DEPARTMENT OF CHEMISTRY

GOVT. DIGVIJAY PG AUTONOMOUS COLLEGE, RAJNANDGAON (C.G.)



M.Sc. Chemistry

Second Semester

2025-26

DEPARTMENT OF CHEMISTRY GOVT. DIGVIJAY PG AUTONOMOUS COLLEGE, RAJNANDGAON

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Syllabus and Marking Scheme for Second Semester Session 2025-26

Paper No.	Title of the Paper	Marks Allotted in Theory		Marks Allotted in Internal Assessment		Credits
		Max	Min	Max.	Min.	
I	TRANSITION METAL COMPLEXES AND DIFFRACTION METHODS	80	16	20	04	04
II	BIOMOLECULES AND STEREOCHEMISTRY	80	16	20	04	04
III	THERMODYNAMICS, ELECTROCHEMISTRY AND SURFACE CHEMISTRY	80	16	20	04	04
IV	SPECTROSCOPY	80	16	20	04	04
V	Lab Course I ORGANIC CHEMISTRY PRACTICAL	100	36			02
IV	Lab Course II ANALYTICAL CHEMISTRY & COMPUTER PRACTICAL	100	36			02
	Total	520		80		20

04 Theory papers

320

04 Internal Assessment

80

02 Practical

200

Total Marks

600

Note: 25 marks = 01 credit in Theory Papers and 50 Marks = 01 Credit in Practical

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SEMESTER - II

2025-26

PAPER-I

TRANSITION METAL COMPLEXES AND DIFFRACTION METHODS

Max. Marks:

80Min. Marks:

16

Unit-I Electronic Spectra of Transition Metal Complexes

Spectroscopic ground states, correlation, Orgel and Tanabe-Sugano diagrams for transition metal complexes (d¹-d⁹ 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.

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 equlibria, quenching of orbital angular momentum by ligand field, Magnetic properties of complexes with A, E and T terms, spin orbit coupling.

Unit -II: Metal clusters

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

Wade's rule, styx number, isolobal analogy, applications of boron compounds, synthesis and structures of S-N cyclic compounds

Unit - III: Lanthanoids and actinoids and Electron Diffraction

Introduction, occurrence, physical and chemical properties, electronic spectra and magnetic properties- oxidation states, term symbols, color transition, organometallic compounds and recent applications.

Electron Diffraction

Scattering intensity vs scattering angle, Wierl equation, measurement technique, elucidation of structure of simple gas phase molecules. Low energy electron diffraction and structure of surfaces.

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Unit-IV X-Ray Diffraction

Bragg condition, Miller indices, Laue method, Bragg method, Debye – Scherrer method of X-Ray structural analysis of crystals, index reflections, identification of unit cells from systematic absences in diffraction pattern. Structure of simple lattices and X-ray intensities, structure factor and its relation to intensity and electron density, phase problem. Ramchandran Diagram.

NeutronDiffraction

Scattering of neutrons by solid and liquids, magnetic scattering, measurement techniques. Elucidation of structure of magnetically ordered unit cell.

LIST OF REFERENCE BOOKS:

- 1. Advanced Inorganic Chemistry, F.A. Cotton and Wilkinson, JohnWiley.
- 2. Inorganic Chemistry, J.E. Huheey, Harpes&Row.
- 3. Chemistry of the Elements, N.N. Greenwood and A. Earnshow, Pergamon.
- 4. Inorganic Electronic Spectrosocopy, A.B.P. Lever, Elsevier.
- 5. Magnetochemistry, R.L. Carlin, SpringerVerlag.
- 6. Comprehensive Coordination Chemistry eds., G. Wilkinson, R.D. Gillars and J.A.

McCleverty, Pergamon.

- 7. Modern spectroscopy, J. M. Hollas, JohnWiley.
- 8. Applied electron spectroscopy for chemical analysis Ed. H. Windawi and F.L. Ho, Wiley Interscience.

	Departmental members	
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Chairperson /H.O.D	a . We i genier	N
Subject Expert A Aluri	1	8
(University Nominee)	2	9
Subject Expert.	3	10
Representative	4	11
(Industry)	5	12
Representative	6	13
(Alumni)	7	14
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(Professor Science Faculty Other Dept.)		- company of the second

SEMESTER - II

2025-26

PAPER- II

REACTIONMECHANISM, REARRENGMENTS AND REAGENTS

Max. Marks: 80Min. Marks:

16

Unit I: Substitution Reactions Aliphatic Electrophilic substitution

Bimolecular mechanisms S_{E1} , S_{E2} and S_{Ei} mechanism, electrophilic substitution accompanied by double bond shifts. Effect of substrates, leaving group and the solvent polarity on the reactivity.

Aromatic Electrophilic substitution

The arenium ion mechanism and important Electrophilic substitution reactions, directing effect, orientation and reactivity, energy profile diagrams. The ortho/para ratio, ipso attack, diazonium coupling.

Aromaticity

Aromaticity in homocyclic and heterocyclic compounds Huckel's rule, antiaromaticity, homo-aromaticity, non-aromaticity, quasi aromatic compounds PMO approach for Aromaticity and Annulenes.

Unit II: 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, Hunsdieckerreaction

Unit III: PericyclicReactions

Molecular orbital symmetry, Frontier orbitals of ethylene, 1,3- butadiene, 1,3,5- hexatriene and allylsystem. Classification of pericyclic reactions. Woodward- Hoffman correlation diagrams. FMO and PMO approach. Electrocyclic reactions- conrotarory and disrotatory motions, 4n, 4n+2 and allylsystems. Cycloadditions-antarafacial and suprafacial additions, 4n and 4n+2 systems, 2+2 addition of ketenes. Sigmatropic rearrangements, suprafacial and antarafacial shifts of H, sigmatropic shifts involving carbon.

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moieties, 3, 3-and 5,5- sigmatropic rearrange-ments. Claisen, Cope and aza-Coperearrangements.

Unit IV Rearrangements:

General mechanistic considerations - nature of migration, migratory aptitude, memory effects. A detailed study of the following rearrangements :Pinacolpinacolone, Wagner-Meerwein, Demjanov, Benzil-Benzilic acid, Favorskii, Arndt-Eistert synthesis, Neber, Beckmann, Hofman, Curtius, Schmidt, Baeyervilliger, Shapiro reaction.

Reagents

Oxidation Oxidation of hydrocarbons, Oxidation of alcohols, Oxidation of aldehydes and ketones

Reduction- Catalytic hydrogenation, Reduction by dissolving metals, Reduction by hydride-transfer reagents

List of Reference Books

- 1. Advanced Organic Chemistry Reaction Mechanism and Structure, Jerry March JohnWiley.
- 2. Handbook of Organic named reactions: Reagents, Mechanisms and Applications, Dakeshwar Kumar Verma, Y Dewangan and CB Verma, ELSEVIER, Netherland, 2023.
- 3. Structure and Mechanism in Organic Chemistry, C.K. Ingold, Cornell University Press.
- 4. Organic Chemistry, R. T. Morrison and R.N. Boyd, PrenticeHall.
- 5. Modern Organic Reactions. H.O. HouseBenjamin
- J.M. Coxon, Blackie, 6. Principles of Organic Synthesis, R.O.C. Normonand Academic&professional.
- 7. Pericyclic reactions, S.M. Mukherji, Macmillan India.
- 8. Reaction Mechanism in Organic Chemistry, S.M. Mukherji and S.P. Singh, Macmillan
- International. 9. Stereo Chemistry of Organic Compounds, D. Nasipuri, NewAge
- 10. Stereo Chemistry of Organic Compounds, P.S. Kalsi, New AgeInternational.
- 11. Organic Chemistry, I.L.Finar, Vol. I & II,EL
- 12. Advanced Organic Chemistry Reaction Mechanism and Structure, Jerry March JohnWiley.
- 13. Advanced Organic Chemistry, F.A. Carey and R.J. Sundbery, Plenum
- 14. Structure and Mechanism in Organic Chemistry, C.K. Ingold, Cornell University Press.
- 15. Organic Chemistry, R. T. Morrison and R.N. Boyd, PrenticeHall.
- 16. Modern Organic Reactions. H.O. House Benjamin Principles of Synthesis, Organic R.O.C. NormonandJ.M. Coxon, Blackie, Academic & professional.
- 17. Pericyclic reactions, S.M. Mukherji, Macmillan India.
- 18. Reaction Mechanism in Organic Chemistry, S.M. Mukherji and S.P. Singh, Macmillan
- 19. Stereo Chemistry of Organic Compounds, D. Nasipuri, New Age International
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SEMESTER - II

2025-26

PAPER- III

THERMODYNAMICS, ELECTROCHEMISTRY AND SURFACE CHEMISTRY

Max. Marks: 80 Min. Marks: 16

ClassicalThermodynamics Unit-I

Brief resume of concept of laws of thermodynamics, free energy ,chemical potential and entropies. Partial molar properties, partial molar free energy, content and partial molar volume and partial molar heat significances.Determination of these quantities.Concept of fugacity and determination of fugacity.Non-Ideal system.Excess function for non-ideal solutions, activity, activity coefficient. Debye-Huckel theory for activity coefficient of electrolyte solution, determination of activity and activity coefficients, ionic strength. Application of phase rule to three componentsystems.

Unit-II Statistical Thermodynamics

Concept of distribution, thermodynamic probability and most probable distribution. Maxwell Boltzmann distribution, Partition functions translational, rotational, vibrational and electronic partition calculation of thermodynamic properties in terms of partition functions. Applications of partitions functions, Fermi-Dirac statistics, Bose-Einstein statistics distributionlaw.

Non-equilibrium Thermodynamics

Irreversible thermodynamics, uncompensated heat, first and second law of thermodynamics, entropy production, Onsager equation, coupled reaction.

Unit - III Electrochemistry

Electrochemistry of solution, Debye-Huckel-Onsager treatment and its interaction, Debye-Huckel-Jerum mode. ion-soivent Thermodynamics of electrified interface equation. Derivation of electrocapillarity.Lippmann equation (surface excess) methods of determination of structure of electrified interfaces.Guoy-Chapman, Stern, Graham-Devanathan-Mottwatts, Tobin, Bockris, Devanathan models. Over potentials, Exchange current density, derivation of Butler-Volmer equation, Semiconductor interfaces theory of double layer at semiconductor, electrolyte solution interface, structure of double layer interfaces, effect of light at semiconductor solutioninterfaces.

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SEMESTER - II

2025-26

PAPER- III

THERMODYNAMICS, ELECTROCHEMISTRY AND SURFACE CHEMISTRY

Max. Marks: 80

Min. Marks: 16

Unit-I ClassicalThermodynamics

Brief resume of concept of laws of thermodynamics, free energy chemical potential and entropies. Partial molar properties, partial molar free energy, partial molar volume and partial molar heat content and their significances. Determination of these quantities. Concept of fugacity and determination of fugacity. Non-Ideal system. Excess function for non-ideal solutions, activity, activity coefficient. Debye-Huckel theory for activity coefficient of electrolyte solution, determination of activity and activity coefficients, ionic strength. Application of phase rule to three componentsystems.

Unit-II 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 distributionlaw.

Non-equilibrium Thermodynamics

Irreversible thermodynamics, uncompensated heat, first and second law of thermodynamics, entropy production, Onsager equation, coupled reaction.

Unit - III Electrochemistry

Electrochemistry of solution, Debye-Huckel-Onsager treatment and its extension, ion-soivent interaction, Debye-Huckel-Jerum mode. Thermodynamics of electrified interface equation. Derivation of electrocapillarity. Lippmann equation (surface excess) methods of determination of structure of electrified interfaces. Guoy-Chapman, Stern, Graham-Devanathan-Mottwatts, Tobin, Bockris, Devanathan models. Over potentials, Exchange current density, derivation of Butler-Volmer equation, Tafel plot. Semiconductor interfaces theory of double layer at semiconductor, electrolyte solution interface, structure of double layer interfaces, effect of light at semiconductor solutioninterfaces.

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Electrocatalysis

Influence of various parameters. Polarography theory-Ilkovic equation, half wave potential and its significance. Introduction to corrosion, homogeneous theory, forms of corrosion, corrosion monitoring and preventionmethods.

UNIT-IV SurfaceChemistry

Adsorption

Surface tension, capillary action, pressure difference across curved surface (Laplace equation), Gibbs adsorption isotherm, BET equation and estimation of surface area using BETequation.

Micelles

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

Macromolecules

Polymer: Definition, types of polymers, electrically conducting polymers, mechanism of polymerization, molecular mass, number and mass average molecular mass, molecular mass determination (osmometry, viscometry, diffusion and light scattering methods), sedimentation, chain configuration of macromolecules, calculation of average dimensions of various chain structures.

LIST OF REFERENCE BOOKS:

- 1. Physical Chemistry, P.W. Atkins, ELBS
- 2. Thermodynamics, S. Glasstone
- 3. Statistical Thermodynamics, M.C. Gupta
- 4. Chemical Thermodynamics, Rastogi & Mishra
- 5. Kintetics and Mechanism of Chemical Transformation, J. Rajaraman J. Kuriacose, McMillan
- 6. Micelles, Theoretical and Applied Aspects, V. Moroi, Plenum
- 7. Modem Electrochemisty Vol.-I and Vol.-II, J.O.M. Bockris and A.K.N. Reddy, Plenum
- 8. Introduction to Polymer Science, V.R. Gowarikar, N.V. Vishwanamanand J. Sridhar, WileyEastern.

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	Departmental members		
Chairperson /H.O.D		A	
Subject Expert Abui	1	8	
(University Nominee)	2	9	
Subject Expert.	3	10	
Representative	4	11	
(Industry)	5	12	
Representative	6	13	
(Alumni)	7. 100	14	
Representative	7		

SEMESTER - II

2025-26

PAPER- IV

SPECTROSCOPY

Max. Marks: 80 Min. Marks: 16

Unit-I

MolecularSpectroscopy

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 radiative decay, internal conversion, spectra of transition metal complex, charge transferspectra.

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.

Unit -II 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.

RamanSpectroscopy

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)

Unit - III 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.

Nuclear Quadruple Resonance Spectroscopy Quadruple nuclei, Quadruple moments, electric field gradient, coupling constant, splitting, applications.

Unit -IV Photoelectron Spectroscopy

Basic principle: photo-electric effect, ionization process, Koopmans theorem, photoelectron spectra of simple molecules, ESCA, chemical information from ESCA.

Photo acoustic Spectroscopy

Basic principles of photo acoustic spectroscopy (PAS), PAS gases and condensed systems, chemical and surface applications.

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.

LIST OF REFERENCE BOOKS:

Modern Spectroscopy J.M. Hollas, Johan Wiley. 1.

Applied Electron Spectroscopy for chemical analysis ed. H. Windawi and F.L. 2. Ho, WileyInterscience.

NMR, NQR EPR and Mossbauer Spectroscopy in Inorganic Chemistry, R.V. 3. Parish. Ellish Harwood.

Physical Methods in Chemistry, R.S. Drago, Saunders Company 4.

Infrared and Raman Spectra: Inorganic and Coordination Compounds, K. 5. Nakamoto, Wiley.

Spectroscopic Methods in Organic Chemistry, D.H. Williams, I. Fleming, Tata 6. McGraw-Hill.

Application of Spectroscopy of Organic Compounds, J.R. Dyer, PrenticeHall. 7.

Organic Spectroscopy, Third Ed., William Kemp, Palgrave Publications. 8.

Fundamentals of Molecular Spectroscopy, C.N. Banwell, Tata McGraw-Hill. 9.

	Departmental members	
Chairperson /H.O.D.		N
Subject Expert Bru	1	8
(University Nominee)	2	9
Subject Expert.	3	10
	4	11
Representative(Industry)	5	12
Representative	6	13
(Alumni)	7	14
Representative	8180	Page and William

M.Sc. Chemistry

[Second Semester]

Laboratory Course I : Organic Chemistry

2025-26

Max. Marks : 100

MAJOR EXPERIMENTS

Organic Synthesis

- Acetylation: Acetylation of cholesterol and separation of cholesteryl acetate by column (i) chromatography.
- Synthesis of β-Naphthyl acetate / Hydroquinonediacetate. (ii)
- Oxidation: Adipie acid by chromic acid oxidation of cyclohexanol
- Grignard reaction: Synthesis of triphenylmethanol from benzoicacid (iv)
- Aldol condensation: Dibenzalacetone from benzyldehyde (v)
- Sandmeyer reaction: p-chlorotoluene from p-toluidine / o- chlorobenzoic acid (vi) from anthranilic acid.
- (vii) Acetoacetic ester Condensation: Synthesis of ethyl-n-butylacetoacetate by A.E.E. condensation.
- (viii) Cannizzaro reaction: 4- chlorobenzaldehyde as substrate / Benzoic acid and benzyl alcohol.
- (ix) Friedel Crafts Reaction:β-Benzoylpropionic acid from succinic anhydride and benzene.
- Aromatic electrophilic sustitutions: Synthesis of p-nitroaniline and bromoaniline. The (x)products may be characterized by spectral techniques.

MINOR EXPERIMENTS

Qualitative Analysis

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

Quantitative Analysis

- Determination of the percentage of number of hydrioxy group in an organic compound by (i) acetylation method.
- Estimation of amines/phenols using bromated bromide solution /or acetylation method. (ii)
- Estimation of carbonyl group by hydrazone formation method (iii)
- Estimation of Glycine by titration method. (iv)
- Determination of equivalent weight of carboxyl compound/ estimation of carboxyl group (v) by titration method/ silver salt method

LIST OF REFERENCE BOOKS:

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

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	Departmental members	
Chairperson /H.O.D.		5/
Subject Expert Ablu	1	8
(University Nominee)	2	9
Subject Expert. Ash	3	10
Representative	4	11
(Industry)	5	12
Representative	6	13
(Alumni)	7	14
Representative	3/00	

M.Sc. Chemistry [Second Semester]

Laboratory Course II: -Analytical Chemistry 2025-26

Max. Marks: 100

MAJOR EXPERIMENTS

Analytical Chemistry

Error Analysis & Statistical Data Analysis

Error, types of errors, minimization of errors, statistical treatment for error analysis, standard deviation liner 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 chromatography

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.

MINOR EXPERIMENTS

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.

LIST OF REFERENCE BOOKS:

- 1. Computer for Chemists, Pundhir&Bansal, PragatiPrakashan;
- 2. Computer and Common Sense, R. Hunt and J. Shelley, PrenticeHall.
- 2. Computational Chemistry, A.C.Norris.
- 3. Computer Programming in FORTRAN IV, V. Rajaraman, PrenticeHall
- 4. B.K Sharma, spectroscopy, Krishnapublication

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	Departmental members		
Chairperson /H.O.D.		19	
Subject Expert	1	8	
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Representative(Professor Science Faculty Other Dept.)	'00	to to make the state of	