DEPARTMENT OF CHEMISTRY

COURSE CURRICULUM & MARKING SCHEME

M.Sc. CHEMISTRY
Semester - II

SESSION : 2023-24

ESTD: 1958

GOVT. V.Y.T. PG AUTONOMOUS COLLEGE, DURG, 491001 (C.G.)

(Former Name – Govt. Arts & Science College, Durg)

NAAC Accredited Grade A+, College with CPE - Phase III (UGC), STAR COLLEGE (DBT)

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Department of Chemistry

Govt. V.Y.T. PG Autonomous

College, Durg (C.G.)

M.Sc. Chemistry

Second Semester

2023-24

Syllabus and Marking Scheme for Second Semester

Session 2023-24

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	05
II	**CONCEPTS IN ORGANIC CHEMISTRY**	80	16	20	04	05
III	**THERMODYNAMICS, ELECTROCHEMISTRY AND SURFACE CHEMISTRY**	80	16	20	04	05
IV	**SPECTROSCOPY**	80	16	20	04	05
V	Lab Course I **ORGANIC CHEMISTRY PRACTICAL**	100	36	-----	-----	04
IV	Lab Course II **ANALYTICAL CHEMISTRY PRACTICAL**	100	36	-----	-----	04
	Total	**520**	-----	**80**	-----	**28**

04 Theory papers - 320

04 Internal Assessment - 80

02 Practical - 200

Total Marks - 600

Note: 20 marks = 01 credit in Theory Papers and 25 Marks = 01 Credit in Practical

The syllabus for M.Sc. Chemistry is hereby approved for the sessions 2023-24 and 2024-25

Name and Signatures	Departmental members **Name and Signatures**
Chairperson /H.O.D	1. .....
Subject Expert ..... (University Nominee)	2. .....
Subject Expert.....	3. .....
Subject Expert.....	4.....
Subject Expert.....	5. .....
Representative ..... (Industry)	6. .....
Representative ..... (Alumni)	7. .....
Representative ..... (Professor Science Faculty Other Dept.)	8. .....
	9. .....
	10. .....
	11. .....
	12. .....

M.Sc. CHEMISTRY

SEMESTER - II

2023-24

PAPER- I

TRANSITION METAL COMPLEXES AND DIFFRACTION METHODS

Max. Marks 80

Min. Marks 16

Unit-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.

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

Unit –III

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.Description of the procedure for an X-ray structure analysis, absolute configuration of molecules, Ramchandran Diagram.

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.

Unit-IV

Neutron Diffraction

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

Metal clusters

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

Isopoly and Heteropoly Acids and Salts

Prepration, properties and structure of isopolyandheteropoly acids of molybdenum and tungsten.

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. Earnshow, Pergamon.
4. Inorganic Electronic Spectrosocopy, 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. McCleverty, Pergamon.
7. Modern spectroscopy, J. M. Hollas, John Wiley.
8. Applied electron spectroscopy for chemical analysis Ed. H. Windawi and F.L. Ho, Wiley Inter science.

Question Paper Format and Distribution of Marks for PG Semester Examination

Question paper format for the Post-Graduate Examination has been revised from the Session 2022-23. The revised format will be applicable for all the question papers of Semester I, II, III & IV. The following are the main points of the new format:

1. The question paper will be of **80 marks**
2. Questions will be asked Unit-wise in each question paper.
3. From each Unit, the questions will be asked as follows:

Q.1 Very short answer type question **(Answer in one or two sentences)** **(02 Marks)**

Q.2 Very short answer type question **(Answer in one or two sentences)** **(02 Marks)**

Q.3 Short answer type question **(Answer in 200-250 words)** **(04 Marks)**

Q.4 Long answer type questions **(Answer in 400-450 words)** **(12 Marks)**

Type of Question	Unit-I	Unit-II	Unit-III	Unit-IV
Very Short (2 Questions) (Maximum two sentences)	**2 x 2 = 4 Marks**	**2 x 2 = 4 Marks**	**2 x 2 = 4 Marks**	**2 x 2 = 4 Marks**
Short (1 Question) 200-250 words	**1 x 4 = 4 Marks**	**1 x 4 = 4 Marks**	**1 x 4 = 4 Marks**	**1 x 4 = 4 Marks**
Long answer (1 Question) 400-450 words	**1 x 12 = 12 Marks**	**1 x 12 = 12 Marks**	**1 x 12 = 12 Marks**	**1 x 12 = 12 Marks**

Note:

1. Question no. 1 and Question 2 will be compulsory.
2. Question no. 3 and 4 will consist of 2 optional questions of which one has to be attempted.
3. As mentioned above, two compulsory very short answer type questions (2+2 marks), one short answer type question with internal choice (4 marks) and one long answer type question with internal choice (12 marks) will be asked from each unit. Thus there will be questions of 20 marks from each unit and of total 80 marks from all the four units of the syllabus/syllab

M.Sc. CHEMISTRY

SEMESTER - II

2023-24

PAPER- II

CONCEPTS IN ORGANIC CHEMISTRY

Max. Marks 80
Min. Marks 16

Unit –I

Nature of Bonding in Organic Molecules

Localized and delocalized chemical bond, conjugation and cross conjugation, bonding infullerenes, Bonds weaker than covalent- addition compounds, crown ether complexes and cryptands, inclusion compounds, cyclodextrins, catenanes and rotaxanes

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.

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, Hunsdiecker reaction

Unit –III

Conformational analysis

Conformational analysis of cycloalkanes, decalins, effect of conformation on reactivity, conformation of sugars, steric strain due to unavoidable crowding.

Stereochemistry

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.

Unit –IV

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- conrotarory and disrotatory motions, 4n, 4n+2 and allyl systems.Cycloadditions- antarafacialand suprafacial additions, 4n and 4n+2 systems, 2+2 addition of ketenes.Sigmatropic rearrangements, suprafacial and antarafacial shifts of H, sigmatropic shifts involving carbon moieties, 3, 3-and 5,5-sigmatropic rearrange-ments. Claisen, Cope and aza-Cope rearrangements.

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. Pericyclic reactions, S.M. Mukherji, Macmillan India.
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.
10. Stereo Chemistry of Organic Compounds, P.S. Kalsi, New Age International.
11. Organic Chemistry, I.L.Finar, Vol. I & II, ELBS.

Question Paper Format and Distribution of Marks for PG Semester Examination

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M.Sc. CHEMISTRY

SEMESTER - II

2023-24

PAPER- III

THERMODYNAMICS, ELECTROCHEMISTRY AND SURFACE CHEMISTRY

Max. Marks 80
Min. Marks 16

Unit-I

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.

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 - distribution law.

Non-equilibrium Thermodynamics

Fundamental concepts, entropy production and entropy flow, phenomenological laws, Onsager's reciprocity relations, and irreversible thermodynamics for coupled reactions.

Unit – III

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.

Thermodynamics of electrified interface equations: Derivation of electro-capillarity, Lippmann equations, determination of surface excess.

Structure of electrified interfaces: Guoy-Chapman and Stern models. Over potentials, exchange current density, derivation of Butler-Volmer equation. Tafelplot.Polarography theory - Ilkovic equation, half wave potential and its significance.

UNIT –IV

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.

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.

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).

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 and 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, Wiley Eastern.

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M.Sc. CHEMISTRY

SEMESTER - II

2023-24

PAPER- IV

SPECTROSCOPY

Max. Marks 80
Min. Marks 16

Unit – I

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.

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.

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)

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, A_2B_2, 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:

1. Modern Spectroscopy J.M. Hollas, Johan Wiley.
2. Applied Electron Spectroscopy for chemical analysis ed. H. Windawiand F.L. Ho, Wiley Interscience.
3. NMR, NQR EPR and Mossbauer Spectroscopy in Inorganic Chemistry, R.V. Parish. Ellish 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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M.Sc. Chemistry
[Second Semester]
Laboratory Course I :Organic Chemistry
2023-24

M. M. 100

MAJOR EXPERIMENTS

Organic Synthesis

(i) Acetylation: Acetylation of cholesterol and separation of cholesteryl acetate by column chromatography.
(ii) Synthesis of β-Naphthyl acetate / Hydroquinone diacetate.
(iii) Oxidation: Adipic acid by chromic acid oxidation of cyclohexanol
(iv) Grignard reaction:Synthesis of triphenylmethanol from benzoic acid
(v) Aldol condensation :Dibenzalacetoneefrombenzyldehyde
(vi) Sandmeyerreaction : p-chlorotoluene from p-toluidine / o- chlorobenzoic acid from anthranilic acid.
(vii) Acetoacetic ester Condensation: Synthesis of ethyl-n-butylacetoacetateby A.E.E. condensation.
(viii) Cannizzaroreaction : 4- chlorobenzaldehyde as substrate / Benzoic acid and benzyl alcohol.
(ix) Friedel Crafts Reaction: β-Benzoyl propionic acid from succinic anhydride and benzene.
(x) Aromatic electrophilic sustitutions: 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.

M.Sc. Chemistry
[Second Semester]
2023-24

Laboratory Course II: -Analytical Chemistry and Computer

M. M. 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^+, Ca^{2+}, SO_4^{2-}, NO_2^-, 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.

Computational Chemistry

Introduction to structure drawing, spread sheet and chemistry related softwares. Brief description of computational methods: 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 - H_2O, CO_2 and NH_3. 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.

The syllabus for M.Sc. Chemistry is hereby approved for the sessions 2023-24 and 2024-25

Name and Signatures	Departmental members **Name and Signatures**
Chairperson /H.O.D	1. .....
Subject Expert ..... (University Nominee)	2. .....
Subject Expert.....	3. .....
Subject Expert.....	4.....
Subject Expert.....	5. .....
	6. .....
Representative ..... (Industry)	7. .....
Representative ..... (Alumni)	8. .....
Representative ..... (Professor Science Faculty Other Dept.)	9. .....
	10. .....
	11. .....
	12. .....