

CHAITANYA SCIENCE AND ARTS COLLEGE
(AUTONOMOUS)
PAMGARH, JANJGIR-CHAMPA (C.G.)



ACCREDITED "A" GRADE BY NAAC

**DEPARTMENT
OF
CHEMISTRY**

**COURSE CURRICULUM & MARKING SCHEME
POSTGRADUATE PROGRAMME
M.Sc. Chemistry**

**PROGRAM CODE: CCMS01
FIRST & SECOND SEMESTER**

Approved By	Board of Studies	Academic Council
Date	30/08/2025	04 SEP 2025

ACADEMIC YEAR 2025-26

**SYLLABUS FRAMED ACCORDING TO THE NEP-2020
UNDER THE SCHEME OF CBCS (CHOICE BASED CREDIT SYSTEM)**

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DEPARTMENT OF CHEMISTRY
CHAITANYA SCIENCE AND ARTS COLLEGE
PAMGARH, DISTT. - JANJGIR-CHAMPA (C.G.)
(AN AUTONOMOUS COLLEGE)

DEPARTMENT OF CHEMISTRY

M.Sc. (CHEMISTRY) PROGRAM CODE: CCMS01

Program Outcome (PO)

Upon completion of the M.Sc. (Chemistry) Program, the students will be able to:

- PO1: Knowledge:** Acquire an overview of concepts, fundamentals and advancements of science across a range of fields, with in-depth knowledge in at least one area of study. Develop focused field knowledge and amalgamate knowledge across different disciplines.
- PO2: Complementary skills:** Students will be able to engage in critical investigation through principal approaches or methods and through effective information search and evaluation strategies. Employ highly developed conceptual, analytical, quantitative and technical skills and are adept with a range of technologies
- PO3: Applied learning:** Students will be able to apply disciplinary or interdisciplinary learning across multiple contexts, integrating knowledge and practice. Recognize the need for information; effectively search for, evaluate, manage and apply that information in support of scientific investigation or scholarly debate
- PO4: Communication:** Communicate effectively on scientific achievements, basic concepts and recent developments with experts and with society at large. Able to comprehend and write reports, documents, make effective presentations by oral and/or written form.
- PO5: Problem-solving:** Investigate, design and apply appropriate methods to solve problems in science, mathematics, technology and/or engineering.
- PO6: Environment and sustainability:** Understand the impact of the solutions in ethical, societal and environmental contexts and demonstrate the knowledge of and need for sustainable development.
- PO7: Teamwork, collaborative and management skills:** Recognize the opportunities and contribute positively in collaborative scientific research. Engage in intellectual exchange of ideas with researchers of other disciplines to address important research issues

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Program Specific Outcome (PSO)

Upon completion of the M.Sc. (Chemistry) Program, the students will be able to:

PSO1: Understand and explain the fundamental concepts in Physical Chemistry, Organic Chemistry, Inorganic Chemistry, Analytical Chemistry and its application.

PSO2: Apply various concepts, interpret/derive/deduce expressions, reaction mechanism, structure etc.

PSO3: Solve problems/numerical using basic chemistry knowledge and concepts.

PSO4: Carry out advanced experiments, investigate and explore through projects, record the observations, present the inference/results and discuss/interpret the result.

Johnson

R. Sub

Sharma

Elum

Reddy

DEPARTMENT OF CHEMISTRY
M.Sc. (CHEMISTRY) PROGRAM CODE: CCMS01 BOARD OF STUDIES ACADEMIC
YEAR: 2025-26

The syllabus for M.Sc. (Chemistry) I & II semester is hereby approved for the academic year 2025-26

Scheme of M. Sc. Chemistry under Semester System
Program Code: CCMS01

Session 2024-25

Semester	Course Code	Course Name	Credit			Total Credit	Marks			
			L	T	P		ESE	CIA	Total	
									MAX	MIN
First	MCHT101	Coordination Chemistry	3	1	-	4	70	30	100	40
	MCHT102	Concepts in Organic Chemistry	3	1	-	4	70	30	100	40
	MCHT103	Mathematics for Chemists, Quantum Chemistry and Chemical Dynamics	3	1	-	4	70	30	100	40
	MCHT104	Group Theory and Computer for Chemists	3	1	-	4	70	30	100	40
	MCHP101	Lab Course I: Inorganic Chemistry	-	-	2	2	-	-	100	40
	MCHP102	Lab Course II: Physical Chemistry	-	-	2	2	-	-	100	40
		Subtotal				20	280	120	600	-
Second	MCHT201	Transition Metal Complexes and Diffraction Methods	3	1	-	4	70	30	100	40
	MCHT202	Organic Reaction Mechanism	3	1	-	4	70	30	100	40
	MCHT203	Thermodynamics, Electrochemistry And Surface Chemistry	3	1	-	4	70	30	100	40
	MCHT204	Spectroscopy	3	1	-	4	70	30	100	40
	MCHP201	Lab Course I: Organic Chemistry	-	-	2	2	-	-	100	40
	MCHP202 A OR MCHP202 B	Lab Course II: Analytical Chemistry OR Social outreach & Skill development field work	-	-	2	2	-	-	100	40
		Subtotal				20	280	120	600	-

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Program	CCMS01, M.Sc. CHEMISTRY	Semester	I
Course Code	MCHT101	Paper	I
Course Title	COORDINATION CHEMISTRY		
Course Type	Theory		
Course Outcomes	<p>CO1: To understand Walsh diagram, bent rule, energetics of hybridization and MOT.</p> <p>CO2: To know structure of carbonyls, nitrosyls, dinitrogen and dioxygen complexes.</p> <p>CO3: To understand energy profile of a reaction and determination of stability constant of transition metal complexes.</p> <p>CO4: To know mechanism and kinetics of substitution and electron transfer reaction in complexes.</p>		
Credit Value	4		
Total Marks	CIA: 30, ESE: 70, Min Passing Marks: 40		

Unit	Contents	Total Hours
I	<p>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,</p> <p>Metal π-Ligand Bonding Limitation of crystal field theory, Jahn-Teller distortions, molecular orbital theory, octahedral, tetrahedral and square planar complexes, Nephelauxetic series, π bonding and molecular orbital theory.</p>	15
II	<p>Metal π-Complexes Metal carbonyls, structure and bonding, vibrational spectra of metal carbonyls for bonding and structural elucidation, important reactions of metal carbonyls.</p> <p>Nitrosyl: Preparation, bonding, structure & important reactions of transition metal nitrosyl, dinitrogen complexes, tertiary phosphine as ligand important reactions of metal carbonyls; preparation, bonding, structure and important reactions of transition metal nitrosyl, dinitrogen and dioxygen complexes.</p>	15
III	<p>Metal Ligand Equilibria in Solution Stepwise and overall formation constants and their interaction, trends in stepwise constants, factors affecting the stability of metal complexes. nature of metal ion and ligand, chelate effect and its thermodynamic origin. Energy profile of a reaction, reactivity of metal complexes, inert and labile complexes, determination of</p>	15

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	binary formation constants by pH- metry and spectrophotometry	
IV	Reaction Mechanism of Transition Metal Complexes Kinetics of octahedral substitution, acid hydrolysis, factors affecting acid hydrolysis, base hydrolysis, conjugate base mechanism, direct and indirect evidence in favor of conjugate mechanism, anation reactions, reactions without metal ligand bond cleavage. Substitution reactions in square planar complexes, the trans effect and its theories, mechanism of the substitution reaction. Redox reactions, electron transfer reactions, mechanism of one electron transfer reactions, outer sphere type reaction, cross reactions and Marcus-Hush theory, inner sphere type reactions.	15
Total No. of Lectures		60

List of Reference Books:

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. Earnshaw, Pergamon.
4. Inorganic Electronic Spectroscopy, A.B.P. Lever, Elsevier.
5. Comprehensive Coordination Chemistry eds., G. Wilkinson, R.D. Gillars and I.A. McCleverty, Pergamon.
6. Mechanisms of Inorganic Reactions, Fred Basalo and Ralph G. Pearson, Wiley Eastern Private Ltd

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Program	CCMS01, M.Sc. CHEMISTRY	Semester	I
Course Code	MCHT102	Paper	II
Course Title	CONCEPTS IN ORGANIC CHEMISTRY		
Course Type	Theory		
Course Outcomes	<p>CO1: Recognize and distinguish between aromatic and antiaromatic compounds by their structures.</p> <p>CO2: Explain different free radicals and mechanisms of different rearrangements via free radicals.</p> <p>CO3: Learn the terminology associated with conformational analysis and stereochemistry of various compounds</p> <p>CO4: Know the basic concept of different types of pericyclic reactions and rules governing them.</p>		
Credit Value	4		
Total Marks	CIA: 30, ESE: 70, Min Passing Marks: 40		

Unit	Contents	Total Hours
I	<p>Nature of Bonding in Organic Molecules Localized and delocalized chemical bond, conjugation and cross conjugation, bonding in fullerenes, Bonds weaker than covalent bond-addition compounds, crown ether complexes and cryptands, inclusion compounds, rotaxanes and catenanes.</p> <p>Aromaticity Aromaticity in benzenoid and non- benzenoid compounds, alternant and non- alternant hydrocarbons, Huckel's rule, energy level of molecular orbitals, annulenes, antiaromaticity, homo-aromaticity, PMO approach.</p>	15
II	<p>Free Radical Reactions Types of free radical reactions, free radical substitution mechanism at an Aromatic substrate, neighboring 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 compound by diazonium salts, Sandmeyer reaction. Free radical rearrangement, Hunsdiecker reaction</p>	15

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III	<p>Conformational analysis Conformational analysis of cycloalkanes, decalins, effect of conformation on reactivity, conformation of sugars, steric strain due to unavoidable crowding.</p> <p>Stereochemistry of Organic Compounds Elements of symmetry, chirality, 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.</p>	15
IV	<p>Pericyclic Reactions Molecular orbital symmetry, Frontier orbitals of ethylene, 1,3-butadiene, 1,3,5-hexatriene and allyl system. Classification of pericyclic reactions. Woodward-Hoffman correlation diagrams. FMO and PMO approach. Electrocyclic reactions- conrotatory and disrotatory motions, $4n$, $4n+2$ and allyl systems. Cycloadditions-antarafacial and suprafacial additions, $4n$ and $4n+2$ systems, 2+2 addition of ketenes. Sigma tropic rearrangements, suprafacial and antarafacial shifts of H, sigma tropic shifts involving carbon moieties, 3, 3-and 5,5-sigmatropic rearrangements. Claisen, Cope and aza-Cope rearrangements.</p>	15
Total No. of Lectures		60

List of Reference Books:

1. Advanced Organic Chemistry — Reaction Mechanism and Structure, Jerry March John Wiley.
2. Advanced Organic Chemistry, F.A. Carey and R.J. Sundbery, Plenum
3. Structure and Mechanism in Organic Chemistry, C.K. Ingold, Cornell University Press.
4. Organic Chemistry, R. T. Morrison and R.N. Boyd, Prentice Hall.
5. Modern Organic Reactions. H.O. House Benjamin
6. Principles of Organic Synthesis, R.O.C. Normon and &professional.
7. Pericyclic reactions, S.M. Mukherji, Macmillan India.
8. Reaction Mechanism in Organic Chemistry, S.M. Macmillan J.M. Coxon, Blackie, Academic Mukherji and S.P. Singh,
9. Stereo Chemistry of Organic Compounds, D. Nasipuri, New Age International.
10. Stereo Chemistry of Organic Compounds, P.S. Kalsi, New Age International.
11. Organic Chemistry, I.L.Finar, Vol. I & II, ELBS.

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Program	CCMS01, M.Sc. CHEMISTRY	Semester	I
Course Code	MCHT103	Paper	III
Course Title	MATHEMATICS FOR CHEMISTS, QUANTUM CHEMISTRY AND THERMODYNAMICS		
Course Type	Theory		
Course Outcomes	<p>CO1: To have basic knowledge of mathematics – vector, matrix algebra, probability, calculus and its application in chemistry which adds value to the program.</p> <p>CO2: To understand the basic postulates of quantum mechanics and solve Schrodinger wave equation for quantum mechanical models variation theorem, perturbation theory and Huckel MO theory and its application.</p> <p>CO3: To discuss the quantum mechanical aspect of angular momentum and spin, Russell-Saunders terms and coupling schemes, atomic states, atomic terms and evaluate term symbols.</p> <p>CO4: To describe different theories of reaction rates, fast reactions and its methods, kinetics and mechanism of photochemical and unimolecular reactions.</p>		
Credit Value	4		
Total Marks	CIA: 30, ESE: 70, Min Passing Marks: 40		

Unit	Contents	Total Hours
I	<p>Vectors, Matrix Algebra and Probability Vectors, dot, cross and triple products. The gradient, divergence and curl. Addition and multiplication; inverse, adjoint and transpose of matrices. Introduction to determinants.</p> <p>Calculus Rules for differentiation, applications of differential calculus including maxima and minima, partial differentiation. Basic rules for integration, integration by algebraic simplification, integration by parts, partial fraction and substitution.</p>	15

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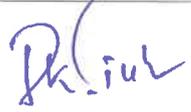
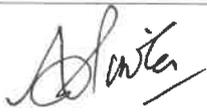
II	<p>Quantum Chemistry Time-independent Schrodinger equation and the postulates of quantum mechanics. Discussion of solutions of the Schrodinger equation to some model systems viz. particle in one-dimensional and three dimensional box, the concept of degeneracy, the harmonic oscillator, the rigid rotors, the hydrogen atom.</p> <p>Approximate Methods The variation method and perturbation theory (first order and non degenerate). Applications of variation method and perturbation theory to hydrogen and helium atom.</p>	15
III	<p>Angular Momentum Ordinary angular momentum, eigen functions and eigen values of angular momentum, ladder operator, the concept of spin, antisymmetric wave functions and Pauli's exclusion principle.</p> <p>Electronic Structure of Atoms Russell-Saunders terms and coupling schemes. Atomic states, atomic terms and term symbols.</p> <p>Molecular Orbital Theory Huckel theory of conjugated systems, Applications to ethylene, butadiene and cyclobutadiene.</p>	15
IV	<p>Classical Thermodynamics Maxwell relations, Partial molar properties- concept, its significance and methods of determination, Concept of chemical Potential, Gibbs Duhem Equation, variation of chemical potential with temperature and pressure. Concept of fugacity, its significance and methods of determination. Non-ideal systems: excess functions for non-ideal solutions. Concept of activity and activity coefficient. Application of phase rule to three component systems: solid-liquid system and liquid-liquid system, salting out effect.</p>	15
Total No. of Lectures		60

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List of Reference Books:

1. Physical Chemistry, P.W. Atkins, ELBS
2. Introduction to Quantum Chemistry, A.K. Chandra, Tata McGraw Hill
3. Quantum Chemistry, Ira N. Levine, Prentice Hall
4. Coulsons Valence R. Me. Weeny, ELBS
5. Thermodynamics, S. Glasstone
6. Mathematical Preparation for Physical Chemistry, F. Daniels, McGraw Hill.
7. Mathematics for Chemists, Bhupendra Singh

    
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Program	CCMS01, M.Sc. CHEMISTRY	Semester	I
Course Code	MCHT104	Paper	IV
Course Title	GROUP THEORY AND COMPUTERS FOR CHEMISTS		
Course Type	Theory		
Course Outcomes	<p>CO1: To understand symmetry properties of compounds, character tables and their uses in spectroscopy.</p> <p>CO2: To know principles involved in interaction of electromagnetic radiation with matter.</p> <p>CO3: To understand basic structure of computers, memory and operating systems and 'C' language.</p> <p>CO4: To learn development of small computer codes involving simple formula in chemistry.</p>		
Credit Value	4		
Total Marks	CIA: 30, ESE: 70, Min Passing Marks: 40		

Unit	Contents	Total Hours
I	<p>Symmetry and Group Theory in Chemistry</p> <p>Symmetry elements and symmetry operation, definition of group, subgroup, relation between order of a finite group and its subgroup. Conjugacy relation and classes. point symmetry group. Schon flies symbols, representations of groups by matrices (representation for the C_n, C_{nv}, C_{nh}, D_{nh} etc. groups to be worked out explicitly). Character of a representation. The great orthogonality theorem (without proof) and its importance. Character tables and their uses in spectroscopy.</p>	15
II	<p>Unifying Principles</p> <p>Electromagnetic radiation, interaction of electromagnetic radiation with matter absorption, emission, transmission, reflection, refraction, dispersion, polarization and scattering. Uncertainty relation and natural line width and natural line broadening, transition probability, results of the time dependent perturbation theory, transmission moment, selection rules, intensity of spectral lines. Born-Oppenheimer approximation, rotational, vibrational and electronic energy levels.</p>	15

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III	Introduction to Computers and Computing Basic structure and functioning of computers with a PC as an illustrative example. Memory, I/O devices. Secondary storage. Computer languages. Operating systems with DOS as an example. Introduction to UNIX and WINDOWS Data processing, principles of programming. Algorithms and flow- charts. Elements of computer language 'C'. Constants and variables. Operations and symbols. Expressions. Arithmetic assignment statement.	15
IV	Computer Programming in 'C' Language Input and Output. Format statement. Termination statements. Branching statements such as IF or GO TO statement. LOGICAL variables. Double precision variables. Subscripted variables and DIMENSION DO statement. FUNCTION and SUBROUTINE. COMMON and DATA Statements. Development of small computer codes involving simple formula in Chemistry, such as Vander Waals equation, pH titration, Kinetics, radioactive decay. Evaluation of lattice energy and ionic radii from experimental data.	15
Total No. of Lectures		60

List of Reference Books:

1. Computers and Common Sense, R. Hunt and J. Shelley Prentice Hall.
2. Computers Chemistry, A.C. Norris.
3. Microcomputer Quantum Mechanics, Killingbeck, Adam Hilger.
4. Computer Programming in FORTRAN IV, V Rajaraman, Prentice Hall
5. An Introduction to Digital Computer Design. V. Rajaraman and T. Radhakrishnan, Prentice Hall.
6. Physical Methods in Chemistry, R.S. Drago, Saunders College
7. Chemical Applications of Group Theory F.A. Cotton.

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Program	CCMS01, M.Sc. CHEMISTRY	Semester	I
Course Code	MCHP101	Paper	L-I
Course Title	INORGANIC CHEMISTRY		
Course Type	Laboratory		
Credit Value	2		
Total Marks	ESE: 100, Min Passing Marks: 40		

MAJOR EXPERIMENTS

Qualitative analysis

Qualitative analysis of mixture containing eight radicals including two less common metals from among the following by semi micro method.

Basic Radicals:

Ag, Pb, Hg Bi, Cu, Cd, As, Sb, Sn, Fe, Al, Cr, Zn, Mn, Co, Ni, Ba, Sr, Ca, Mg, Na, K, Ce, Th, Zr, W, Te, Ti, Mo, U, V, Be, Li, Au, Pt.

Acidic Radicals:

Carbonate, Sulphite, Sulphide, Nitrite, Nitrate, Acetate, Fluoride, Chloride, Bromide, Iodide, Sulphate, Borate, Oxalate, Phosphate, Silicate, Thiosulphate, Ferricyanide, Sulphocyanide, Chromate, Arsinat and Permanganate.

Quantitative Analysis

Separation and determination of two metal ions in ores, alloys, or mixtures in solution, one by volumetric and the other by gravimetric methods.

MINOR EXPERIMENTS

Estimations

- Phosphoric acid in commercial orthophosphoric acid.
- Boric acid in borax.
- Ammonia in an ammonium salt.
- Manganese dioxide in pyrolusite.
- Available chlorine in bleaching powder.
- Hydrogen peroxide in a commercial sample.

Preparations

Preparation of selected inorganic compounds and their study by I.R. Electronic spectra, Mossbauer, E.S.R. and magnetic susceptibility measurements, Handling of air and moisture sensitive compounds. Theoretical study of structure and their identification of some preparations by spectral analysis

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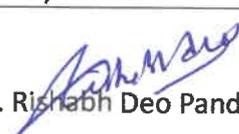
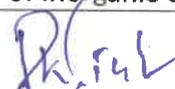
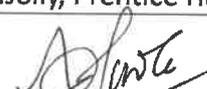
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2. $\text{TiO}(\text{C}_9\text{H}_8\text{NO})_2 \cdot 2\text{H}_2\text{O}$
 3. $\text{Cis-K}[\text{Cr}(\text{C}_2\text{O}_4)_2(\text{H}_2\text{O})_2]$
 4. $\text{Na}[\text{Cr}(\text{NH}_3)_2(\text{SCN})_4]$
 5. $\text{Mn}(\text{acac})_3$
 6. $\text{K}_3[\text{Fe}(\text{C}_2\text{O}_4)_3]$
 7. Prussian Blue, Turnbull's Blue.
 8. $[\text{Co}(\text{NH}_3)_6][\text{Co}(\text{NO}_2)_6]$
 9. $\text{Cis-}[\text{Co}(\text{trien})(\text{NO}_2)_2]\text{Cl} \cdot \text{H}_2\text{O}$
 10. $\text{Hg}[\text{Co}(\text{SCN})_4]$
 11. $[\text{Co}(\text{Py})_2\text{Cl}_2]$
 12. $[\text{Ni}(\text{NH}_3)_6]\text{Cl}_2$
 13. $\text{Ni}(\text{DMG})_2$
- $[\text{Cu}(\text{NH}_3)_4]\text{SO}_4 \cdot \text{H}_2\text{O}$

List of Reference Books:

1. Vogel's Text Book of Qualitative Analysis, revised, J. Bassett, R.C. Denney, G.H. Jeffery and J. Mendham, ELBS.
2. Synthesis and Characterization of Inorganic Compounds, W.L. Jolly, Prentice Hall.

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Program	CCMS01, M.Sc. CHEMISTRY	Semester	I
Course Code	MCHP102	Paper	LII
Course Title	PHYSICAL CHEMISTRY		
Course Type	Laboratory		
Credit Value	2		
Total Marks	ESE: 100, Min Passing Marks: 40		

MAJOR EXPERIMENTS

Adsorption

1. To study surface tension — concentration relationship for solution (Gibb's equation).
2. To study the adsorption of oxalic acid on charcoal and to verify Freundlich adsorption isotherm.

Chemical Kinetics

1. Determination of the effect of (a) Change of temperature (b) Change of concentration of reactants and catalyst and (c) ionic strength of the media on the velocity constant of hydrolysis of an ester/ionic reactions.
2. Determination of the rate constant for the oxidation of iodide ions by hydrogen peroxide studying the kinetics as an iodine clock reaction.

Spectrophotometry

1. Verification of Lambert- Beer Law. Determination of metal ions e.g. Fe, Cu, Zn, Pb etc. using inorganic reagents and organic chelating agent.

MINOR EXPERIMENTS

Phase Equilibria

1. Determination of congruent composition and temperature of a binary system (e.g. diphenylamine- benzophenone system.)
2. Determination of glass transition temperature of a given salt (e.g., CaCl₂)
3. To construct the phase diagram for three component system (e.g., chloroform —acetic acid- water).

Solutions

1. Determination of molecular weight of non-electrolyte/electrolyte by cryoscopic method and to determine the activity coefficient of an electrolyte.
2. Determination of molecular weight of non-volatile substances by Landsberger's method.

Conductometry/Colorimeter

1. To determine the basicity of an organic acid.
2. Determination of solubility and solubility product of sparingly soluble salts (e.g. PbSO₄, BaSO₄) conductometrically.

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3. Determination of the strength of strong and weak acids in a given mixture conductometrically.
4. Determination of pK_a of acetic acid and verification of Ostwald Dilution law

Potentiometry/pH metry

1. Determination of the strength of strong and weak acids in a given mixture using a potentiometer /pH meter.
2. Determination of temperature dependence of EMF of a cell.
3. To determine pK_a of the given monobasic acid by pH metric titration.

Determination of the dissociation constant of monobasic/dibasic acid by Albert- Serjeant method.

List of Reference Books:

1. Practical Physical Chemistry, A.M. James and F.E. Prichard, Longman.
2. Findley's Practical Physical Chemistry, B.Plevitt, Longman.
3. Experimental Physical Chemistry ,R.C.Das and B. Behra, Tata McGraw Hill.

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Program	CCMS01, M.Sc. CHEMISTRY	Semester	II
Course Code	MCHT201	Paper	I
Course Title	TRANSITION METAL COMPLEXES AND DIFFRACTION METHODS		
Course Type	Theory		
Course Outcomes	CO1: To understand how to interpret electronic spectra of complexes. CO2: To know magnetic properties of complexes of different geometry. CO3: To understand principle of X-ray diffraction and their uses in structure determination of compounds. CO4: To understand metal cluster and metal polyacids.		
Credit Value	4		
Total Marks	CIA: 30, ESE: 70, Min Passing Marks: 40		

Unit	Contents	Total Hours
I	Electronic Spectra of Transition Metal Complexes Spectroscopic ground states, correlation, Orgel and Tanabe-Sugano diagrams for transition metal complexes (d^1 - d^9 states), calculations of Dq , B and parameters, charge transfer spectra, spectroscopic method of assignment of absolute configuration in optically active metal chelates and their stereochemical information.	15
II	Magnetic Properties of Transition Metal Complexes Magnetic properties of octahedral, tetrahedral, tetragonally distorted square planar, trigonal bipyramidal and square bipyramidal complexes based on CFT, spin equilibrium, spin free and spin paired equilibria, quenching of orbital angular momentum by ligand field, Magnetic properties of complexes with A, E and T terms, spin orbit coupling.	15
III	X-Ray diffraction Bragg condition, Miller indices, Diffraction methods-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, Ramchandran Diagram.	15

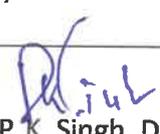
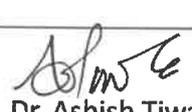
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IV	Metal clusters Higher boranes, carboranes, metallo boranes and metallocarboranes. Metal carbonyls and halide clusters, compounds with metal-metal multiple bonds. Isopoly and Heteropoly Acids and Salts Preparation, properties and structure of isopoly and heteropoly acids of molybdenum and tungsten.	15
	Total No. of Lectures	60

List of Reference Books:

1. Advanced Inorganic Chemistry, F.A. Cotton and Wilkinson, John Wiley.
2. Inorganic Chemistry, J.E. Huheey, Harpes & Row.
3. Chemistry of the Elements, N.N. Greenwood and A. Earnshaw, Pergamon.
4. Inorganic Electronic Spectroscopy, A.B.P. Lever, Elsevier.
5. Magnetochemistry, R.L. Carlin, Springer Verlag.
6. Comprehensive Coordination Chemistry eds., G. Wilkinson, R.D. Gillars and J.A.
7. McCleverty, Pergamon.
8. Modern spectroscopy, J. M. Hollas, John Wiley.
9. Applied electron spectroscopy for chemical analysis Ed. H. Windawi and F.L. Ho, Wiley Inter science.


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Program	CCMS01, M.Sc. CHEMISTRY	Semester	II
Course Code	MCHT202	Paper	II
Course Title	ORGANIC REACTION MECHANISM		
Course Type	Theory		
Course Outcomes	<p>CO1: To understand the basic concepts and explain the mechanism and stereochemical aspects of elimination reactions.</p> <p>CO2: To understand the mechanism and stereochemistry of nucleophilic substitution reactions.</p> <p>CO3: To acquire the knowledge of mechanism of electrophilic substitution in aliphatic as well as aromatic compounds.</p> <p>CO4: To understand the mechanistic and stereochemical concepts of addition reactions.</p>		
Credit Value	4		
Total Marks	CIA: 30, ESE: 70, Min Passing Marks: 40		

Unit	Contents	Total Hours
I	<p>Reaction Mechanism : Structure and Reactivity Types of mechanism, types of reaction, thermodynamic and kinetic requirements, kinetic and thermodynamic control, Hammond's postulate, Curtin Hamnett principle, potential energy diagram, transition states, intermediates, methods of determining mechanism , isotopic effects. Effect of structure on reactivity - resonance and field effects, steric effects and quantitative treatment. The Hammett equation and linear free energy relationship, substituent and reaction constants, Taft equation.</p> <p>Elimination Reactions The E2, E1 and E1cB mechanisms. Orientation of the double bond. Reactivity -effects of substrate structures, attacking base, the leaving group and the medium. Mechanism and orientation in pyrolytic elimination.</p>	15

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II	<p>Aliphatic Nucleophilic Substitution The S_N1, S_N2, mixed S_N1 and S_N2 and SET mechanisms. The neighbouring group mechanism, neighbouring group participation by π and σ bonds. Classical and non-classical carbocations, norbornyl system, common carbocation rearrangements.</p> <p>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, regioselectivity.</p> <p>Aromatic Nucleophilic substitution 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.</p>	15
III	<p>Aliphatic Electrophilic substitution Bimolecular mechanisms SE_2, SE_i and SE_1 mechanism, electrophilic substitution accompanied by double bond shifts. Effect of substrates, leaving group and the solvent polarity on the reactivity.</p> <p>Aromatic Electrophilic substitution The arenium ion mechanism, orientation and reactivity, energy profile diagrams. The ortho/para ratio, ipso attack, diazonium coupling, Vilsmeier reaction.</p>	15
IV	<p>Addition to carbon - carbon multiple bonds Mechanistic and stereochemical aspects of addition reactions involving electrophiles, nucleophiles and free radicals, regio- and chemoselectivity, orientation and reactivity. Hydrogenation of aromatic rings, hydrogenation of double and triple bonds.</p> <p>Addition to Carbon-Hetero multiple bonds Mechanism of metal hydride reduction of saturated and unsaturated carbonyl compounds. Acids, esters and nitriles. Addition of Grignard reagent, organozinc and organolithium reagents to carbonyl and unsaturated carbonyl compounds, Wittig reaction. Mechanism of condensation reaction involving enolates — Claisen, Mannich, Benzoin, Perkin and Stobbe reactions.</p>	15
Total No. of Lectures		60





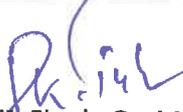


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List of Reference Books:

1. Advanced Organic Chemistry — Reaction Mechanism and Structure, Jerry March John Wiley.
2. Advanced Organic Chemistry, F.A. Carey and R.J. Sundbery, Plenum
3. Structure and Mechanism in Organic Chemistry, C.K. Ingold, Cornell University Press.
4. Organic Chemistry, R.T. Morrison and R.N. Boyd, Prentice Hall.
5. Modern organic Reactions. H.O. House Benjamin
6. Principles of Organic Synthesis, R.O.C. Normon and J.M. Coxon, Blackie, Academic & Professional.
7. Organic Reactions and their mechanism, S. Kalsi, New Age International.
8. Reaction Mechanism in Organic Chemistry, S.M. Mukherji and S.P. Singh, Macmillan
9. Stereo Chemistry of Organic Compounds, D. Nasipuri, New Age International.

    
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Program	CCMS01, M.Sc. CHEMISTRY	Semester	II
Course Code	MCHT203	Paper	III
Course Title	CHEMICAL DYNAMICS, STATISTICAL THERMODYNAMICS, ELECTROCHEMISTRY AND SURFACE CHEMISTRY		
Course Type	Theory		
Course Outcomes	<p>CO1: To have knowledge and understanding of basic concepts in classical thermodynamics – partial molar properties, fugacity, activity and activity coefficient, construct and apply phase diagrams to 3-component systems.</p> <p>CO2: To illustrate the concepts in statistical thermodynamics – distribution, thermodynamic probability, partition function and its application and to compare various statistics. fundamental concepts of irreversible thermodynamics and discuss the application of its laws.</p> <p>CO3: To explain and derive equations related to the theory of strong electrolytes – Debye- Huckel law and its extensions, structure/models and thermodynamics of electrified interfaces, polarography and its applications.</p> <p>CO4: To describe and interpret various adsorption isotherms and its applications, concept and various aspects of micelles and macromolecules.</p>		
Credit Value	4		
Total Marks	CIA: 30, ESE: 70, Min Passing Marks: 40		

Unit	Contents	Total Hours
I	<p>Chemical Dynamics</p> <p>Methods of determining rate laws, Arrhenius equation, collision theory of reaction rates, steric factor, activated complex theory, kinetic salt effects, steady state kinetics. Photochemical reactions (Hydrogen-bromine and hydrogen-chlorine reactions), kinetics of enzyme reactions, fast reactions, study of fast reactions by flow method, flash photolysis and the nuclear magnetic resonance method. Dynamics of unimolecular reactions (Lindmann-Hinshelwood and Rice - Ramsperger- Kassel – Marcus [RRKM] theories of unimolecular reactions.</p>	15

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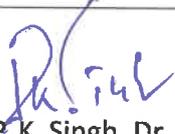
II	<p>Statistical Thermodynamics Concept of distribution, thermodynamic probability and most probable distribution. Maxwell Boltzmann distribution, Partition functions - translational, rotational, vibrational and electronic partition functions, calculation of thermodynamic properties in terms of partition functions. Applications of partitions functions, Fermi-Dirac statistics, Bose-Einstein statistics- distribution law.</p> <p>Non-equilibrium Thermodynamics Fundamental concepts, entropy production and entropy flow, phenomenological laws, Onsager's reciprocity relations, and irreversible thermodynamics for coupled reactions.</p>	15
III	<p>Electrochemistry Electrochemistry of solutions: ion- solvent interactions, Debye-Huckel theory for activity coefficient of electrolyte solutions, ionic strength, Debye-Huckel limiting law, Debye-Huckel-Onsager treatment and its extension.</p> <p>Thermodynamics of electrified interface equations: Derivation of electro-capillarity, Lippmann equations.</p> <p>Structure of electrified interfaces: Guoy-Chapman and Stern models. Over potentials, exchange current density, derivation of Butler-Volmer equation. Tafel plot. Polarography theory - Ilkovic equation, half wave potential and its significance.</p>	15
IV	<p>Surface Chemistry Adsorption Surface tension, capillary action, pressure difference across curved surface (Laplace equation), Gibbs adsorption isotherm, BET equation and estimation of surface area using BET equation.</p> <p>Micelles Surface active agents, classification of surface active agents, micellization, critical micellar concentration (CMC), factors affecting the CMC of surfactants, counter ion binding to micelles, thermodynamics of micellization, reverse micelles.</p> <p>Macromolecules Polymer: definition, types of polymers, free radical mechanism of polymerization, molecular mass, number and mass average molecular mass, molecular mass determination (osmometry, viscometry and sedimentation).</p>	15
Total No. of Lectures		60

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List of Reference Books:

1. Physical Chemistry, P.W. Atkins, ELBS
2. Chemical Kinetics, K.J. Laidler, McGraw-Hill
3. Statistical Thermodynamics, M.C.Gupta
4. Kinetics and Mechanism of Chemical Transformation, J. Rajaraman and J. Kuriacose, McMillan.
5. Chemical Thermodynamics, R.P. Rastogi & R.R. Mishra
6. Kinetics and Mechanism of Chemical Transformation, J. Rajaraman and J. Kuriacose, McMillan
7. Micelles, Theoretical and Applied Aspects, V. Moroi, Plenum
8. Modern Electrochemistry Vol.-I and Vol.-II, J.O.M. Bockris and A.K.N.Reddy, Plenum
9. Introduction to Polymer Science, V.R. Gowariker, N.V. Vishwanamanand J. Sridhar, Wiley Eastern.

    
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Program	CCMS01, M.Sc. CHEMISTRY	Semester	II
Course Code	MCHT204	Paper	IV
Course Title	SPECTROSCOPY		
Course Type	Theory		
Course Outcomes	<p>CO1: To gain insight into the basic principle of molecular spectra and discuss rigid rotor, energy levels, origin of rotational spectra and its applications.</p> <p>CO2: To understand the theories/principles, predict the functional groups and differentiate between IR and Raman spectra</p> <p>CO3: To acquire knowledge of principle, technique, interpretation and applications of NMR spectroscopy.</p> <p>CO4: To interpret the principle and applications of photo electron, photo acoustic and ESR spectroscopy.</p>		
Credit Value	4		
Total Marks	CIA: 30, ESE: 70, Min Passing Marks: 40		

Unit	Contents	Total Hours
I	<p>Molecular Spectroscopy Energy levels, molecular orbital, vibronic transitions, vibration progressions and geometry of the excited states, Franck - Condon principle, electronic spectra of polyatomic molecules. Emission spectra: radiative and non-radiative decay, internal conversion, spectra of transition metal complex, charge transfer spectra.</p> <p>Microwave Spectroscopy Classification of molecules, rigid rotor model, effect of isotopic substitution on the transition frequencies, intensities, non-rigid rotor. Stark effect, nuclear and electron spin interaction and effect of external field. Applications of microwave spectroscopy.</p>	15

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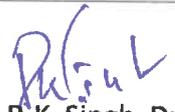
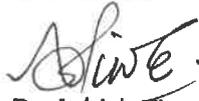
II	<p>Infrared spectroscopy Review of linear harmonic oscillator, vibrational energy of diatomic molecules, zero point energy, force constant and bond strengths, anharmonicity. Morse potential energy diagram, vibration – rotation Spectroscopy, P, Q, R, branches. Breakdown of Oppenheimer approximation, vibration of polyatomic molecules. Selection rules, normal modes of vibration, group frequencies, overtones, hot bands, factors affecting the band positions and intensities, far IR region, metal ligand vibrations, normal co-ordinate analysis.</p> <p>Raman Spectroscopy Classical and quantum theories of Raman effect- Pure rotational, vibrational and vibrational- rotational Raman spectra, selection rules, mutual exclusion principle. Resonance Raman Spectroscopy, coherent anti stokes Raman Spectroscopy (CARS)</p>	15
III	<p>Nuclear Magnetic Resonance Spectroscopy Nuclear spin, nuclear resonance, saturation, shielding of magnetic nuclei, chemical shift and its measurements, factors influencing chemical shift, deshielding, spin- spin interactions , factors including coupling constant 'J'. Classification (ABX, AMX, ABC, A₂B₂, etc), spin decoupling. Basic ideas about instruments, FT NMR, advantages of FT NMR, use of NMR in medical diagnostics.</p> <p>Nuclear Quadruple Resonance Spectroscopy Quadruple nuclei, Quadruple moments, electric field gradient, coupling constant, splitting, applications of NQR spectroscopy.</p>	15
IV	<p>Photoelectron Spectroscopy Basic principle: photo-electric effect, ionization process, Koopmans theorem, photoelectron spectra of simple molecules, ESCA, chemical information from ESCA.</p> <p>Photo acoustic Spectroscopy Basic principles of photo acoustic spectroscopy (PAS), PAS gases and condensed systems, chemical and surface applications.</p> <p>Electron Spin Resonance Spectroscopy Basic principles, zero field splitting and Kramer's degeneracy, factors affecting the 'g' value. Isotropic and anisotropic hyperfine coupling constants, spin Hamiltonian, spin densities and McConnell relationship, measurement techniques, applications of ESR spectroscopy.</p>	15
Total No. of Lectures		60

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List of Reference Books:

1. Modern Spectroscopy J.M. Hollas, Johan Wiley.
2. Applied Electron Spectroscopy for chemical analysis ed. H. Windawiand F.L. Ho, Wiley Inter science.
3. NMR, NQR EPR and Mossbauer Spectroscopy in Inorganic Chemistry, R.V. Parish. Elish Harwood.
4. Physical Methods in Chemistry, R.S. Drago, Saunders Company
5. Infrared and Raman Spectra: Inorganic and Coordination Compounds, K. Nakamoto, Wiley.
6. Spectroscopic Methods in Organic Chemistry, D.H. Williams, I. Fleming, Tata McGraw-Hill.
7. Application of Spectroscopy of Organic Compounds, J .R. Dyer, Prentice Hall.

    
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Program	CCMS01, M.Sc. CHEMISTRY	Semester	II
Course Code	MCHP201	Paper	L-I
Course Title	ORGANIC CHEMISTRY		
Course Type	Laboratory		
Credit Value	2		
Total Marks	ESE: 100, Min Passing Marks: 40		

MAJOR EXPERIMENTS

Organic Synthesis

1. Acetylation: Acetylation of cholesterol and separation of cholesteryl acetate by column chromatography.
2. Synthesis of 1,3-Naphthyl acetate / Hydroquinone diacetate.
3. Oxidation: Adipic acid by chromic acid oxidation of cyclohexanol
4. Grignard reaction: Synthesis of triphenylmethanol from benzoic acid
5. Aldol condensation :Dibenzalacetone from benzyldehyde
6. Sandmeyer reaction p-chlorotoluene from p-toluidine / o- chlorobenzoic acid from anthranilic acid.
7. Acetoacetic ester Condensation: Synthesis of ethyl-n-butylacetoacetateby A.E.E. condensation.
8. Cannizzaro reaction : 4- chlorobenzaldehyde as substrate / Benzoic acid and benzyl alcohol.
9. Friedel Crafts Reaction: 13-Benzoyl propionic acid from succinic anhydride and benzene.
10. Aromatic electrophilic substitutions: Synthesis of p-nitroaniline and bromoaniline. The products may be characterized by spectral techniques.

MINOR EXPERIMENTS

Qualitative Analysis

Separation, purification and identification of compounds of binary mixtures (solid-solid, liquid-solid) using TLC and column chromatography, chemical tests; IR spectra to be used for functional group identification.

List of Reference Books:

1. Practical Organic Chemistry by A.I. Vogel.
2. Practical Organic Chemistry by Mann and Saunders.
3. Practical Organic Chemistry by Garg and Salija.

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Program	CCMS01, M.Sc. CHEMISTRY	Semester	II
Course Code	MCHP201	Paper	LII
Course Title	ANALYTICAL AND COMPUTATIONAL CHEMISTRY		
Course Type	Laboratory		
Credit Value	2		
Total Marks	ESE: 100, Min Passing Marks: 40		

MAJOR EXPERIMENTS

Analytical Chemistry

Error Analysis & Statistical Data Analysis

Error, types of errors, minimization of errors, statistical treatment for error analysis, standard deviation, linear least squares. Calibration of volumetric apparatus, burettes, pipette, standard flask, weight box, etc.

Volumetric Analysis

Basic Principle

Determination of iodine and saponification values of oil sample. Determination of DO, COD, BOD. Hardness of water samples.

Chromatography

Separation of cations and anions by Paper chromatograph, Column chromatography

Flame Photometry / AAS / FIA

Determination of cations / anions and metal ions e.g. Na⁺, K⁺, Ca²⁺, SO₄²⁻, NO₂⁻, Fe, Mo, Ni, Cu, Zn, etc.

Spectrophotometry

Verification of Beer-Lambert law

Molar absorptivity calculation, plotting graph to obtain λ_{max} etc.

Effect of pH in aqueous coloured system.

Determination of metal ions e.g. Fe, Cu, Zn, Pb, etc. using inorganic reagent like SCN, an organic chelating agent like dithizone, cupferron, 8-hydroxyquinoline, etc. in aqueous / organic phase in the presence of surface active agents.

Nephelometry / Turbidimetry

Determination of chloride, sulphate, phosphate, turbidity, etc.

MINOR EXPERIMENTS

Use of Computer Programs

The students will learn how to operate a PC and how to run standard Programs with data preferably from physical Chemistry laboratory. Further, the student will operate Word Processing software such as WORDSTAR / MS-WORD.

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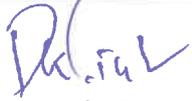
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Computational Chemistry

Introduction to structure drawing, spread sheet and chemistry related softwares. Brief description of computational methods: QSAR tools, *ab-initio*, semi empirical molecular mechanics. Introduction to SCF MO wave functions for open shell state RHF, ROHF and URHF methods. Basis sets TO and GTF. Introductory DFT, Z-matrix of simple molecules - H₂O, CO₂ and NH₃. Web resources.

List of Reference Books:

1. Computer and Common Sense, R. Hunt and J. Shelley, Prentice Hall.
2. Computational Chemistry, A.C. Norris.
3. Computer Programming in FORTRAN IV, V. Rajaraman, Prentice Hall.

    
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