DEPARTMENT OF CHEMISTRY

COURSE CURRICULUM & MARKING SCHEME

M.Sc. CHEMISTRY

Semester - I

SESSION : 2024-25

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)

Phone : 0788-2212030

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Department of Chemistry

Govt. V.Y.T. PG Autonomous College

Durg (C.G.)

Syllabus

M.Sc. Chemistry

First and Second Semester (2024--25)

DEPARTMENT OF CHEMISTRY

GOVT. V.Y.T. PG AUTONOMOUS COLLEGE, DURG

Approved syllabus for M.Sc. Chemistry by the Members of Board of Studies for Sessions 2024-25

The syllabus with the paper combinations is as under:

Semester I:

Paper I: MCH-101 COORDINATION CHEMISTRY	Paper II: MCH-102 ORGANIC REACTION MECHANISM
Paper III: MCH-103 MATHEMATICS FOR CHEMISTS,QUANTUM CHEMISTRY AND CHEMICAL DYNAMICS	Paper IV: MCH-104 GROUP THEORY AND COMPUTER FOR CHEMISTS
Lab Course I: MCHL-01 INORGANIC CHEMISTRY PRACTICAL	Lab Course II: MCHL-02 PHYSICAL CHEMISTRY PRACTICAL

Semester II:

Paper I: MCH-201 TRANSITION METAL COMPLEXES AND DIFFRACTION METHODS	Paper II: MCH-202 CONCEPTS IN ORGANIC CHEMISTRY
Paper III: MCH-203 THERMODYNAMICS, ELECTROCHEMISTRY AND SURFACE CHEMISTRY	Paper IV: MCH-204 SPECTROSCOPY
Lab Course I: MCHL-03 ORGANIC CHEMISTRY PRACTICAL	Lab Course II: MCHL-04 ANALYTICAL CHEMISTRY PRACTICAL

Semester III:

Paper I: MCH-301 APPLICATIONS OF SPECTROSCOPY	Paper II: MCH-302 BIO-ORGANIC CHEMISTRY
Paper III: MCH-303 ENVIRONMENTAL CHEMISTRY	Paper IV: Elective-A: MCH-304(A) BIO-INORGANIC AND SUPRAMOLECULAR CHEMISTRY Elective-B: MCH-304(B) NATURAL PRODUCTS Elective-C: MCH-304(C) POLYMER AND NANOCHEMISTRY Elective-D: MCH-304(D) NANOMATERIALS AND NANOTECHNOLOGY
Lab Course I: MCHL-05 GENERAL PRACTICAL	Lab Course II: MCHL -06(A), MCHL-06(B), MCHL-06(C) ELECTIVE PRACTICAL (A, B OR C)

Semester IV:

Paper I: MCH-401 **SOLID STATE AND PHOTOCHEMISTRY**	**Paper II: MCH-402** **BIO-PHYSICAL CHEMISTRY**
Paper III: MCH-403 **ANALYTICAL CHEMISTRY**	**Paper IV:** **Elective-A: MCH-404(A)** **ORGANOTRANSITION METAL CHEMISTRY** **Elective-B: MCH-404(B)** **MEDICINAL CHEMISTRY** **Elective-C: MCH-404 (C)** **CHEMICAL KINETICS AND NUCLEAR CHEMISTRY** **Elective-D: MCH-404 (D)** **POLYMER CHEMISTRY**
Lab Course I: MCHL-07 **PROJECT**	**Lab Course II: MCHL-08(A), MCHL-08(B), MCHL-08(C)** **ELECTIVE PRACTICAL (A, B OR C)**

Note: Industrial Visit/Training is mandatory for all students as part of curriculum

The syllabus for M.Sc. Chemistry is hereby approved for the Session 2024-25

Name and Signatures	Departmental members **Name and Signatures**
Chairperson /H.O.D Dr. Anupama Asthana	
Subject Expert .... Dr. Arun Mishra 05/7/24 (University Nominee)	1. ..... Dr. V.S. Geele .....
Subject Expert. Dr. S.C. Tiwari	2. ..... Dr. Sunitha Mathew
Subject Expert..... H. Mohabey (Dr. Hemlata Mohabey)	3. ....
Subject Expert..... 05.07.24 (Dr. Anju Jha)	4..... .....
Representative ..... (Industry)	5. ....
Representative ..... Dr. Bhawna Jain	6. ....
(Alumni)	7. ....
Representative ..... 5/7/24 (Professor Science Faculty Other Dept.) (Dr. S.D. Deshmukh)	8. ....
	9. ....
	10. ....
	11. ....
	12. ..... Dr. A. Tiwary

GENERAL INSTRUCTIONS FOR STUDENTS

1. The candidate has to obtain minimum 20% marks in each theory paper and internal assessment separately.
2. The candidate has to secure minimum 36% marks as an aggregate in order to pass that semester examination.
3. The internal assessment shall include class test, home assignment and seminar presentation.
4. Internal Assessment Examination will be as follows:
   i. Internal Test in each paper (20 marks)
   ii. Seminar (Power point presentation) in any one of the paper (20 marks). The marking of seminar shall be in terms of hard copy submission (10 marks) and presentation and open discussion (10 marks).
   iii. Assignment in each of the remaining papers (excluding the paper of Seminar. (20 marks)
   iv. Average of marks obtained in internal test + seminar in any one paper and marks obtained in internal test + assignment in rest of the papers will be calculated and taken into consideration.
5. The grading system will be followed in all semesters.

CREDIT ALLOTMENTS

- Theory Paper = 05 credits (04+01)
- Practical = 04 credits

TOTAL CREDITS/ SEMESTER

- 04 theory papers (100 each) and two practicals (100 each) in Semester - I, II & III : **20 + 08 = 28 credits**
- 04 theory papers (100 each) and one practical and one project in lieu of one practical (100 each) in Semester - IV: **20 + 08 = 28 credits**

TOTAL CREDITS / PROGRAMME

- 16 Theory + 08(Practical + Project work) – 80 + 32 = 112 credits

EVALUATION PATTERN

Theory 80 marks = 04 Credits

Question paper format for the Post-Graduate Examination has been revised from the Session 2018-19. 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/syllabi.

Internal Assessment 20 marks = 01 credit

- Unit test – One class test in each theory paper comprising 20 marks
- Seminar presentations (Power point) – Comprising 20 marks in any one paper
- Home assignments – Assignment of total 20 marks comprising of two long answer type questions of 10 marks each from rest the theory paper (excluding the seminar paper) The answer should be prepared with the help of standard reference books. (The titles of those books, authors, year of publication and publishers details should be mentioned in an appropriate way, at the end of each assignment).

Practical/Project work in lieu of practical of 100 marks =04 credits

Department of Chemistry

Programme 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.

Department of Chemistry

Govt. V.Y.T. PG Autonomous College

Durg (C.G.)

M.Sc. Chemistry

First Semester

2024-25

Syllabus and Marking Scheme for First Semester Session 2024-25

Paper No.	Title of the Paper	Marks Allotted in Theory		Marks Allotted in Internal Assessment		Credits
		Max	Min	Max.	Min.	
I	MCH-101 COORDINATION CHEMISTRY	80	16	20	04	05
II	MCH-102 ORGANIC REACTION MECHANISM	80	16	20	04	05
III	MCH-103 MATHEMATICS FOR CHEMISTS, QUANTUM CHEMISTRY AND CHEMICAL DYNAMICS	80	16	20	04	05
IV	MCH-104 GROUP THEORY AND COMPUTER FOR CHEMISTS	80	16	20	04	05
V	MCHL-01 Lab Course I INORGANIC CHEMISTRY PRACTICAL	100	36	------	-----	04
IV	MCHL-02 Lab Course II PHYSICAL CHEMISTRY PRACTICAL	100	36	-----	-----	04
	Total	**520**	----	**80**	-----	**28**

04 Theory papers - 320

04 Internal Assessments - 80

02 Practical - 200

Total Marks - 600

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

Note: Industrial Visit/Training is mandatory for all students as part of curriculum

M.Sc. CHEMISTRY

SEMESTER – I

2024-25

PAPER- I

MCH-101: COORDINATION CHEMISTRY

Course Outcome (CO):

After completion of the course, students would be able:

CO1: To understand Walsh diagram, bent rule, energetics of hybridization and MOT.

CO2: To know structure of carbonyls, nitrosyls, dinitrogen and dioxygen complexes.

CO3: To understand energy profile of a reaction and determination of stability constant of transition metal complexes.

CO4: To know mechanism and kinetics of substitution and electron transfer reaction in complexes.

M.Sc. CHEMISTRY
SEMESTER - I
2024-25
PAPER- I
MCH-101: COORDINATION CHEMISTRY

Max. Marks 80
Min. Marks 16

Unit - 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.

Metal π-Ligand Bonding

Limitation of crystal field theory, molecular orbital theory, octahedral, tetrahedral and square planar complexes, π- bonding and molecular orbital theory.

Unit –II

Metal π -Complexes

Metal carbonyls, structure and bonding, vibrational spectra of metal carbonyls for bonding and structural elucidation, important reactions of metal carbonyls; preparation, bonding, structure and important reactions of transition metal nitrosyl, dinitrogen and dioxygen complexes; tertiary phosphine as ligand.

Unit –III

Metal Ligand Equilibria in Solution

Stepwise and overall formation constants and their interaction, trends in stepwise constants, factors affecting the stability of metal complexes with reference to the nature of metal ion and ligand, chelate effect and its thermodynamic origin, determination of binary formation constants by pHmetry and spectrophotometry. Energy profile of a reaction, reactivity of metal complexes, inert and labile complexes, kinetic application of valence bond and crystal field theories.

Unit –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 evidences in favour of conjugate mechanism, anation reactions, reactions without metal ligand bond cleavage. Substitution reactions in square planar complexes, the trans effect, mechanism of the substitution reaction. Redox reactions, electron transfer reactions, mechanism of one electron transfer reactions, outersphere type reaction, cross reactions and Marcus-Hush theory, inner sphere type reactions.

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. Earnshow, Pergamon.
4. Inorganic Electronic Spectrosocopy, A.B.P. Lever, Elsevier.
5. Magnetochemistry, R.L. Carlim, 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 Interscience.
9. Mechanisms of Inorganic Reactions, Fred Basalo and Ralph G. Pearson, Wiley Eastern Private Ltd

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 2018-19. 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/syllabi.

M.Sc. CHEMISTRY
SEMESTER-I
2024-25
PAPER- II
MCH-102: ORGANIC REACTION MECHANISM

Course Outcome (CO):

After completion of the course, the students would be able:

CO1: To understand the basic concepts and explain the mechanism and stereochemical aspects of elimination reactions.

CO2: To understand the mechanism and stereochemistry of nucleophilic substitution reactions.

CO3: To acquire the knowledge of mechanism of electrophilic substitution in aliphatic as well as aromatic compounds.

CO4: To understand the mechanistic and stereochemical concepts of addition reactions.

M.Sc. CHEMISTRY
SEMESTER-I
2024-25
PAPER- II
MCH-102: ORGANIC REACTION MECHANISM

Max. Marks 80
Min. Marks 16

Unit -I

Reaction Mechanism: Structure and Reactivity

Types of mechanism, types of reaction, thermodynamic and kinetic requirements, kinetic and thermodynamic control, Hammond's postulate, Curtin Hammett 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.

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.

Unit-II

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, phenonium ions, nor-bornyl system, common carbocation rearrangements. 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.

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.

Unit - III

Aliphatic Electrophilic substitution

Bimolecular mechanisms S_E2, S_Ei and S_E1 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, orientation and reactivity, energy profile diagrams. The ortho/para ratio, ipso attack, diazonium coupling, Vilsmeir reaction.

Unit-IV

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.

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, organo zinc and organo lithium reagents to carbonyl and unsaturated carbonyl compounds, Wittig reaction. Mechanism of condensation reaction involving enolates – Claisen, Mannich, Benzoin, Perkin and Stobbe reactions.

REFERENCE BOOKS:

1. Adv. Organic Chem., 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 Univ. Press.
4. Organic Chemistry, R.T. Morrison and R.N. Boyd, Prentice Hall.
5. Modern organic Reactions. H.O. House Benjamin
6. Organic Reactions and their mechanism, S. Kalsi, New Age International.
8. Reaction Mechanism in Org. Chemistry, S.M. Mukherji and S.P. Singh, Macmillan

Question Paper Format and Distribution of Marks for PG Semester Examination

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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/syllabi.

M.Sc. CHEMISTRY
SEMESTER - I
2024-25
PAPER- III
MCH-103: MATHEMATICS FOR CHEMISTS, QUANTUM CHEMISTRY AND CHEMICAL DYNAMICS

Course Outcome (CO):

After completion of the course, the students would be able:

CO1: To have basic knowledge of mathematics – vector, matrix algebra, probability, calculus and its application in chemistry which adds value to the program.

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.

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.

CO4: To describe different theories of reaction rates, fast reactions and its methods, kinetics and mechanism of photochemical and unimolecular reactions.

M.Sc. CHEMISTRY
SEMESTER - I
2024-25
PAPER- III
MCH-103: MATHEMATICS FOR CHEMISTS, QUANTUM CHEMISTRY AND CHEMICAL DYNAMICS

Max. Marks 80
Min. Marks 16

Unit-I

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, special matrices (symmetric, skew-symmetric, Hermitian, skew-Hermitian, unit, diagonal, unitary) and their properties. Introduction to determinants.

Permutations and combinations and probability.

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.

First-order differential equations, homogeneous, exact and linear equations.

Unit-II

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, concept of degeneracy, the harmonic oscillator, the rigid rotor, the hydrogen atom.

Approximate Methods

The variation theorem and perturbation theory (first order and non-degenerate). Applications of variation method and perturbation theory to hydrogen and helium atom.

Unit-III

Angular Momentum

Ordinary angular momentum, eigen functions and eigen values of angular momentum, ladder operator, concept of spin, antisymmetry and Pauli's exclusion principle.

Electronic Structure of Atoms

Russell-Saunders terms and coupling schemes. Atomic states, atomic terms and term symbols.

Molecular Orbital Theory

Huckel theory of conjugated systems, Applications to ethylene, butadiene and cyclobutadiene.

Unit – IV

Chemical Dynamics

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, general features of 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.

REFERENCE BOOKS:

1. Physical Chemistry, P.W. Atkins, ELBS
2. Introduction to Quantum Chemistry, A.K. Chandra, Tata McGraw HillQuantum Chemistry, Ira N. Levine, Prentice Hall
3. Coulsons Valence R. Mc. Weeny, ELBS
4. Chemical Kinetics, K.J. Laidler, McGraw-Hill
5. Kinetics and Mech. of Chemical Transformation, J. Rajaramanand J. Kuriacose, McMillan.
6. Mathematical Preparation for Physical Chemistry, F. Daniels, McGraw Hill.
7. Mathematics for Chemists, Bhupendra Singh

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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.
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Thus there will be questions of 20 marks from each unit and of total 80 marks from all the four units of the syllabus/syllabi.

M.Sc. CHEMISTRY

SEMESTER – I

2024-25

PAPER- IV

MCH-104: GROUP THEORY AND COMPUTERS FOR CHEMISTS

Course Outcome (CO):

After completion of the course, students would be able:

CO1: To understand symmetry properties of compounds, character tables and their uses in spectroscopy.

CO2: To know principles involved in interaction of electromagnetic radiation with matter.

CO3: To understand basic structure of computers, memory and operating systems and 'C' language.

CO4: To learn development of small computer codes involving simple formula in chemistry.

M.Sc. CHEMISTRY
SEMESTER – I
2024-25
PAPER- IV
MCH-104: GROUP THEORY AND COMPUTERS FOR CHEMISTS

Max. Marks 80
Min. Marks 16

Unit I **Symmetry and Group Theory in Chemistry**

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. Schonflies symbols, representations of groups by matrices (representation for the Cn, Cnv, Cnh, Dnh 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.

Unit –II **Unifying Principles**

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.

Unit –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. Arithmatic assignment statement.

Unit – 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.

REFERENCE BOOKS:

1. Computers and Common Sense, R. Hunt and J. Shelley Prentice Hall.
2. Computers Chemistry, A.C. Norris.
3. Microcomputer Quantum Mechanics, Killngbeck, Adam Hilger.
4. Computer Programming in FORTRAN IV, V Rajaraman,Prentice Hall
5. An Introd. to Digital Computer Design. V. Rajaraman and T. Radhakrishan, 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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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/syllabi.

M.Sc. Chemistry [First Semester]
MCHL-01: Laboratory Course I
Inorganic Chemistry
2024-25

Course Outcome (CO):

After completion of the course, students would be able:

CO1: To understand the basic principles involved in separation and estimation of acidic and basic radicals in inorganic mixture.
CO2: To apply the knowledge of qualitative and quantitative estimations in real sample analysis.
CO3: To get 'Hands on Training' and develop skill for synthesis of various inorganic compounds.
CO4: To identify and characterize prepared compounds by spectral analysis.

M.Sc. Chemistry [First Semester] MCHL-01
Laboratory Course I Inorganic Chemistry
2024 - 25

M. M. 100

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, Arsinate 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

(a) Phosphoric acid in commercial orthophosphoric acid.
(b) Boric acid in borax.
(c) Ammonia in an ammonium salt.
(d) Manganese dioxide in pyrolusite.
(e) Available chlorine in bleaching powder.
(f) 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 ofsome preparations by spectral analysis

1. $VO(acac)_2$
2. $TiO(C_9H_8NO)_2 2H_2O$
3. Cis-K $[Cr(C_2O_4)_2(H_2O)_2]$
4. $Na[Cr(NH_3)_2(SCN)_4]$
5. $Mn(acac)_3$
6. $K_3[Fe(C_2O_4)_3]$
7. Prussian Blue, Turnbull's Blue.
8. $[Co(NH_3)_6][Co(NO_2)_6]$
9. Cis-$[Co(trien)(NO_2)_2]Cl.H_2O$
10. $Hg[Co(SCN)_4]$
11. $[Co(Py)_2Cl_2]$
12. $[Ni(NH_3)_6]Cl_2$
13. $Ni(DMG)_2$
14. $[Cu(NH_3)_4]SO_4.H_2O$

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.

M.Sc. Chemistry

[First Semester]

MCHL-02: Laboratory Course II

Physical Chemistry

2024 - 25

Course Outcome (CO):

After completion of the course, students would be able:

CO1: To understand basic concepts in Physical Chemistry through experiential learning.
CO2: To acquaint with the basic principles of equipment/instruments and its applications.
CO3: To develop observation skill and analytical skill through diverse practicals.
CO4: To develop teamwork spirit, scientific temper and logical thinking.

M.Sc. Chemistry
[First Semester]
Laboratory Course II
Physical Chemistry
2024-25

M. M. 100

Number of hours for each experiment: 3-4 hours

A list of experiments under different headings is given below. Typical experiments are to be selected from each type.

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.

Polarimetry

1. Determine the specific and molecular rotation of optically active substance.
2. To determine the concentration of a solution of an optically active substance.

Thermodynamics

1. To determine heat of neutralization of an acid using Dewar flask.
2. To determine heat of solution of a substance by solubility method.
3. To determine the partial molar volume of solute and solvent in aqueous solutions at room temperature.
4. Determination of the temperature dependence of the solubility of a compound in two solvents (benzoic acid in water and in DMSO-water mixture) and calculate the partial molar heat of solution.

MINOR EXPERIMENTS

Surface tension

1. To determine surface tension of an organic liquid by drop method.
2. To compare cleansing power of detergents.
3. To study the variation of surface tension with temperature.
4. To determine the critical micelle concentration of a soap by surface tension measurements.

Viscosity

1. To determine viscosity of an organic liquid using Ostwald viscometer.
2. To verify Kendall's equation.
3. To study the variation of viscosity with temperature.

Phase Equilibria

1. Determination of congruent composition and temperature of a binary system (e.g. diphenylamine benzophenone system.)
2. Determination of distribution coefficient of succinic acid between ether and water.
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.

Spectrophotometry

1. Verification of Beer-Lambert law and determination of concentration of unknown solution.
2. Effect of pH in aqueous coloured system.

Conductometry

1. To determine the basicity of an organic acid.
2. Determination of solubility and solubility product of sparingly soluble salts (e.g. $PbSO_4$, $BaSO_4$) conductometrically.
3. Determination of pK_a of acetic acid and verification of Ostwald Dilution law

Potentiometry/pH metry

1. Determination of temperature dependence of EMF of a cell.
2. To determine pK_a of the given monobasic acid by pHmetric titration.
3. Determination of the dissociation constant of monobasic/dibasic acid by Albert- Serjeant method.

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.

The syllabus for M.Sc. Chemistry is hereby approved for the Session 2024-25

Name and Signatures	Departmental members **Name and Signatures**
Chairperson /H.O.D Dr. Anupama Asthana	1. Dr. V.S Geel
Subject Expert Dr. Arun Mishra 05/7/24 (University Nominee)	2. 05.07.24 Dr. Sunitha B. Mathew
Subject Expert Dr. S.C. Tiwari	3.
Subject Expert (Dr. Hemlata Mohabey)	4.
Subject Expert 05/07/24 (Dr. Anju Jha)	5. Dr. Prerna Kathane 05/7/24
Representative (Industry)	6.
Representative Dr. Bhawna Jain (Alumni)	7.
Representative Dr. S.D. Deshmukh (Professor Science Faculty Other Dept.)	8. Dr. A. Kashyap
	9. Dr. A.K. Pillai
	10.
	11.
	12.