for reactions between atoms and reactions between molecules in terms of partition function. Influence of ionic strength and dielectric constant. Explosive reactions.
- Electrolytes: Limitation of Arrhenius theory of electrolytic dissociation. Role of solvent and inter-ionic forces. Activity and activity coefficients, determination of activity coefficients, Debye- Huckel Theory of the structure of dilute ionic solution, charge density and electrical potential. Properties of ionic cloud, activity coefficients from Debye-Huckel theory. Limiting law and its verification. Debye-Huckel theory to more concentrated solutions. Partial molar quantities of electrolytic solutions, determination of partial molar volume.

# IV Statistical Thermodynamics:

Quantum states and complexions. The combinatory rule, system with definite total energy. Degeneracy of energy levels, probability and most probable distribution, in distinguishability, Maxwell-Boltzmann statistics, partition function, translational, rotational, vibrational, nuclear and electronic partition functions. Internal energy and heat capacity in terms of partition function.

# V Chemistry of Macromolecules:

VI

Introduction, type of polymers. Step polymerization, kinetics of step polymerization.

Statistical approach to Gelation, Molecular weight distribution in linear poly condensation (Derivation of size distribution), Molecular weight averages. Methods of determining molecular weight by osmotic pressure, light scattering, sedimentation and viscosity methods.

Solid State: Crystal structures, Bragg's law and applications. Band structure of solid.

#### **Paper Name: Polymer Chemistry**

**Paper CODE: B020707T** Marks: 100 (ETE 75 & CIE 25)

#### I. Basics

Importance of polymers, basic concepts :monomers, degree of polymerization. Linear branched and network polymers. Classification of polymers. Polymerization: condensation, addition/radical chain-ionic and co-ordination and copolymerization. Polymerization conditions and polymer reactions. Polymerization in homogeneous and heterogeneous systems.

#### II. Polymer Characterization

Polydispersion-average molecular weight concept. Number, weight and viscosity average molecular weights. Polydispersity and molecular weight distribution. The practical significance of molecular weight. Measurement of molecular-weights. Endgroup, viscosity, light scattering, osmotic and ultracentrifugation methods.

## III. Analysis and testing of polymers

Chemical analysis of polymers, spectroscopic methods, X-ray diffraction study. Thermal analysis and physical testing-tensile strength. Fatigue, impact tear resistance, hardness and abrasion resistance.

#### IV. Inorganic Polymers

A general survey and scope of inorganic polymers special characteristics, classification, homo and hetero atomic polymers. Structure, properties and applications of (1) Polymers based on boron-borazines, boranes and carboranes. (2) Polymers based on silicon, silicones, polymetalloxanes and polymetallosiloxanes, silazanes.

# V. Structure, Properties and Application of

- Polymers based on Phosphorous-Phosphazenes, Polyphosphates.
- Polymers based on Sulphur-tetrasulphurtetranitride and related compounds.
- Co-ordination and metal chelate polymers.

Paper Name: Techniques of Chemistry -I

**Paper CODE: B020708T**Marks: 100 (ETE 75 & CIE 25)

#### 1. Data handling in Analysis:

Accuracy and precision. Errors, determinate and indeterminate errors, significant figures. Rounding off figures, standard deviation, regression analysis.

#### 2. Separation Techniques:

Principles and applications of solvent extraction. Quantitative treatments of extraction equilibria. Solvent extraction of metals. Solid phase extraction.

# 3. Chromatography:

Introduction, principle, and experimental setup of chromatography. Partition and Adsorption chromatography: Principle of partition and adsorption chromatography. Mobile and stationary phases. liquid-liquid, gas-liquid, gas-solid and liquid-solid chromatography. Reversed phase partition chromatography, paper and thin layer chromatography Applications of partition and adsorption chromatography., HPLC.

#### 4. Ion Exchange resins:

Mechanism of ion exchange. Factors affecting the selection of ion exchange resins. Techniques in ion exchange methods and analytical applications.

#### 5. Spot tests:

Spot tests for metal ions, spot tests for identification of functional groups-hydroxyl, carboxylic, nitro, nitroso, azo and amino.

#### 6. Thermal Methods of Analysis:

Principle, methodology and applications: Thermogravimetric and differential thermal Analysis, thermometric titrations. Thermal stability of polymers. Decomposition Pattern and decomposition reactions- examples.

**Paper Name: Medicinal Chemistry** 

**Paper CODE: B020709T** Marks: 100 (ETE 75 & CIE 25)

#### I. Drug Design

Development of new drugs, procedures followed in drug design, concept of lead compound and end modification, concepts of prodrugs and soft drugs, structure-activity relationship (SAR). Factors affecting bioactivity: Theories of drugs activity- occupancy theory, rate theory, induced fit theory. Quantitative structure activity relationship. History and development of QSAR. Concepts of drugs receptors and drug receptors. Elementary treatment of drug interactions. Physico-chemical parameters: lipophilicity, partition coefficient, electronic ionization constants, steric, Shelton surface activity parameter and redox potentials. LD-50, ED-50 (Mathematical derivations of equations excluded). Basic ideas about Pharmacokinetics and Pharmacodynamics.

II. Antineoplastic Agents

Introduction, cancer chemotherapy. Role of alkylating agents and antimetabolites in treatment of cancer. Mention of carcinolytic antibiotics and mitoptic inhibitors. Synthesis of mechlorethamine, mustards and 6- mercaptopurine. Recent developments in cancer chemotherapy.

III. Cardiovascular Drugs

Introduction, cardiovascular diseases, drug inhibitors of peripheral sympathetic function. Central intervention of cardiovascular output. Direct acting arteriolar dilators. Synthesis of amyl nitrate, hydrolaxine methyldopa and diazoxide propanol.

IV. Local Anti-infective Drugs

Anti-tubercular drugs and Anti-malerial drugs: Introduction and general mode of action. Synthesis of sulphonamides, norfloxacin, dapsone, chloroquin and primaquin.

V. Psychoactive Drugs-The Chemotherapy of mind

CNS depressants, general anesthetics, mode of action, hypnotics, sedatives, anti-anxiety drugs, benzodiazepines, antipsychotic drugs. Synthesis of diazepam, alprazolam and barbiturates.

VI. Antibiotics

General introduction, structure and synthesis of penicillin G & chloramphenicol.

#### VI. Metals in Medicines

Metal deficiency and diseases, toxic effects of metals, metals for diagnosis and chemotherapy.