

Hindi Vidya Prachar Samiti's Ramniranjan Jhunjhunwala College of Arts, Science & Commerce (Autonomous College)

Affiliated to

UNIVERSITY OF MUMBAI

Syllabus for the M.Sc. Program: M.Sc. (Chemistry)

Program Code: RJSPGCHE

CBCS: 2020 - 2021

M.Sc. CHEMISTRY SEMESTER I

Course	Nomenclature	re Credit Topics	
		S	
RJSPGCHE101	Paper I (Physical Chemistry)	4	 Thermodynamics-I Quantum Chemistry Chemical Dynamics-I Electrochemistry Recapitulation – basics of electrochemistry.
RJSPGCHE102	Paper II (Inorganic Chemistry)	4	 Chemical Bonding Molecular Symmetry and Group Theory Materials Chemistry and Nanomaterials Solid State Chemistry Nanomaterials Characterization of Coordination compounds
RJSPGCHE103	Paper III (Organic Chemistry)	4	 Physical Organic Chemistry Thermodynamic and kinetic requirements of a reaction. Determining mechanism of a reaction. Acids and Bases Nucleophilic substitution reactions and Aromaticity. Stereochemistry. Oxidation and Reduction
RJSPGCHE104	Paper IV (Analytical Chemistry)	4	 Language of Analytical Chemistry Quality in Analytical Chemistry Calculations based on Chemical Principles. Optical Methods Recapitulation and FT Technique Molecular Ultraviolet and Visible Spectroscopy Infrared Absorption Spectroscopy. Thermal Methods Automation in chemical analysis

RJSPGCHEPR101	Physical Chemistry Practical		Physical Chemistry Practical
RJSPGCHEPR102	Inorganic Chemistry Practical		Inorganic Chemistry Practical
RJSPGCHEPR103	Organic Chemistry	8	Organic Chemistry Practical
RJSPGCHEPR104	Practical Analytical Chemistry		Analytical Chemistry Practical
NOFUCHERRIU4	Practical		

Theory semester I

Course Code	Title	Credits
RJSPGCHE101	Physical Chemistry	4
Uni	Unit – I	
Thermodynamics-I		
1.1. State function and exact differentials. Maxwell equations, Maxwell thermodynamic Relations; it's significance and applications to ideal gases, Joule Thomson experiment, Joule Thomson coefficient, inversion temperature, Joule Thomson coefficient in terms of van der Waals constants.		
1.2.Recapitulation of first, second and third law of thermodynamics, Entropy change for a phase transition, absolute entropies, determination of absolute entropies in terms of heat capacity, standard molar entropies and their dependence on molecular mass and molecular structure, residual entropy.		
Uni	t – II	1
Quantum Chemistry:		
2.1 Classical Mechanics, failure of classical mechanics: Need for Quantum Mechanics.		
[Recapitulation: Different phenomena such as Photoelectric effect, Blackbody radiation, Compton effect etc. should be highlighted in understanding the evolution of Quantum mechanics in above points.]		

- 2.2 Particle waves and Schrödinger wave equation, wave functions, properties of wave functions, Normalization of wave functions, orthogonality of wave functions
- 2.3 Operators and their algebra, linear and Hermitian operators, operators for the dynamic variables of a system such as, position, linear momentum, angular momentum, total energy, eigen functions, eigen values and eigen value equation, Schrödinger wave equation as the eigen value equation of the Hamiltonian operator, average value and the expectation value of a dynamic variable of the system, Postulates of Quantum Mechanics, Schrödinger's Time independent wave equation from Schrödinger's time dependent wave equation.
- 2.4 Application of quantum mechanics to the following systems:
- a) Free particle, wave function and energy of a free particle.
- b) Particle in a one, two and three dimensional box, separation of variables, Expression for the wave function of the system, expression for the energy of the system, concept of quantization, introduction of quantum number, degeneracy of the energy levels.
- c) Harmonic oscillator, approximate solution of the equation, Hermite polynomials, expression for wave function, expression for energy, use of the recursion formula.

Unit III

1

3.1 Composite Reactions:

Recapitulation: Rate laws, Differential rate equations Consecutive reactions,

Steady state Approximation, rate determining steps, Microscopic Reversibility and Detailed Balanced Chain reactions-chain initiation processes. Some inorganic mechanisms: formation and decomposition of phosgene, decomposition of ozone, Reaction between Hydrogen and Bromine and some general examples Organic Decompositions: Decomposition of ethane, decomposition of acetaldehyde Gas phase combustion: Reaction between hydrogen and oxygen, Semenov – Hinshelwood and Thompson mechanism, Explosion limits and factors affecting explosion limits.

- 3.2 Polymerization reactions: Kinetics of stepwise polymerization, Calculation of degree of polymerization for stepwise reaction. Kinetics of free radical chain polymerization, Kinetic chain length and estimation of average no. of monomer units in the polymer produced by chain polymerization.
- 3.3 Reaction in Gas Phase

Unimolecular Reactions: Lindeman-Hinshelwood theory, Rice-Ramsperger-Kassel (RRK) theory, Rice-Ramsperger-Kassel Marcus (RRKM) theory.

Unit IV

1

Electrochemistry

Recapitulation – basics of electrochemistry.

- 4.1 Debye-Hückel theory of activity coefficient, Debye-Hückel limiting law and it's extension to higher concentration (derivations are expected).
- 4.2 Electrolytic conductance and ionic interaction, relaxation effect. Debye-Hückel-Onsager equation (derivation expected). Validity of this equation for aqueous and non-aqueous solution, deviations from Onsager equation, Debye -Falkenhagen effect (dispersion of conductance at high frequencies), Wien effect.
- 4.3 Batteries: Alkaline fuel cells, Phosphoric acid fuel cells, High temperature fuel cells [Solid –Oxide Fuel Cells (SOFC) and Molten Carbonate Fuel Cells]
- 4.4 Bio-electrochemistry: Introduction, cells and membranes, membrane potentials, theory of membrane potentials, interfacial electron transfer in biological systems, adsorption of proteins onto metals from solution, electron transfer from modified metals to dissolved protein in solution, enzymes as electrodes, electrochemical enzyme-catalyzed oxidation of styrene. Goldmann equation. (derivations are expected)

M. Sc.	Semester I Theory	
RJSPGCHE101	Course Outcomes: After completion of course students will be able to:	
Paper I	study the advanced thermodynamics Maxwell equation, its application	
Physical Chemistry	to ideal gases, the concept of different laws of thermodynamics.	
	2. learn the concepts of quantum mechanics and be able to solve the problems related to 1D, 2D and 3D box, explain the role of operators in quantum mechanics.	
	3. study the kinetics of various complex reactions, understand the different theories of chemical kinetics.	

4. learn the theories dealing with ionic conductance, different types of batteries, study metal and bimolecular interactions.

Learning Outcomes:

On successful completion of this course students will be able to

- 1. understand the utility of Maxwell equations to predict the thermodynamic parameters for the ideal gases, predict the natural trend by studying different laws of thermodynamics.
- 2. understand the significance of the concept learnt in predicting still complicated quantum systems, predict the mechanical parameters concerning them with the simple mathematics aided by its beautiful approximations.
- 3. inculcate the skill of simplifying complicated reaction mechanisms, develop strategies to control gaseous reactions.
- 4. understand implementation the concept of ionic conductance, understand the development of commercial batteries, study the role of metal electrochemical interactions. With biomolecules.

References:

- 1. Peter Atkins and Julio de Paula, Atkin's *Physical Chemistry*, 7^aEdn., Oxford University Press, 2002.
- 2. K.J. Laidler and J.H. Meiser, *Physical Chemistry*, 2-Ed., CBS Publishers and Distributors, New Delhi, 1999.
- 3. Robert J. Silby and Robert A. Alberty, *Physical Chemistry*, 3-Edn., John Wiley and Sons (Asia) Pte. Ltd., 2002.
- 4. Ira R. Levine, *Physical Chemistry*, 5 Edn., Tata McGraw-Hill New Delhi, 2002.
- 5. G.W. Castellan, *Physical Chemistry*, 3-Edn., Narosa Publishing House, New Delhi, 1983.
- 6. S. Glasstone, Text Book of Physical Chemistry, 2-Edn., McMillan and Co. Ltd., London, 1962
- 7. B.K. Sen, Quantum Chemistry including Spectroscopy, Kalyani Publishers, 2003.
- 8. A.K. Chandra, Introductory Quantum Chemistry, Tata McGraw Hill, 1994.
- 9. R.K. Prasad, Quantum Chemistry, 2-Edn., New Age International Publishers, 2000.
- 10. S. Glasstone, *Thermodynamics for Chemists*, Affiliated East-West Press, New Delhi, 1964.
- 11. W.G. Davis, *Introduction to Chemical Thermodynamics A Non Calculus Approach*, Saunders, Philadelphia, 19772.

- 12. Peter A. Rock, *Chemical Thermodynamics*, University Science Books, Oxford University Press, 1983.
- 13. Ira N. Levine, *Quantum Chemistry*, 5^aEdn., Pearson Education (Singapore) Pte. Ltd., Indian Branch, New Delhi, 2000.
- 14. Thomas Engel and Philip Reid, Physical Chemistry, 3-Edn., Pearson Education Limited 2013.
- 15. D.N. Bajpai, Advanced Physical Chemistry, S. Chand 1-Edn., 1992.
- 16. *Bockris*, John O'M., *Reddy*, Amulya K.N., Gamboa-Aldeco, Maria E., Modern Electrochemistry, 2A, Plenum Publishers, 1998.
- 17. Physical Chemistry by Gurtu and Gurtu
- 18. A Text book of Physical Chemistry by K L kapoor Vol 5, 2 Edn

Course Code	Title	Credits
RJSPGCHE102	Inorganic Chemistry	4
Chemical Bonding	Unit I	1
_	aybridization Derivation of wave functions for sp , sp^2 , $sp3$ orbital considering only sigma bonding.	
	ement of d orbitals in various types of hybridizations. Concept of e energy, derivation expected. Formal charge with examples.	
1.3 Critical analysis of VB	т.	
1.4 Molecular Orbital Theory for diatomic species of First transition Series.		
1.5Molecular Orbital Theory for Polyatomic species considering σ bonding for SF ₆ , CO ₂ , B ₂ H ₆ , I ₃ - molecular species.		
1.6 Weak forces of attraction: Hydrogen bonding - concept, types, properties, methods of detection and importance. Van der Waal's forces, ion-dipole, dipole-dipole, London forces.		
	Unit-II	1
Molecular Symmetry and Group Theory:		
2.1Symmetry criterion of optical activity, symmetry restrictions on dipole moment. A systematic procedure for symmetry classification of molecules.		

- 2.2Concepts of Groups, Sub-groups, Classes of Symmetry operations, Group Multiplication Tables. Abelian and non-Abelian point groups.
- 2.3Representation of Groups: Matrix representation of symmetry operations, reducible and irreducible representations. The Great Orthogonality Theorem and its application in construction of character tables for point groups C₂v, C₃v and D_{2h}, structure of character tables.
- 2.4Applications of Group Theory
- (a) Symmetry adapted linear combinations (SALC), symmetry aspects of MO theory, sigma bonding in AB_n (Ammonia, CH₄) molecule.
- (b) Determination of symmetry species for translations and rotations.
- (c) Mulliken's notations for irreducible representations.
- (d) Reduction of reducible representations using reduction formula.
- (e) Group-subgroup relationships.
- (f) Descent and ascent in symmetry correlation diagrams showing relationship between different groups.

Unit: III

1

Materials Chemistry and Nanomaterials

3.1Solid State Chemistry

- 3.1.1 Electronic structure of solids and band theory, Fermi level, K Space and Brillouin Zones.
- 3.1.2 Structures of Compounds of the type: AB [nickel arsenide (NiAs), AB_{2:} fluorite (CaF₂) and anti-fluorite structures, rutile (TiO₂) structure and layer structure [cadmium chloride and iodide (CdCl₂, Cdl₂)].
- 3.1.3 Methods of preparation for inorganic solids: ceramic method, precursor method, sol-gel method (applications in Biosensors), microwave synthesis (discussion, principles, examples, merits and demerits are expected)

3.2 Nanomaterials

- 3.2.1 **Preparative methods:** Chemical methods, Solvothermal, Combustion synthesis, Microwave, Co-precipitation, Langmuir Blodgett (L-B) method, biological methods, synthesis using microorganisms.
- 3.2.2 Applications in the field of: solar cells, nanoelectronics and medicines.

M.Sc. Semester I Chemistry Syllabus

Unit IV Characterization of Coordination compounds

- 4.1 Structure elucidation of coordination compounds based on UV, IR, NMR and ESR spectroscopic techniques and magnetic measurements.
- 4.2 Spectral calculations using Orgel and Tanabe-Sugano diagram, calculation of electronic parameters such as Δ , B, C, Nephelauxetic ratio.
- 4.3 Determination of formation constants of metal complexes (Overall and Stepwise): Comparative studies of Potentiometric and spectral methods.

M.Sc.	Semester I Theory
RJSPGCHE102	Course Outcome:
Paper II	After completion of course students will be able to:
Inorganic Chemistry	Recapitulation of the concept of hybridization, understand molecular orbital theory and hydrogen bond.
	2.To adopt a systematic procedure for studying the symmetry of molecules.
	3. To understand the electronic structure of solids and methods for its preparation. Study nanomaterials and its application in different fields.
	4.Characterize the coordination compounds with the help of various spectroscopic techniques.
	Learning Outcome:
	On successful completion of this course students will be able to:
	1. Apply the concept of hybridization and derive the wave functions for sp, sp ² and sp ³ types involving sigma bonds, concept of resonance, resonance energy and formal charge calculations.
	2. Apply molecular orbital theory for various polyatomic species and finally to elaborate on hydrogen bond concept, its types, properties, methods of detection and its importance.
	3. Interpret the concepts of Groups, sub-groups, classes of symmetry and matrix representation of symmetry operations. To apply the concept of group theory to construct character table for different point groups and comprehend the applications of Group Theory.
	4. Students will be able to predict the electronic structure of AB, AB ₂ , antifluorite and rutile type solids and to learn the synthesis of inorganic solids by ceramic, precursor and sol-gel method.

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M.Sc. Semester I Chemistry Syllabus

- 5. To extend the above method for synthesizing nano materials and to study its application in the field of semiconductors and solar cells.
- 6. To characterize the coordination compounds with the help of various spectroscopic techniques and understand calculations of the formation constant of metal complexes and certain parameters like Nephelauxetic ratio from spectral data.

References:

Unit I

- 1. B. R. Puri, L. R. Sharma and K. C. Kalia, Principles of Inorganic Chemistry, Milestone Publishers, 2013-2014.
- 2. W. W. Porterfield, Inorganic Chemistry-A Unified Approach, 2-Ed., Academic Press, 1993.
- 3. B. W. Pfennig, Principles of Inorganic Chemistry, Wiley, 2015.
- 4. C. E. Housecroft and A. G. Sharpe, Inorganic Chemistry, Pearson Education Limited, 2-Edition 2005.
- 5. J. Huheey, F. A. Keiter and R. I. Keiter, Inorganic Chemistry–Principles of Structure and Reactivity, 4-Ed., Harper Collins, 1993.
- 6. P. J. Durrant and B. Durrant, Introduction to Advanced Inorganic Chemistry, Oxford University Press, 1967.
- 7. R. L. Dekock and H.B.Gray, Chemical Structure and Bonding, The Benjamin Cummings Publishing Company, 1989.
- 8. G. Miessler and D. Tarr, Inorganic Chemistry, 3-Ed., Pearson Education, 2004.
- 9. R. Sarkar, General and Inorganic Chemistry, Books & Allied (P) Ltd., 2001.
- 10. C. M. Day and J. Selbin, Theoretical Inorganic Chemistry, Affiliated East West Press Pvt. Ltd., 1985.
- 11. J. N. Murrell, S. F. A. Kettle and J. M. Tedder, The Chemical Bond, Wiley, 1978.
- 12. G. A. Jeffrey, An Introduction to Hydrogen Bonding, Oxford University Press, Inc., 1997.

Unit II

- 1. F. A. Cotton, Chemical Applications of Group Theory, 2-Edition, Wiley Eastern Ltd., 1989.
- 2. H. H. Jaffe and M. Orchin, Symmetry in Chemistry, John Wiley & Sons, New York, 1996.
- 3. R. L. Carter, Molecular Symmetry and Group Theory, John Wiley & Sons, New York, 1998.
- 4. K. V. Reddy. Symmetry and Spectroscopy of Molecules, 2-Edition, New Age International Publishers, New Delhi, 2009.
- 5. A. SalahuddinKunju and G. Krishnan, Group Theory and its Applications in Chemistry, PHI Learning, 2012.
- 6. P. K. Bhattacharya, Group Theory and its Chemical Applications, Himalaya Publishing House. 2014.

7. S. Swarnalakshmi, T. Saroja and R. M. Ezhilarasi, A Simple Approach to Group Theory in Chemistry, Universities Press, 2008.

Unit III

- 1. Solid State Chemistry Introduction, Lesley E. Smart, Elaine A. Moore, ISBN 0-203-49635-3, Taylor & Francis Group, LLC.
- 2. Nanomaterials & Nanochemistry, 2007, Catherine Brechignac, Philippe Houdy, Marcel Lahmani, ISBN 978-3-540-72992-1 Springer Berlin Heidelberg New York.
 - 3. Nanomaterials Chemistry, Recent Developments and New Directions C.N.R. Rao, A. Muller, and A.K. Cheetham, ISBN 978-3-527-31664-9, 2007 WILEY-VCH Verlag GmbH & Co. KGaA, Weinheim.
- 4. Nano-Surface Chemistry, 2001, Morton Rosoff, ISBN: 0-8247-0254-9, Marcel Dekker Inc. New York.
 - 5. The Chemistry of Nanomaterials, CNR Rao, Muller Cheetham, WILEY-VCH Verlag GmbH & Co. KGaA, Weinheim, 2004.
 - 6. Semiconductor Nanomaterials, Challa S.S.R. Kumar, ISBN: 978-3-527-32166-7, WILEY-VCH Verlag GmbH & Co. KGaA, Weinheim, 2010.

Unit IV

- 1. J. E. Huheey, E. A. Keiter and R. L. Keiter; Inorganic Chemistry: Principles of Structure and Reactivity, Pearson Education, 2006.
- 2. D. Banerjea ,Coordination Chemistry
- 3. Geary Coordination reviews
- 5. P.W. Atkins, T. Overton, J. Rourke, M. Weller and F. Armstrong; Shriver & Atkins: Inorganic Chemistry, 4-ed. Oxford University Press, 2006. (Physical methods in inorganic chemistry,topic.no.8,pg.223-253)
- 6. F. A. Cotton, G. Wilkinson, C. A. Murillo and M. Bochmann; Advanced Inorganic Chemistry, 6-ed. Wiley, 1999,
- 7. B. Douglas, D. McDaniel and J. Alexander. *Concepts and Models of Inorganic Chemistry* (3rd edn.), John Wiley & Sons (1994).
- 8. 7.J.D Lee, Concise Inorganic chemistry, ELBS. (Chapter 32, Spectra, Pg. 938-971)
- 9. 8.R.S.Drago ,Physical methods in inorganic chemistry,

Course Code	Title	Credits
COURT OF CHARGE CONTROL OF CHARGE CHA		4
	Unit I	1
Physical Organic Chem	istry:	
constants, reaction coor activated complex, Ha	d kinetic requirements of a reaction: rate and equilibrium rdinate diagram, transition state (activated complex), nature of mmond postulate, Reactivity vs selectivity, Curtin-Hammett versibility, Kinetic vs thermodynamic control of organic reactions.	
isotopes (Kinetic isotope	Inism of a reaction: Product analysis, kinetic studies, use of effect – primary and secondary kinetic isotope effect). Detection diates, crossover experiments and stereochemical evidence.	
effect, resonance, bond solvation. Comparative s	tors affecting acidity and basicity: Electronegativity and inductive strength, electrostatic effects, hybridization, aromaticity and study of acidity and basicity of organic compounds on the basis ffect and non-aqueous solvents. Acid and base catalysis – general h examples.	
	Unit II	1
Nucleophilic substitution	reactions and Aromaticity	
2.1Nucleophilic substitut	ion reactions:	
SET mechanisms. SN robonds. Factors affecti	c substitution: SN^1 , SN^2 , SN^i reactions, mixed SN^1 and SN^2 and eactions involving NGP - participation by aryl rings, α -and ping these reactions: substrate, nucleophilicity, solvent, sterication, leaving group. Ambident nucleophiles. S_NcA , S_N1' and S_N2' ylic) carbon.	
2.1.2 Aromatic nucleophilic substitution: SN ^{Ar,} SN ¹ , benzyne mechanisms. Ipso, cine, tele and vicarious substitution.		
2.1.3 Ester hydrolysis: Classification, nomenclature and study of all eight mechanisms of acid and base catalyzed hydrolysis with suitable examples.		
2.2 Aromaticity:		
2.2.1 Structural, thermochemical, and magnetic criteria for aromaticity, including NMR characteristics of aromatic systems. Delocalization and aromaticity.		

- 2.2.2 Application of HMO theory to monocyclic conjugated systems. Frost-Musulin diagrams. Huckel's (4n+2) and 4n rules.
- 2.2.3 Aromatic and antiaromatic compounds up-to 18 carbon atoms. Homoaromatic compounds. Aromaticity of all benzenoid systems, heterocycles, metallocenes, azulenes, annulenes, aromatic ions and Fullerene (C₆₀).

Unit-III

1

Stereochemistry:

- 3.1 **Concept of Chirality:** Recognition of symmetry elements.
- 3.2 **Molecules with tri- and tetra-coordinate centers:** Compounds with carbon, silicon, nitrogen, phosphorous and sulphur chiral centers, relative configurational stabilities.
- 3.3 Molecules with two or more chiral centers: Constitutionally unsymmetrical molecules: erythro-threo and syn-anti systems of nomenclature. Interconversion of Fischer, Sawhorse, Newman and Flying wedge projections. Constitutionally symmetrical molecules with odd and even number of chiral centers: enantiomeric and meso forms, concept of stereo genic, chirotopic, and pseudo asymmetric centers. R-S nomenclature for chiral centres in acyclic and cyclic compounds.
- 3.4 **Axial and planar chirality:** Principles of axial and planar chirality. Stereochemical features and configurational descriptors (R, S) for the following classes of compounds: allenes, alkylidene cycloalkanes, spirans, biaryls (buttressing effect) (including BINOLs and BINAPs), ansa compounds, cyclophanes, trans-cyclooctenes.
- 3.5 **Prochirality:** Chiral and prochiral centres; prochiral axis and prochiral plane. Homotopic, heterotopic (enantiotropic and diastereotropic) ligands and faces. Identification using substitution and symmetry criteria. Nomenclature of stereoheterotropic ligands and faces. Symbols for stereoheterotropic ligands in molecules with i) one or more prochiral centres ii) a chiral as well as a prochiral center, iii) a prochiral axis iv) a prochiral plane v) pro-pseudo asymmetric center. Symbols for enantiotropic and diastereotropic faces.

Unit-IV

1

- **4.1 Oxidation:** General mechanism, selectivity, and important applications of the following:
- 4.1.1 **Dehydrogenation:** Dehydrogenation of C-C bonds including aromatization of six membered rings using metal (Pt, Pd, Ni) and organic reagents (chloranil, DDQ).
- 4.1.2 **Oxidation of alcohols to aldehydes and ketones:** Chromium reagents such as K₂Cr₂O₇/H₂SO₄ (Jones reagent), CrO₃-pyridine (Collin's reagent), PCC (Corey's reagent) and PDC (Cornforth reagent), hypervalent iodine reagents (IBX, Dess-Martin periodinane). DMSO based reagents (Swern oxidation), Corey-Kim oxidation advantages over Swern and limitations; and Pfitzner-Moffatt oxidation-DCC and DMSO and Oppenauer oxidation.
- 4.1.3 **Oxidation involving C-C bonds cleavage:** Glycols using HIO₄; cycloalkanones using CrO₃; carbon-carbon double bond using ozone, KMnO₄, CrO₃, NaIO₄ and OsO₄; aromatic rings using RuO₄ and NaIO₄.

- 4.1.4 **Oxidation involving replacement of hydrogen by oxygen:** oxidation of CH₂ to CO by SeO₂, oxidation of aryl methanes by CrO₂Cl₂ (Étard oxidation).
- 4.1.5 **Oxidation of aldehydes and ketones:** with H₂O₂ (Dakin reaction), with peroxy acid (Baeyer-Villiger oxidation)
- **4.2 Reduction:** General mechanism, selectivity, and important applications of the following reducing reagents:
- 4.2.1 **Reduction of CO to CH₂ in aldehydes and ketones-** Clemmensen reduction, Wolff-Kishner reduction and Huang-Minlon modification.
- 4.2.2 **Metal hydride reduction:** Boron reagents (NaBH₄, NaCNBH₃, diborane, 9-BBN, Na(OAc)₃BH, aluminium reagents (LiAlH₄, DIBAL-H, Red Al, L and K- selectrides).
- 4.2.3 NH₂NH₂ (diimide reduction) and other non-metal-based agents including organic reducing agents (Hantzsch dihydropyridine).
- 4.2.4 **Dissolving metal reductions:** using Zn, Li, Na, and Mg under neutral and acidic conditions, Li/Na-liquid NH₃ mediated reduction (Birch reduction) of aromatic compounds and acetylenes.

M.Sc.	Semester I Theory	
RJSPGCHE103	Course Outcomes:	
Damar III	After completion of course students will be able to:	
Paper-III	1.Understand Physical concept of organic reactions	
Organic chemistry	2. Understand mechanism of nucleophilic substitution reactions including factors affecting these reactions.	
	3. Comprehend the concept of chirality in a molecule having more than one asymmetric center.	
	4. understand the reagents used for oxidation and reduction	
	Learning Outcomes:	
	After studying this unit students will be able to:	
	1. 1.Understand the principles of thermodynamic and kinetic requirement of reaction.	
	2. understand different methods to determine the reaction mechanisms.	
	3. the factor affecting acidity and basicity	
	4. To understand aliphatic and aromatic nucleophilic substitution reactions.	
	5. To recognize structural, thermochemical, and magnetic criteria for aromaticity including application of HMO theory monocyclic	

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- conjugated system.
- 6. To understand the concept of aromaticity, anti-aromaticity and homo aromaticity in annulenes, charged rings, fused ring systems and heterocycles.
- 7. To study the concept of chirality with respect to the molecules having two or more chiral centers.
- 8. To explore the concept of axial and planar chirality and prochirality
- 9. To explore general mechanism, selectivity, and important applications of different oxidizing and reducing agents in organic reactions. 2.Undestand the use of different oxidizing and reducing agents in terms of industrial applications

Reference Books:

- 1. Physical Organic Chemistry, Neil Isaacs
- 2. Modern Physical Organic Chemistry, Eric V. Anslyn and Dennis A. Dougherty
- 3. Comprehensive Organic chemistry, Barton and Ollis, Vol 1
- 4. Organic Chemistry, J. Claydens, N. Greeves, S. Warren and P. Wothers, Oxford University Press.
- 5. Advanced Organic Chemistry, F.A. Carey and R.J. Sundberg, Part A and B, Plenum Press.
- 6. Stereochemistry: Conformation and mechamism, P.S. Kalsi, New Age International, New Delhi.
- 7. Stereochemistry of carbon compounds, E.L Eliel, S.H Wilen and L.N Manden, Wiley.
- 8. Stereochemistry of Organic Compounds- Principles and Applications, D. Nasipuri. New International Publishers Ltd.
- 9. March's Advanced Organic Chemistry: Reactions, Mechanisms and Structure, Michael B. Smith, Jerry March, Wiley.
- 10. Advanced Organic Chemistry: Reactions and mechanism, B. Miller and R. Prasad, Pearson Education.
- 11. Advanced Organic Chemistry: Reaction mechanisms, R. Bruckner, Academic Press.
- 12. Understanding Organic Reaction Mechanisms, Adams Jacobs, Cambridge University Press.
- 13. Writing Reaction Mechanism in organic chemistry, A. Miller, P.H. Solomons, Academic Press.
- 14. Principles of Organic Synthesis, R.O.C. Norman and J.M Coxon, Nelson Thornes.
- 15. Advanced Organic Chemistry: Reactions and mechanism, L.G. Wade, Jr., Maya Shankar Singh, Pearson Education.
- 16. Mechanism in Organic Chemistry, Peter sykes, 6th edition onwards.
- 17. Modern Methods of Organic Synthesis, W. Carruthers and Iain Coldham, Cambridge University Press.
- 18. Organic Synthesis, Jagdamba Singh, L.D.S. Yadav, PragatiPrakashan.

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RJSPGCHE104	Analytical Chemistry	4
Course Code	Title	Credits

Unit I:

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1.1 Language of Analytical Chemistry

- 1.1.1 Analytical perspective, Common analytical problems, terms involved in analytical chemistry (analysis, determination, measurement, techniques, methods, procedures and protocol)
- 1.1.2 An overview of analytical methods, types of instrumental methods, instruments for analysis, detectors, fundamental characteristic of detectors with respect to spectral response and linearity, quantum efficiency, dynamic range, response time, noise, transducers and sensors, performance characteristic of instruments: Figures of merit like precision, bias, sensitivity, detection limit, dynamic range and selectivity. Calibration and standardization
- 1.1.3 Errors, determinate and indeterminate errors. Types of determinate errors, Calibration and standardization, minimization of errors.
- 1.1.4 Quantitative methods of analysis: calibration curve, standard addition and internal standard method.

1.2 Quality in Analytical Chemistry:

1.2.1 Quality Management System (QMS):

Evolution and significance of Quality Management, types of quality standards for laboratories, total quality management (TQM), philosophy implementation of TQM (reference of Kaizen, Six Sigma approach & 5S), quality audits and quality reviews, responsibility of laboratory staff for quality and problems.

1.2.2 Safety in Laboratories:

Basic concepts of Safety in Laboratories, Personal Protection Equipment (PPE), OSHA, Toxic Hazard (TH) classifications

1.2.3 Accreditations:

Accreditation of Laboratories, Introduction to ISO series, Indian Government Standards (ISI, Hallmark, AGMARK)

1.2.4 Good Laboratory Practices (GLP)

Principle, Objective, OECD guidelines, The US FDA 21CFR58, Klimisch score

Unit II:

1

1

Calculations based on Chemical Principles

The following topics are to be covered in the form of numerical problems only:

- a) Concentration of a solution based on volume and mass units.
- b) Calculations of ppm, ppb and dilution of the solutions, concept of mmol.
- c) Stoichiometry of chemical reactions, concept of kg mol, limiting reactant, theoretical and practical yield.
- d) Solubility and solubility equilibria, effect of presence of common ion.
- e) Calculations of pH of acids, bases, acidic and basic buffers.
- f) Oxidation number, rules for assigning oxidation number, redox reaction in term of

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oxidation number, oxidizing and reducing agents, equivalent weight of oxidizing and reducing agents, stoichiometry of redox titration (Normality of a solution of a oxidizing / reducing agent and its relationship with molarity).

Unit: III

1

Optical Methods

3.1Recapitulation and FT Technique

- 3.1.1 Recapitulation of basic concepts, Electromagnetic spectrum, Sources, Detectors, sample containers.
- 3.1.2 Laser as a source of radiation, Fibre optics.
- 3.1.3 Introduction of Fourier Transform.

3.2 Molecular Ultraviolet and Visible Spectroscopy

NUMERICALS ARE EXPECTED

3.2.1Derivation of Beer- Lambert's Law and its limitations, factors affecting molecular absorption, types of transitions [emphasis on charge transfer absorption], pH, temperature, solvent and effect of substituents.

Applications of Ultraviolet and Visible spectroscopy:

- 1) On charge transfer absorption
- 2) Simultaneous spectroscopy
- 3) Derivative Spectroscopy
- 3.2.2 Dual spectrometry Introduction, Principle, Instrumentation and Applications

3.3 Infrared Absorption Spectroscopy

- 3.3.1 Instrumentation: Sources, Sample handling, Transducers, Dispersive, non-dispersive instrument
- 3.3.2 FTIR and its advantages
- 3.3.3 Applications of IR [Mid IR, Near IR, Far IR]: Qualitative with emphasis on "Finger print" region, Quantitative analysis, Advantages and Limitations of IR.
- 3.3.4 Introduction and basic principles of diffuse reflectance spectroscopy.

Unit: IV

1

4.1 Thermal Methods:

- 4.1.1 **Introduction:** Recapitulation of types of thermal methods, comparison between TGA and DTA.
- 4.1.2 **Differential Scanning Calorimetry:** Principle, comparison of DTA and DSC, Instrumentation, Block diagram, Nature of DSC Curve, Factors affecting curves (sample size, sample shape, pressure).
- 4.1.3 **Applications:** Heat of reaction, Specific heat, Safety screening, Polymers, liquid crystals, Percentage crystallinity, oxidative stability, Drug analysis, Magnetic transition. e.g. Analysis of Polyethylene for its crystallinity.

4.2 Automation in chemical analysis:

Need for automation, Objectives of automation, An overview of automated instruments and instrumentation, process control analysis, flow injection analysis, discrete automated systems, automatic analysis based on multilayered films, gas monitoring equipments, Automatic titrators. **Beckman analyzer, Dupont analyzer**,

M. Sc.	Semester I theory
RJSPGCHE104 Analytical	Course outcomes:
Chemistry	1. The young talents will be able to understand the language of analytical chemistry, basic principles & its applications.
	2. Students will be introduced to the concept of 'quality' in analytical chemistry, safety in laboratories, accreditations and GLP.
	3. Students will understand, solve & interpret the problems based on chemical principles, employing statistical tools.
	4. Students will be introduced to automation in chemical analysis in order to bring best opportunities to each student, enabling them to get dream position in the industry.
	5. Students will be encouraged to pursue research in the frontier areas of analytical chemistry.
	Learning Outcomes:
	 After learning this unit, students will understand the types of errors, sources of error, parameters used to indicate accuracy & precision of methods, methods used for quantification, Quality Management System, Safety measures in Laboratories, Accreditation of Laboratories & Good Laboratory Practices. After learning this unit, students will be able to understand, solve & interpret the problems based on chemical principles, employing
	 statistical tools. 3. After learning this unit, students will be able to understand the basic concepts of Molecular Ultraviolet and Visible Spectroscopy, IR spectroscopy and advantages of FT techniques. 4. After learning this unit, students will be able to understand the basic information about thermal methods, principle and working of Differential Scanning Calorimetry, need and objectives of Automation in chemical analysis.

M.Sc. Semester I Chemistry Syllabus

References

Unit I

- 1. Modern Analytical Chemistry by David Harvey, McGraw-Hill Higher Education
- 2. Principles of Instrumental Analysis Skoog, Holler and Nieman, 5-Edition, Ch. 1.
- 3. Fundamentals of Analytical Chemistry, By Douglas A. Skoog, Donald M. West, F. James Holler, Stanley R. Crouch, 9-Edition, 2004, Ch: 5.
- 4. Undergraduate Instrumental Analysis, 6-Edition, J W Robinson, Marcel Dekker, Ch:1.
- 5. ISO 9000 Quality Systems Handbook, Fourth Edition, David Hoyle. (Chapter: 3 & 4) (Free download).
- 6. Quality in the Analytical Laboratory, Elizabeth Pichard, Wiley India, Ch. 5, Ch. 6 & Ch. 7.
- 7. Quality Management, Donna C S Summers, Prentice-Hall of India, Ch:3.
- 8. Quality in Totality: A Manager's Guide To TQM and ISO 9000, ParagDiwan, Deep & Deep Publications, 1st Edition, 2000.
- 9. Quality Control and Total Quality Management P.L. Jain-Tata McGraw-Hill (2006) Total Quality Management Bester field Pearson Education, Ch:5.
- 10. Industrial Hygiene and Chemical Safety, M H Fulekar, Ch:9, Ch:11 & Ch:15.
- 11. Safety and Hazards Management in Chemical Industries, M N Vyas, Atlantic Publisher, Ch:4, Ch:5 & Ch:19.
- 12. Staff, World Health Organization (2009) Handbook: Good Laboratory Practice (GLP)
- 13. OECD Principles of Good Laboratory Practice (as revised in 1997)". OECD Environmental Health and Safety Publications.OECD.1. 1998.
- 14. Klimisch, HJ; Andreae, M; Tillmann, U (1997). "A systematic approach for evaluating the quality of experimental toxicological and eco-toxicological data". doi:10.1006/rtph.1996.1076. PMID 9056496.

Unit II

1. 3000 solved problems in chemistry, Schaums Solved problem series, David E. Goldbers, McGraw Hill international Editions, Chapter 11,15,16,21,22

Unit III

- 1. D. A. Skoog, F. J. Holler, T. A. Nieman, Principles of Instrumental Analysis, 5-Edition, Harcourt Asia Publisher. Chapter 6, 7.
- 2. H. H. Willard, L. L. Merritt, J. A. Dean, F. A. Settle, Instrumental Methods of Analysis,6 th Edition, CBS Publisher. Chapter 2.
- 3. R. D. Braun, Introduction to Instrumental Analysis, McGraw Hill Publisher. Chapter 8.
- 4. D. A. Skoog, F. J. Holler, T. A. Nieman, Principles of Instrumental Analysis, 5 th Edition, Harcourt Asia Publisher. Chapter 13, 14.
- 5. H. H. Willard, L. L. Merritt, J. A. Dean, F. A. Settle, Instrumental Methods of Analysis,6 th Edition, CBS Publisher. Chapter 2.
- 6. R. D. Braun, Introduction to Instrumental Analysis, McGraw Hill Publisher. Chapter 5.
- 7. G. W. Ewing, Instrumental Methods of Chemical Analysis, 5 th Edition, McGraw Hill Publisher, Chapter 3.
- 8. M. Ito, The effect of temperature on ultraviolet absorption spectra and its relation to hydrogen bonding, J. Mol. Spectrosc. 4 (1960) 106-124.

- 9. A. J. Somnessa, The effect of temperature on the visible absorption band of iodine inseveral solvents, Spectrochim. Acta. Part A: Molecular Spectroscopy, 33 (1977) 525-528.
- 10. D. A. Skoog, F. J. Holler, T. A. Nieman, Principles of Instrumental Analysis, 5 th Edition, Harcourt Asia Publisher. Chapter 16, 17.
- 11. R. D. Braun, Introduction to Instrumental Analysis, McGraw Hill Publisher. Chapter 12
- 12. Z. M. Khoshhesab (2012). Infrared Spectroscopy- Materials Science, Engineering and Technology. Prof. Theophanides Theophile (Ed.). ISBN: 978-953-51-0537-4, InTech,(open access)

Unit IV

- 1. Introduction to instrumental methods of analysis by Robert D. Braun, Mc. Graw Hill (1987): Chapter 27
- 2. Thermal Analysis-theory and applications by R. T. Sane, Ghadge, Quest Publications
- 3. Instrumental methods of analysis, 7 th Edition, Willard, Merrit, Dean: Chapter 25
- 4. Instrumental Analysis, 5 th Edition, Skoog, Holler and Nieman: Chapter 31
- 5. Quantitative Chemical Analysis, 6 th Edition, Vogel: Chapter 12
- 6. Analytical Chemistry by Open Learning: Thermal Methods by James W. Dodd & Dodd & Tonge Tonge
- 7. Instrumental methods of analysis, 7 th Edition, Willard, Merrit, Dean: Chapter 26
- 8. Instrumental Analysis, 5th Edition, Skoog, Holler and Nieman: Chapter 33
- 9. Introduction to instrumental methods of analysis by Robert D. Braun, Mc. GrawHill (1987): Chapter 28

Course Code	Practical Title	Credits
RJSPGCHEPR101	Physical Chemistry Practical	2

Non – Instrumental:

- 1. To determine the heat of solution (ΔH) of a sparingly soluble acid (benzoic /salicylic acid) from solubility measurement at three different temperatures.
- 2. To study the variation of calcium sulphate with ionic strength and hence determine the thermodynamic solubility product of CaSO₄ at room temperature.
- 3. To investigate the reaction between acetone and iodine.
- 4. To study the variation in the solubility of Ca(OH)₂ in presence of NaOH and hence to determine the solubility product of Ca(OH)₂ at room temperature.
- 5. Graph Plotting of mathematical functions –linear, exponential and trigonometry and identify whether functions are acceptable or non-acceptable?

Instrumental:

- 1. To determine the mean ionic activity coefficient of an electrolyte by e.m.f. measurement.
- 2. To study the effect of substituent on the dissociation constant of acetic acid conductometrically.
- 3. To determine pKa values of phosphoric acid by potentiometric titration with sodium hydroxide using glass electrode.
- 4. To verify Ostwald's dilution law and to determine the dissociation constant of a weak monobasic acid conductometrically.

M.Sc	Semester I Practical
RJSPGCHEPR101	Course Outcome:
Practical I	Students will be able to determine:
Physical	
Chemistry	1. ΔH, Ksp, order of reaction/reactant, solubility variation, acceptable function, mean ionic activity coefficient, effect of substituent, pKa values, dissociation constants by simple and convenient instrumental/non-instrumental methods.
	Learning Outcomes: On successful completion of this course students will be able to:
	1. understand the reactivity of species on the basis of these parameters, select the right function representing the quantum system and develop the skills to study analogous systems.

References:

- 1 Practical Physical Chemistry, B. Viswanathan and P.S. Raghavan, Viva Books Private Limited, 2005.
- 2 Practical Physical Chemistry, A.M. James and F.E. Prichard, 3-Edn., Longman Group Ltd., 1974.
- 3 Experimental Physical Chemistry, V.D. Athawale and P. Mathur, New Age International Publishers, 2001.

Course Code	Practical Title	Credits
RJSPGCHEPR102	Inorganic Chemistry Practical	2

Ores and Alloys

- 1) Analysis of Devarda's alloy.
- 2) Analysis of Cu Ni alloy.
- 3) Analysis of Tin Solder alloy.
- 4) Analysis of Limestone.

Instrumentation

- 1) Estimation of Copper using Iodometric method potentiometrically.
- 2) Estimation of Fe³⁺ solution using Ce(IV) ions potentiometrically

M.Sc	Semester I Practical
RJSPGCHEPR102	Course Outcomes:
Practical II	1. Students will learn to analyze ore and alloys.
Inorganic Chemistry	2. Learn to estimate metal ions potentiometrically.
	Learning outcomes:
	On successful completion of this course students will be able to:
	1. Learn to do the analysis of alloys and estimate the percentage of metal content by volumetric and gravimetric methods.
	2. Estimate the metal ions (like Fe ³⁺ and Ce ⁴⁺) present in the given solution potentiometrically.

Reference:

- 1. Advanced experiments in Inorganic Chemistry., G. N. Mukherjee., 1-Edn., 2010., U.N.Dhur& Sons Pvt Ltd
- 2. The Synthesis and Characterization of Inorganic Compounds by William L. Jolly
- 3. Inorganic Chemistry Practical Under UGC Syllabus for M.Sc. in all India Universities By: Dr Deepak Pant

	RJSPGCHEPR103	Organic Chemistry Practical	2
(Course Code	Practical Title	Credits

One step preparations (1.0 g scale)

- 1. Bromobenzene to p-nitrobromobenzene
- 2. Anthracene to anthraquinone
- 3. Benzoin to benzil
- 4. Anthracene to Anthracene maleic anhydride adduct
- 5. 2-Naphthol to BINOL
- 6. p-Benzoquinone to 1,2,4-triacetoxybenzene
- 7. Ethyl acetoacetate to 3-methyl-1-phenylpyrazol-5-one
- 8. o-Phenylenediamine to 2-methylbenzimidazole
- 9. o-Phenylenediamine to 2,3-diphenylqunooxaline
- 10. Urea and benzil to 5,5-diphenylhydantoin

M.Sc	Semester I
RJSPGCHEPR103	Course Outcomes:
Practical III	1. Students will be able to plan the synthesis and study reaction parameters including stoichiometry and safety aspect. Students will also understand the process of purification of product by crystallization and checking its purity by TLC and melting point.
	Learning Outcomes: Students will acquire in-depth knowledge of how to Design and carry out synthesis as well as accurately record the results of synthesis.

Course Code	Practical Title	Credits
RJSPGCHEPR104	Analytical Chemistry Practical	2

- 1. To carry out assay of the sodium chloride injection by Volhard's method. Statistical method.
- 2. To determine (a) the ion exchange capacity (b) exchange efficiency of the given cation exchange resin.
- 3. To determine amount of Cr(III) and Fe(II) individually in a mixture of the two by titration with $FDT\Delta$
- 4. To determine the breakthrough capacity of a cation exchange resin.
- 5. To determine the lead and tin content of a solder alloy by titration with EDTA.
- 6. To determine amount of Cu(II) present in the given solution containing a mixture of Cu(II) and Fe(II).
- 7. To determine number of nitro groups in the given compound using TiCl₃.

M.Sc.	Semester I Practical
RJSPGCHEPR104 Practical /V	 Course Outcome: The students will be exposed to the various methods of titrations such as precipitation titration, complexometric titration; and ion exchange chromatography. Learning Outcomes: After performing experiments students will understand the concept of primary and secondary standards, how to carry out assay of commercial samples, preparation of ion exchange column and determination of capacity of resin.

References:

- 1. Quantitative Inorganic Analysis including Elementary Instrumental Analysis by A. I. Vogels, 3rdEd. ELBS (1964)
- 2. Vogel's textbook of quantitative chemical analysis, Sixth Ed. Mendham, Denny, Barnes, Thomas, Pearson education
- 3. Standard methods of chemical analysis, F. J. Welcher
- 4. Standard Instrumental methods of Chemical Analysis, F. J. Welcher
- 5. W.W.Scott."Standard methods of Chemical Analysis", Vol.I, Van Nostrand Company, Inc., 1939.
- 6. E.B.Sandell and H.Onishi, "Spectrophotometric Determination of Traces of Metals", Part-II, 4th Ed., A Wiley Interscience Publication, New York, 1978

M.Sc. Semester I Chemistry Syllabus

M.Sc. (Chemistry) Semester - I &II

Paper Pattern

Internal Exam

1. Class Test: 20 marks

2. Presentation: 20 marks

Paper Pattern for Semester End Examination

Maximum Mark: 60 Duration: 2Hrs

There will be 5 questions each of 12 marks.

Q.1 from Unit I, Q.2 from Unit II, Q.3 from Unit III and Q.4 from Unit IV.

The pattern for above questions is as follows:

- > Each question will have five sub questions of 4 marks each.
- ➤ Learners have to attempt any 3 questions out of 5.
- Q. 5 will have 8 sub questions of 3 marks each (2 questions will be from each unit).

Learners have to attempt any 4 questions out of 8.

Practical Exam

Practical exam will be of 50 marks.

> Experiment: 40 marks

> Journal : 5 marks

➤ Viva : 5 marks