**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: RJSPGCHEP

## CBCS: 2020 -2021

# M.Sc. (Physical Chemistry) Semester – IV

| Course | Nomenclature | Credits | Topics |
|---|---|---|---|
| RJSPGCHEP401 | Paper - I<br>Polymer, Green, Biophysical and Applied | 4 | Polymer Chemistry II<br>Polymer Chemistry-III.<br>Bio-physical Chemistry and Green Chemistry.<br>Photochemistry-II: Kinetics and Applications<br>Photophysical Kinetics of bimolecular processes.<br>Solar Cells. |
| RJSPGCHEP402 | Paper - II<br>Material Science, Network and Irreversible Thermodynamics | 4 | Metals and alloys.<br>Mechanical properties of solid materials.<br>Lasers and superconductors.<br>Non-equilibrium thermodynamics |
| RJSPGCHEP403 | Paper - III<br>Symmetry & Spectroscopy | 4 | Symmetry in Chemistry.<br>N.M.R. Spectroscopy-I.<br>ESR and Mossbauer Spectroscopy.<br>$^{13}C$ N.M.R. Spectroscopy |
| RJSPGCHEP404 | Paper - IV<br>Intellectual Property Rights & Cheminformatics | 4 | Introduction to Intellectual Property.<br>Patents, Industrial Designs, Copyrights, Trade Marks, Geographical Indications.<br>Trade Secrets<br>IP Infringement issue and enforcement.<br>Economic Value of Intellectual Property.<br>Different International agreements.<br>Introduction to Chem informatics<br>Representation of molecules and chemical reactions .<br>Searching Chemical Structures.<br>Applications |

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| RJSPGCHEPRP401 | Practical-I | 8 | Polymer, Green, Biophysical And Applied Practical |
| RJSPGCHEPRP402 | Practical-II | | Material Science, Network and Irreversible Thermodynamics Practical |
| RJSPGCHEPRP403 | Practical-III | | Symmetry & Spectroscopy Practical |
| RJSPGCHEPRP404 | Practical-IV | | Intellectual Property Rights & Cheminformatics Practical |

**Theory semester IV**

| Course Code | Title | Credits |
|---|---|---|
| **RJSPGCHEP401** | **Paper – I Polymer, Green, Biophysical and Applied** | 4 |
| **Unit – I**<br>**Polymer Chemistry II**<br>**1.1 Polymers in solid state** – Transitions (glass transition and crystalline melting temperature), crystalline behaviour, factors affecting crystallinity, polymer blends and Alloys.<br>**1.2 Identification and characterization of polymers**: Chemical analysis- End group analysis; Physical analysis by Spectral methods: IR, UV, Raman, NMR, X-ray diffraction analysis, microscopic methods: SEM, TEM, Thermal analysis-TGA, DTA & DSC.<br>**1.3 Properties of polymers**: Thermal (glass transition temperature, and its determination), mechanical (deformation and fracture) effects in polymers, visco elasticity surface (surface tension, hardness, friction, abrasion), physical (Impact strength, Tensile strength, solubility) of polymers, weather ability, rheology and mechanical models, mechanical behavior, Rubber elasticity.<br>**1.4 Polymer degradation and stabilization**: Oxidative, thermal, radiation, Biodegradation | | 1 |

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| **Unit II:**<br>**Polymer Chemistry-III**<br><br>**2.1 Techniques of polymerization**: Bulk polymerization, solution polymerization, suspension polymerization, emulsion polymerizations,<br>**2.2 Thermodynamics of polymer solutions**: Solubility parameter, thermodynamics of mixing**,** theta temperature<br><br>**2.1 Polymer technology**:<br>**2.1.1** Polymer auxiliaries, plasticizers, heat Stabilizers, colorants, flame retardants. fillers, rein for cements,<br>**2.1.2** Elastomers: Introduction, Processing, Rubber Types, Vulcanization, Properties, Reclaiming.<br>**2.1.3** Fibers: introduction, production, Fiber spinning, Textile fibers, Industrial fibers,<br>recycling.<br>**2.1.4** Films sheets: Introduction and processing techniques (injection and blow Moulding extrusion), Recycling of plastics.<br>**2.2 Properties and applications of some commercially important polymers**. Carbochain polymers- Polyolefins, ABS group, elastomers, vinyl polymers, acrylic polymers, heterochain polymers- polyethers, polycarbonates, polysaccharides, polyamides fluoropolymers, Resins (epoxy, alkyd, phenol-formaldehyde and urea-formaldehyde), Silicones, polyphosphazenes, sulphur containing polymers. | 1 |

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| **UNIT-III**<br>**Bio-physical Chemistry and Green Chemistry**<br><br>**Biophysical Chemistry**<br>**3.1.1** Introduction to Complex Biomolecules: Proteins, enzymes, DNA, RNA, polysaccharides and lipids. chirality and pH dependence of biomolecules.<br>**3.1.2** Biosensors: Enzyme based, Electrochemical, immunosensor, fluorescence, optical, Piezoelectric Biosensors.<br>**3.1.3** Electrophoresis (Technique for bio-molecular study): Principle and factors affecting electro-phoretic mobility, zone electrophoresis, Paper electrophoresis, cellulose acetate electrophoresis, Gel electrophoresis. capillary Electrophoresis, Application of electrophoresis.<br><br>**3.2 Green Chemistry:**<br>**3.2.1** Recapitulation of principles of green chemistry, Waste minimization techniques.<br>**3.2.2** Catalysis and Green Chemistry: Phase transfer catalysts, biocatalyst, photo catalysis. Organic solvents, solvent free system, supercritical fluid, ionic liquid, their characteristics, use as catalyst and solvents. Alternative energy sources for initiation and execution of chemical reaction: Microwave and sonochemistry. | 1 |
| **UNIT-IV**<br><br>**Photochemistry-II: Kinetics and Applications**<br>**4.1: Photophysical Kinetics of bimolecular processes.**<br>4.1.1: Mechanism of fluorescence quenching.<br>4.1.2: Collisions in solutions<br>4.1.3: Kinetics of collisional quenching and Stern-Volmer equation and deviations from Stern Volmer equation,<br>4.1.4: Concentration dependence of quenching and excimer formation<br>4.1.5: Quenching by added substances–charge transfer mechanism and energy transfer mechanism.<br>**4.2: Solar Cells:** photovoltaic and photo galvanic cells; photoelectron chemistry, prospects of solar energy conversion and storage, organic solar cells. | 1 |

| M.Sc. | Semester IV Theory |
|---|---|
| **RJSPGCHEP401**<br><br>Paper I<br><br>**Polymer, Green, Biophysical and Applied** | **Course Outcomes:**<br><br>1. To understand properties of polymers in solid state, characterization of polymers and chemical analysis by spectral methods and.<br>2. To understand the properties and importance of surface-active agents, micelles and emulsion and to learn the applications of surface chemistry for the storage of graphene, fullerenes and nanomaterials.<br>3. To learn the principles of photo physical processes in electronically excited molecules and mechanism of their relaxation by fluorescence and phosphorescence.<br>4. To understand application of photochemical reactions in organic systems (conjugated olefins and aromatic compounds).<br><br>***Learning Outcomes:***<br>*After completing this course student will be able to:*<br>1. apply principles of different spectroscopic, microscopic and thermal methods to identify and characterize polymers.<br>2. understand polymer technology, thermodynamics of polymer solution.<br>3. learn applications and properties of commercially available polymers.<br>4. understand the use of properties of biomolecules in biosensors.<br>5. learn electrophoresis, gel electrophoresis and their application to characterize protein and DNA.<br>6. understand the different techniques and applications of green chemistry.<br>7. Understand the effect of dielectric constant, viscosity on fluorescence sensing in solutions.<br>8. Study different ways of energy transfer to other substances by potential energy of surfaces.<br>9. Find the kinetic parameters by Stern-Volmer equation.<br>10. Learn the upcoming solar cell methodologies. |

**Reference Books: Unit II**


1. P. Bahadur and N. V. Sastry, Principles of Polymer Science, second edition,Narosa Publishing House,2005.
2. C. E. Carraher, Jr., Carraher's Polymer Chemistry, 8th edition, CRC Press, New York,2010.
3. JoelR.Fried,Polymer Science and Technology, Prentice-Hall of IndiaPvt.Ltd., 2000.
4. V.R.Gowarikar,H.V.Viswanathan and J.Sreedhar,PolymerScience.NewAge International Pvt.Ltd.,NewDelhi,1990.
5. F. W. Billmeyer Jr., Text Book of Polymer Science, 3rd edition, John Wiley and Sons,1984.
6. V.K.Ahluwalia & A. Mishra, Polymer Science, A text book,Ane Books Pvt. Ltd,2008.
7. R.Sinha, Outline of Polymer Technology manufacture of Polymers, Prenticehall ofIndiaPvt.Ltd.2000
8. F.J.Davis,Polymer Chemistry,Oxford university Press,2000.
9. D.Walton&P.lotimer,Polymer,Oxford university Press,2000.
10. R.Ypung,Introduction to Polymers,Chapman & Hall,reprint,1989.
11. V.Jain.OrganicPolymer Chemistry,I V Y Publishing House,2003.
12. A.Singh, Polymer Chemistry,Campus Book International,2003.


**Reference Books: Unit III**


**1.** U.N Dash,.AText Book of Biophysical Chemistry,Macmillan IndiaLtd
**2.** Gurtu and Gurtu,Biophysical Chemistry,Pragati Prakashan.
**3.** R.P.Budhiraja,Separation chemistry,New Age International(P)Limited,Publisher
**4.** Avinash Upadhyay,Kakoti Upadhyay,Nirmalendu Nath.Biophysical Chemistry Principles and Techniques Himalaya
**5.**Susan R.Mikkelson ,Eduardo Corton, Bioanalytical Chemistry,Wiley Interscience.08Science,2nd ed.,Kluwer Academic/Plenum Publishers,New York,2000.
**6.** Mike Lancaster,Green Chemistry An IntroductoryText,Royal Societyof Chemistry.
**7.** V.K.Ahluwalia, M.Kidwai, Kluwer Academic Publisher.


**Reference Book: Unit IV**


K.K.Rohatgi-Mukherjee. Fundamentals of Photochemistry.Reprint 2002. New Age International Publisher,1978.

| Course Code | Title | Credits |
|---|---|---|
| **RJSPGCHEP402** | **Paper – II Material Science, Network and Irreversible Thermodynamics** | 4 |
| **UNIT-I**<br>**Metals and alloys**:<br>**1.1 Solidification of metals and alloys:** homogeneous and heterogeneous nucleation growth of crystals, growth of silicon single crystal.<br>**1.2 Metallic solid solutions:** substitutional and interstitial solid solutions.<br>**1.3 Crystal imperfections:** point, line and boundary defects.<br>**1.4 Atomic diffusions in solids:** diffusion mechanisms, steady state and non-steady state diffusions, impurity diffusion into silicon wafers for integrated circuits. | | 1 |
| **Unit-II**<br>**Mechanical properties of solid materials**<br>**2.**1 Stress and strain in metals- Engineering stress and engineering strain, shear stress and shear strain, the tensile test and engineering stress -strain diagram, modulus of elasticity, yield strength.<br>**2.2** Hardness and hardness testing, plastic deformations of metals in single crystals, plastic deformation of polycrystalline metals, solid solution strengthening of metals.<br>**2.3** Fracture of metals-ductile and brittle fracture, toughness and impact testing, fatigue of metals, the creep test, creep-rupture test. | | 1 |
| **Unit III**<br>**Lasers and superconductors**<br>**3.1 Lasers in chemistry**<br>**3.1.1 General principles of LASER Action:** Population Inversion, cavity and mode characteristics, Q-switching, Mode Locking.<br>**3.1.2 Practical Lasers: Solid State Lasers-Ruby**, neodymium, gas lasers-He-Ne, Ar, Kr, Carbon dioxide, Chemical and exciplex Lasers, Dye lasers, LED and Semiconductor Lasers**.**<br>**3.1.3 Applications of Lasers in chemistry:** Spectroscopy at high photon fluxes, collimated beams, Precision specified transitions, Isotope separation, Study of fast reactions using pulsed techniques**.**<br>**3.2 Superconducting solid materials**<br>Band theory of electrical conductivity, Bardeen-Cooper-Schrieffer Theory of super conductivity, the super conducting state, High critical temperature superconductors, magnetic properties of superconductors. | | 1 |

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| **Unit IV**<br><br>**Non-equilibrium thermodynamics**<br>**4.1.1** Features of non-equilibrium thermodynamics, second law of thermodynamics, uncompensated heat and its relation to thermodynamics function.<br><br>**4.1.2** Entropy production and its rate. Entropy production in heat transfer process and during mixing of gases. Entropy production and efficiency of galvanic cell.<br><br>**4.1.3**Onsagers theory: Reciprocal relation, principle of microscopic reversibility. Coupled and uncoupled reactions and their condition.<br><br>**4.1.4** Transport phenomena across membranes. Electro kinetic effect and thermo mechanical effects. | 1 |

| M.Sc. | Semester IV Theory |
|---|---|
| **RJSPGCHEP402**<br><br>Paper II<br><br>**Material Science, network and irreversible thermodynamics** | **Course Outcome:**<br>1. To learn the methods of preparation, properties and defects of metals and alloys.<br>2. To understand the mechanical properties and to apply different test to assess mechanical strength of polymers.<br>3. To understand the LASER, their principles and applications.<br>4. To introduce non equilibrium thermodynamics and different theories controlling these reactions.<br>**Learning Outcome:**<br>*After completing this course students will be able to:*<br>1. understand Solidification of metals and alloys.<br>2. distinguish substitutional and interstitial solid solutions.<br>3. evaluate solid imperfections and their effect on properties of metals and alloys.<br>4. Learn different types of stress, strain and strength of solid materials.<br>5. Understand the fractures in metals and their effect on the quality of metals.<br>6. Learn different terms used in LASERS, their working, principles and applications.<br>7. Understand the theories, requirements and applications of superconducting behavior of solids.<br>8. Apply Non equilibrium processes in daily routines.<br>9. solve problems related to non-equilibrium processes |

**Reference Books : Unit II**


1. WilliamF.Smith,Principles of Material Science and Engineering,3rd edition, McGraw–Hill Inc.1996.
2. Keer H.V,Principles of the Solid State,first reprint,Wiley Eastern Limited, 1994.
3. Principles of Material science and engineering,3rd edition,McGraw–Hill Inc.1996.


**Reference Book: Unit III**


Atkins P.W, Physical Chemistry, Oxford University Press, 6th edition, 1998.


**Reference Books: Unit IV**


1. D.A.Mc Quarrie and J.D.Simon,Molecular Thermodynamics,Viva Books Private Limited, First Indian Ed.,2004.
2. D.A.Mc Quarrie and J.D.Simon,Physical Chemistry,a Molecular Approach, Viva Books Private Limited,First South Asian Ed.,1998.Chap.
3. E.D.Kaufmann, Advanced Concepts in Physical Chemistry,McGraw-Hill,1966.
4. Robert P.H.Gasser and W.Graham Richards,An Introduction to Statistical Thermodynamics, World ScientificPublishingCo.Pte.Ltd.,1995.
5. C.Kalidas and M.V.Sangaranarayan,Non-Equilibrium Thermodynamics, Principlesand Applications, Mc Millan India Ltd.,2002.

| Course Code | Title | Credits |
|---|---|---|
| **RJSPGCHEP403** | **Paper – III Symmetry & Spectroscopy** | 4 |
| **UNIT-I:**<br>**Symmetry in Chemistry**<br>**1.1** Recapitulation: point groups, character tables<br>**1.2** Reduction formula, application of reduction formula to vibrational modes of water molecule**.**<br>**1.3** Application in vibrational spectroscopy, selection rules for IR spectroscopy for molecules such as $H_2O$, $CO_2$, HF, $H_2$<br>**1.4** Application to Raman spectra, selection rules, comparison of IR and Raman selection rules, general approach to vibrational spectroscopy.<br>**1.5** Symmetry in chemical bonding: symmetry adapted linear combination of molecular orbitals, $H_2^+$, $H_2$, LiH, $BeH_2$, $BH_3$, $CH_4$, molecular orbital energy, and bond order. | | 1 |
| **UNIT-II**<br>**N. M. R. Spectroscopy-I**<br>**2.1** A review of one-dimensional NMR spectroscopy.<br>**2.2** Spin-relaxation. Nuclear Over Hauser Effect (NOE), polarization transfer.<br>**2.3** Two-dimensional NMR. Correlated spectroscopy (COSY)<br>**2.4** Nuclear Over Hauser effect Spectroscopy (NOESY)<br>**2.5** Heteronuclear correlation Spectroscopy (HETCOR)<br>**2.6** Solid-state NMR<br>**2.7** Magnetic Resonance Imaging (MRI) | | 1 |

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| **UNIT-III**<br>**ESR and Mossbauer Spectroscopy**<br>**3.1 Electron spin Resonance Spectroscopy:**<br>**3.1.1** Basic principle, hyper fine splitting (isotropic systems);<br>**3.2.2** G-value and the factors affecting there of; interactions affecting electron energies in paramagnetic complexes (Zero-field splitting and Kramer's degeneracy);<br>**3.3.3** Anisotropic effects (the g-value and the hyper fine couplings); The EPR of triplet states; Structural applications to transition metal complexes.<br>**3.1.1** Fundamentals and hyperfine splitting, application to study of free radicals spin densities McConnell relationship Zero field splitting.<br>**3.2 Mossbauer Spectroscopy:**<br>Principles, Recoilless emission and absorption of γ-rays, experimental methods, isomer shift, hyperfine structure (quadrupole interaction), magnetic hyper fine interaction, applications. | 1 |
| **UNIT-IV**<br>**$^{13}$C N. M.R. Spectroscopy**<br>**4.1** Elementary ideas, instrumental difficulties, FT technique advantages and disadvantages. proton noised e-coupling technique advantages and disadvantages, off-resonance technique.<br>**4.2** Chemical shifts of solvents, factors affecting chemical shifts, analogy with $^{1}$H NMR.<br>4.3 **Calculations of chemical shift of hydrocarbons, effect of substituents on chemical shifts, different types of carbons (alkene, alkyne and allene).**<br>**4.4** Chemical shift of aromatic carbon sand effect of substituent.<br>**4.5** Chemical shifts of carbonyl, nitrile and oxime carbons. | 1 |

| M.Sc | Semester IV Theory |
|---|---|
| **RJSPGCHEP403**<br><br>Paper-III<br><br>**Symmetry & Spectroscopy** | Course Outcomes:<br><br>1. Learn to construct character tables and application to different polyatomic molecules.<br>2. Understand two-dimensional NMR and high order of NMR techniques.<br>3. To understand principles and applications of ESR and Mossbauer spectroscopy<br>4. To understand principles and applications of 13C NMR spectroscopy<br><br>*Learning Outcomes:*<br><br>*After completing this course students will be able to:*<br><br>1. Apply Reduction formula, application of reduction formula to vibrational modes of water molecule**.**<br>2. Learn selection rules of IR and Raman spectroscopy.<br>3. understand symmetry adapted linear combination of molecular orbitals, molecular orbital energy, and bond order.<br>4. Learn about instrumentation and principles heteronuclear correlation spectroscopy, solid state NMR.<br>5. Understand applications of NMR in medical field (MRI).<br>6. Understand G-value and Anisotropic effects.<br>7. Apply ESR principles on the study of free radicals and spin densities<br>8. Learn McConnell relationship, zero field splitting.<br>9. Understand Chemical shifts of solvents, factors affecting chemical shifts.<br>10. Calculate Calculations of chemical shift of hydrocarbons, effect of substituent's on chemical shifts, different types of carbons (alkene, alkyne and allene). |

**Reference Books : Unit I**


**1.** K.Veera Reddy,Stmmetry and Spectroscopy of molecules,2nd ed,new age International publishers.
**2.** U.C.Agarwala, H/L/Nigam,S Agarwal,S.S.Kalra,Molecular symmetry in Chemistry via group theory,2013,Ane BooksPvt.ltd.
**3.** H.N.Dass,symmetry and group theory for chemists,2004 Asian Books Pvt.Ltd.
**4.** K.V.Raman,group theory and its applications to Chemistry,1980,Tata Mac Graw hill Pub.Co.Pvt.Ltd.
**5.** P/K.Bhattacharya,Group theory and its chemical applications,1999,Himalaya, Pub.House.
**6.** F.A.Cotton,Chemical applications of Group Theory,Wiley Student Ed., 2006,John Wiley and Sons, (Asia)Pvt. Ltd.
**7.** R.L.Carter,Molecular symmetry and Group theory,Wiley Student Ed.,1996,John Wiley and Sons, (Asia)Pvt. Ltd.
**8.** S.Swarnalakshmi,T.saroja,R.M.Ezhilarisi,A simple approach to Group theory in chemistry,2008, Universities Press( India)Pvt. Ltd.


**Reference Books: Unit III**


1. C.N.Banwell and E.M.Mc Cash,Fundamentals of Molecular Spectroscopy,4th Ed., Tata-McGraw-Hill,1994.
2. M. L. Gupta, Atomic and Molecular Spectroscopy, New Age International Publishers, 2001.
3. H.S.Randhawa, Modern Molecular Spectroscopy,McMillan India Ltd., 2003
4. G.Aruldas, Molecular Structure and Spectroscopy,Prentice-Hall of India, 2001.
5. J.Michael Hollas, Modern Spectroscopy, 4thEd., JohnWiley and Sons, 2004.


**Reference Books: Unit IV**


1. A.E. Derome, Modern NMR Techniques for Chemistry Research, Pergamon,Oxford(1987)
2. J.K.M. Sanders and B.K. Hunter, Modern NMR Spectroscopy, 2nd Oxford University Press, Oxford.edition (1993),
3. R.K.Harris, Nuclear Magnetic Resonance Spectroscopy,(1986)Addison-Wesley, Longman Ltd., London
4. Organic spectroscopy by William Kemp, 3rd Edition, ELBS,1996.

| Course Code | Title | Credits |
|---|---|---|
| **RJSPGCHEP404** | **Paper – IV**<br>**Intellectual Property Rights & Cheminformatics** | 4 |
| **Unit I:**<br>**Introduction to Intellectual Property:**<br>Historical Perspective, Different types of IP, Importance of protecting IP.<br>**Patents:**<br>Historical Perspective, Basic and associated right, WIPO, PCT system, Traditional Knowledge, Patents and Health care-balancing promoting innovation with public health, Software patents and their importance for India.<br>**Industrial Designs:**<br>Definition, How to obtain, features, International design registration.<br>**Copyrights:**<br>Introduction, How to obtain, Differences from Patents.<br>**Trade Marks:**<br>Introduction, How to obtain, Different types of marks – Collective marks, certification marks, service marks, trade names etc.<br>**Geographical Indications:**<br>Definition, rules for registration, prevention of illegal exploitation, importance to India. | | 1 |
| **Unit II:**<br>**Trade Secrets:**<br>Introduction and Historical Perspectives, Scope of Protection, Risks involved and legal aspects of Trade Secret Protection.<br>**IP Infringement issue and enforcement:**<br>Role of Judiciary, Role of law enforcement agencies – Police, Customs etc.<br>**Economic Value of Intellectual Property:**<br>Intangible assests and their valuation, Intellectual Property in the Indian context – Various Laws in India Licensing and Technology transfer.<br>**Different International agreements:**<br>**(a) World Trade Organization (WTO):**<br>(i) General Agreement on Tariffs and Trade (GATT), Trade Related Intellectual Property Rights (TRIPS) agreement<br>(ii) General Agreement on Trade Related Services (GATS) Madrid Protocol.<br>(iii) Berne Convention<br>(iv) Budapest Treaty<br>**(b) Paris Convention**<br>**WIPO** and **TRIPS, IPR** and Plant Breeders Rights, IPR and Biodiversity. | | 1 |

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| **Unit III:**<br>**Introduction to Chem informatics:**<br>History and evolution of cheminformatics, Use of Cheminformatics, Prospects of cheminformatics, Molecular modeling and structure elucidation.<br><br>**Representation of molecules and chemical reactions:**<br>Nomenclature, Different types of notations, SMILES coding, Matrix representations, Structure of Mol files and Sd files, Libraries and toolkits, Different electronic effects, Reaction classification.<br><br>**Searching Chemical Structures:**<br>Full structure search, sub-structure search, basic ideas, similarity search, three-dimensional search methods, basics of computation of physical and chemical data and structure descriptors, data visualization. | 1 |
| **Unit IV:**<br>**Applications:**<br>Prediction of Properties of Compound, Linear Free Energy Relations, Quantitative Structure – Property Relations, Descriptor Analysis, Model Building, Modeling Toxicity, Structure – Spectra correlations, Prediction NMR, IR and Mass spectra, Computer Assisted Structure elucidations, Computer assisted Synthesis Design, Introduction to drug design, Target Identification and Validation, Lead Finding and Optimization, analysis of HTS data, Virtual Screening, Design of Combinatorial Libraries, Ligand based and Structure based Drug design, Application of Chem informatics in Drug Design. | 1 |

| M.Sc. | **Paper – IV**<br>**Intellectual Property Rights & Cheminformatics** |
|---|---|
| **RJSPGCHEP404 Intellectual Property Rights & Cheminformatics** | Course outcomes:<br>1. To create awareness and understanding the terms like intellectual property, patents, copyright, industrial designs, trademarks, geographical indications etc.<br>2. To know trade secrets, IP infringement issues, economic value of intellectual property and study of various related international agreements.<br>3. To explore cheminformatics to facilitate molecular modeling and structure elucidations.<br>4. To apply the knowledge gained about various chemistry principles, techniques and tools in drug designing, target identification and validation, lead finding and optimization.<br><br>*Learning Outcomes:*<br>*After completing this course student will be able to:*<br>1. Apply for Patents, their related norms.<br>2. Obtain industrial design and trademarks.<br>3. Aware themselves about copyright rules.<br>4. Learn rules for registration, prevention of illegal exploitation, importance to India<br>5. understand Trade Secrets.<br>6. learn economic value of IPR.<br>7. learn history, evolution of nomenclature, different types of Notations.<br>8. Search chemical structure and data related to physical data of compounds.<br>9. Understand the application of cheminformatics in detail |

**REFERENCES:**

1. Andrew R. Leach & Valerie J. Gillet (2007) *An Introduction to Cheminformatics.* Springer: The Netherlands.
2. Gasteiger, J. & Engel, T. (2003) *Cheminformatics: A textbook*. Wiley–VCH

3. Gupta, S. P. *QSAR and Molecular Modeling.* Springer-Anamaya Pub.: New Delhi.

| Course Code | Practical Title | Credits |
|---|---|---|
| **RJSPGCHEPRP401** | **PRACTICAL – I (Polymer, Green, Biophysical and Applied)** | 2 |

1. To determine the formula of the zinc (II) ammonia complex by partition method.
2. Determination of the transport no. of silver(I) ions by Hittorf's method.

**Conductometry**.

1. To determine the composition of a mixture of hydrochloric acid, potassium chloride and ammonium chloride by titration with sodium hydroxide and silver nitrate.
2. To determine ΔG, ΔHand ΔS of dissolution of a sparingly soluble salt by conductometry.

**pH metry**

1. To determine K1 and K2 of a dibasic acid by titration with a base.
2. To determine dissociation constant of p-nitro phenol.

| M.Sc. | Physical Chemistry, Paper I Practical |
|---|---|
| **RJSPGCHEPRP401** Practical I<br><br>**Polymer, Green, Biophysical and Applied** | Course Outcome:<br>1. To learn complex formation by instrumental and non-instrumental methods.<br>2. To determine transport number by Hittorf's method.<br><br>*Learning Outcomes:*<br>*After completing this course student will be able to:*<br>1. Determine the formula of the complex by partition method.<br>2. Determine the transport no. of ions by Hittorf's method.<br>3. Determine ΔG, ΔH and ΔS of dissolution of a sparingly soluble salt by conductometry.<br>4. Determine dissociation constant of p-nitro phenol. |

| Course Code | Practical Title | Credits |
|---|---|---|
| **RJSPGCHEPRP402** | **PRACTICAL – II (Material Science, Network and Irreversible Thermodynamics)** | 2 |

1. To construct the phase diagram for a two-component system forming a compound
2. To determine the energy of activation and other thermodynamic parameters of activation for the reaction between persulphate and potassium iodide.
3. To determine the effect of ionic strength of a solution on the reaction between potassium persulphate and potassium iodide.
4. To study the order of the reaction between bromate and bromide.
5. To determine the Van't Hoff's factor by cryoscopic method.

**Potentiometry**

To determine the liquid junction potential with a concentration cell with and without transference.

| M.Sc | Physical Chemistry , Paper II Practical |
|---|---|
| Practical II<br><br>**RJSPGCHEPRP402**<br><br>**Material Science, Network and Irreversible Thermodynamics** | Course Outcomes:<br><br>1. To understand the standard operating procedure of various instruments.<br>2. To learn phase rule of two component system by drawing phase diagram.<br><br>Learning outcomes:<br><br>*After completing this course student will be able to:*<br><br>1. construct the phase diagram for a two-component system forming a compound<br>2. determine the energy of activation and other thermodynamic parameters of activation for the reaction between persulfate and potassium iodide.<br>3. determine the liquid junction potential with a concentration cell with and without transference. |

| Course Code | Practical Title | Credits |
|---|---|---|
| **RJSPGCHEPRP403** | **PRACTICAL – III (Symmetry & Spectroscopy)** | 2 |

**Interpretation of spectra/data:**

1. Interpretation of vibrational-rotational spectra of rigid and non-rigid diatomic molecules
2. Interpretation of electronic spectra of diatomic molecules.
3. Interpretation of electronic spectra of simple polyatomic molecules.
4. Interpretation of NMR,ESR spectra.
5. Interpretation of Mossbauer spectra.
6. Analysis of XRD pattern of cubic system
7. Interpretation of DTA, TG, and DTG curves

| M.Sc | Physical Chemistry, Paper III Practical |
|---|---|
| **RJSPGCHEPRP403**<br>Practical III<br>**Symmetry & Spectroscopy** | Course Outcomes:<br>1. To learn interpretation of spectra and analysis of data.<br><br>*Learning Outcomes:*<br><br>*After completing this course student will be able to:*<br><br>1. Learn to interpret vibrational-rotational spectra of rigid and non-rigid diatomic molecules<br>2. Learn to interpret electronic spectra of diatomic molecules.<br>3. Learn to interpret electronic spectra of simple polyatomic molecules.<br>4. Learn to interpret NMR, ESR spectra.<br>5. Learn to interpret Mössbauer spectra. |

| Course Code | Practical Title | Credits |
|---|---|---|
| **RJSPGCHEPRP404** | **PRACTICAL – IV (Intellectual Property Rights & Cheminformatics)** | 2 |
| **Project Evaluation** | | |

| M.Sc | Semester IV Practical |
|---|---|
| **RJSPGCHEPRP404**<br><br>Practical *IV*<br><br>**Intellectual Property Rights & Cheminformatics** | Course Outcome:<br><br>1. learn to write project objectives, methodology and interpretation of data based on project.<br><br>*Learning Outcomes:*<br><br>*After completing this course student will be able to:*<br><br>1. write result and future direction for a long term project. |

**Reference Books for Practicals**:


1. B.Vishwanathan and P.S.Raghavan, Practical Physical Chemistry,Viva BooksPrivateLimited,2005.
2. A.M.James and F.E.Prichard,Practical Physical Chemistry,3rd ed., Longman,1974.
3. B.P.Lewitt(ed.),Findlay's Practical Physical Chemistry,9th ed.,1973.
4. C.D.Brennanand C.F.H.Tipper,A Laboratory Manual of Experiments in Physical Chemistry,McGraw-Hill,1967.
5. F.Daniel & Others, Experimental Physical Chemistry,1965, Kogakasha Co. Ltd.,Tokyo.

Hindi Vidya Prachar Samiti's

# Ramniranjan Jhunjhunwala College

# of Arts, Science & Commerce

# (Autonomous College)

Affiliated to

# UNIVERSITY OF MUMBAI

## Syllabus for the M.Sc. Part – II

## Program: M.Sc. (Inorganic Chemistry)

## Program Code: RJSPGCHEI

## CBCS: 2020 -2021

# M.Sc. (Inorganic Chemistry) Semester – IV

| Course | Nomenclature | Credits | Topics |
|---|---|---|---|
| RJSPGCHEI401 | Paper I<br>Properties of Inorganic Solids and Group Theory | 4 | 1. Electrical Properties<br>2. Magnetic Properties<br>3. Thermal and Optical Properties.<br>4. Applications of group theory to – Electronic structures |
| RJSPGCHEI402 | Paper II<br>Organometallics And Main Group Chemistry | 4 | 1. Organometallic Chemistry<br>2. Applications of Organometallic Compounds<br>3. Inorganic cluster and cage compounds.<br>4. Inorganic ring and chain compounds |
| RJSPGCHEI403 | Paper III<br>Instrumental Methods in Inorganic Chemistry | 4 | 1. Spectroscopy<br>Infrared spectroscopy.<br>Raman spectroscopy.<br>Applications of Group theory in Infrared and Raman spectroscopy.<br>Nuclear Magnetic Resonance Spectroscopy.<br>2. Microscopy of Surface Chemistry-I<br>3. Microscopy of Surface Chemistry-II<br>4. Thermal Methods |
| RJSPGCHEI404 | Paper IV<br>Intellectual Property Rights & Cheminformatics | 4 | 1. Introduction to Intellectual Property.<br>Patents, Industrial Designs, Copyrights, Trade Marks, Geographical Indications.<br>2. Trade Secrets<br>IP Infringement issue and enforcement.<br>Economic Value of Intellectual Property.<br>Different International agreements.<br>3. Introduction to Chem informatics<br>Representation of molecules and chemical reactions.<br>Searching Chemical Structures.<br>3. Applications |

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|---|---|---|---|
| RJSPGCHEPRI401 | Practical – I | 8 | Properties of Inorganic Solids and Group Theory Practical |
| RJSPGCHEPRI402 | Practical – II | | Organometallics And Main Group Chemistry Practical |
| RJSPGCHEPRI403 | Practical - III | | Instrumental Methods in Inorganic Chemistry Practical |
| RJSPGCHEPRI404 | Practical - IV | | Intellectual Property Rights & Cheminformatics Practical |

**Theory semester IV**

| Course Code | Title | Credits |
|---|---|---|
| **RJSPGCHEI401** | **Paper - I**<br>**Properties of Inorganic Solids and Group Theory** | 4 |
| **Unit I**<br>**Electrical Properties-**<br>(**a) Electrical properties of solids:**<br>(i) Conductivity: Solid Electrolytes; Fast Ion Conductors; Mechanism of Conductivity; Hopping Conduction.<br><br>**(b) Other Electrical Properties:** Thomson and Seebeck Effects; Thermocouples and their Applications; Hall Effect; Dielectric, Ferroelectric, Piezoelectric and Pyrroelectric Materials and their Inter-relationships and Applications | | 1 |
| **Unit II**<br>**Magnetic Properties.**<br>(a) Behaviour of substances in magnetic field, mechanism of ferromagnetic and antiferromagnetic ordering, super exchange, Hysteresis, Hard and soft magnets, structures and magnetic Properties of Metals and Alloys; Transition metal Oxides; Spinels, garnets, Ilmenites; Perovskite and Magneto plumbites, Application in transformer cores, information storage, magnetic bubble memory devices and as permanent magnets. | | 1 |

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| **UNIT-III**<br>**Thermal and Optical Properties**<br>**a) Thermal Properties:** Introduction, Heat Capacity and its Temperature Dependance; Thermal Expansion of Metals; Ceramics and Polymers and Thermal Stresses.<br>**(b) Optical properties:** Color Centres and Birefringence; Luminescent and Phosphor Materials; Coordinate Model; Phosphor Model; Anti Stokes Phosphor; Ruby Laser; Neodymium Laser | 1 |
| **UNIT-IV**<br>**Applications of group theory to –Electronic structures**<br>(a) Recapitulation of Points groups and Character tables.<br>(b) Transformation Properties of Atomic Orbitals;<br>(c) Sigma and pi- molecular orbitals for AB4 (tetrahedral) and AB6(octahedral) molecules;<br>(d) **Ligand Field Theory:** Electronic structures of free atoms and ions; Splitting of levels and terms in a chemical environment; Construction of energy level diagrams; Direct product; Correlation diagrams for $d^2$ ions in octahedral and tetrahedral ligand field; Methods of Ascending and Descending Symmetry; Hole formalism. | 1 |

| M.Sc | Semester IV Theory<br>**Properties of Inorganic Solids and Group Theory** |
|---|---|
| **RJSPGCHEI401**<br><br>Paper I<br><br>**Properties of Inorganic Solids and Group Theory** | **Course Outcomes:**<br><br>Students learn in detail about the electrical, magnetic, thermal, and optical properties of solid structures. They also study the symmetry aspects of the crystal structures, sigma and pi bonding in octahedral and tetrahedral coordination complexes, spectroscopic terms and splitting of energy level.<br><br>***Learning Outcomes:***<br>1) Understand the electrical properties of solids<br>2) Gain knowledge about thermocouples and its applications.<br>3) understand Thomson, Seebeck and Hall effect.<br>4) Know the properties of Ferro, Piezo and pyro electric materials.<br>5) Understand the magnetic properties of solid substances.<br>6) Gain knowledge on ferro, ferri and antiferro magnetic properties.<br>7) study certain phenomenon like Hysteresis, magnetic ordering & super exchange.<br>8) understand certain applications of magnetic solids in different fields.<br>9) Understand the thermal and optical properties of solids.<br>10) Gain knowledge about heat capacity and temperature dependance of solids.<br>11) Learn thermal expansion in metals, ceramics and polymers.<br>12) Understand the phenomenon of thermal stress.<br>13) Understand point groups for different molecules. |

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| | 14) write character table for different symmetry operations<br>15) Understand sigma and pi bonding in tetrahedral and octahedral molecules.<br>16) Learn the splitting of energy levels and spectroscopic terms for different ions. |

**REFERENCE BOOKS**

1. L. E. Smart and E. A. Moore, Solid State Chemistry-Anintroduction, 3rd edition, Taylor and Francis, 2005.

2. A.R.West, Solid State Chemistry and Its Applications, John Wiley& sons, 1987.

3. C.N.R. Rao and J.Gopalkrishnan New Directons in Solid StateChemistry, 2nd Ed., Combridge University Press. 1997

4. L.V. Azaroff, Introductionn to solids, Tata-McGraw Hill Book Ce.New Dehli, 1977.

5. . D.W. Bruce and Dermont O Hare, Inorganic Chemistry, 2nd Ed.Wiely and sons, New York, 1966.

6. J.M. Hollas, Symmetry in Molecuies, Chapman adn Hall Ltd.,1972.

7. Reboert L carter, Molecular Symmeetry and Group Hohn Wileyand Sons, New York, 1988.

8. Ulrich Muller, Inorganic structural Chemistry, 2nd edition, JohnWiley and Sons, Chichester, 1993.

9. .R.N.Kutty and J.A.K.Tareen, Fundamentals of Crystal Chemistry,Universities Press (India) Ltd., 2001..

10. H.V.Keer, Principles of the Solid state, Wiley Eastern Ltd., 1993.Gary L.Miessler and Donald A.Tarr, Inorganic Chemistry, 3rd edition , Pearson Education, Inc., 2004.

11. .D.K.Chakraborty, Solid State Chemistry, New Age InternationalPublishers, 1996.

12. 12. A. Earnshaw, Introduction to Magnetochemistry, Acad.Press,N.Y. (1966)

| Course Code | Title | Credits |
|---|---|---|
| **RJSPGCHEI402** | **Paper - II**<br>**Organometallics and main group Chemistry** | 4 |
| **Unit – I**<br>**Organometallic Chemistry**<br>(a) Metal-Metal Bonding and Metal Clusters.<br>(b) Electron Count and Structures of Clusters.<br>(c) Isolobal Analogy.<br>(d) Organopalladium and Organoplatinum complexes (preparations, properties and applications.). | | 1 |
| **Unit II**<br>**Applications of Organometallic Compounds**<br>(a) Catalysis-Homogenous and Heterogenous catalysis: Comparison, Fundamental Reaction Steps.<br>(b) Organometallics as Catalysts in Organic Reactions:<br>(i) Hydrosilation, (ii) Hydroboration. (iii) Water gas Shifts Reaction (iv) Wacker process (Oxidation of alkenes)<br>(v) Alcohol carbonylation<br>(c) Coupling reactions :(i) Heck's reaction (ii) Suzuki reaction | | 1 |
| **UNIT-III**<br>**Inorganic cluster and cage compounds**<br>(i) Introduction, (ii) Bonding in boranes, (iii) Heteroboranes (iv) Carboranes (v) cluster compounds, (vi) electron precise compounds sand their relation to clusters. | | 1 |
| **UNIT-IV**<br>**Inorganic ring and chain compounds**<br>(a) Silicates, polysilicates and aluminosilicates.<br>(b) Phosphazenes, phosphazene polymers.<br>(c) Polyanionic and polycationic compounds. | | 1 |

| M. Sc. | Semester IV Theory |
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| **RJSPGCHEI402**<br>Paper II<br>**Organometallics and main group Chemistry** | **Course Outcomes:**<br>A) Students learn<br>Metal clusters, Wades rules,<br>Important coordination compounds as catalysts.<br>B) Application of organometallic compounds as catalysts.<br>C)Students will be familiar with the structure and bonding involved in an inorganic cage, cluster, ring, and chain compounds. |

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| | ***Learning Outcomes:***<br><br>A) Students learn to define metal clusters, predict their structure based on Wade's Rules.<br><br>B) important catalytic reactions such as hydroboration, hydrosilylation, Wacker process, Heck and Suzuki reactions are understood.<br><br>Students will understand the structure and applications of the inorganic clusters, cage, ring, and chain compounds. |

**REFERENCES:**

1. Gary Wulfsberg, Inorganic Chemistry ; Viva Books PA Ltd., NewDelhi; 2002.
2. F.A. Cotton and Wilkinson, Advanced Inorganic Chemistry, 3rdedition.
3. James E.Huheey, Inorganic Chemistry, 3rd edition, Harper &Row,Publishers, Asia, Pte Ltd., 1983.
4. W.W.Porterfield,Inorganic Chemistry-An UnifiedApproach,Academic press(1993);
5. D.F.Shriver, P.W.Atkins and C.H. Langford, InorganicChemistry,3rd edition Oxford University Press, 1999.
6. AsimK.Das, Fundamental Concepts of InorganicChemistry,(Volumes-I,II and III)CBS Pub.(2000)
7. N.N.Greenwood and A.Earnshaw, Chemistry of Elements,Pergamon, 1984.
8. J.M.Hollas, Symmetry in Chemistry, Chapmanad Hall Ltd., NY,1972.\
9. F.A.Cotton, Chemical Applications of Group Theory, 2nd edition,Wiley Eastern Ltd., New Delhi , 1976
10. C.J.Ballhausen and H.B.Gray, Molecular Orbital Theory,MCGraw-Hill, New York, 1965.
11. H. Sisler, Chemistry in Non-aqueous Solvents: New York ReinholdPubl. 1965.
12. . J.J. Lagowski, The Chemistry of Non-aqueous Solvents,Academic press, New york and London.
13. . C.M. Day and Joel Selbin, Theoretical InorganicChemistry,Affiliated East West Press Pvt.Ltd., 1985.
14. L.E.Orgel, An Introduction to Ligand Field Theory , Methuen &Co.Ltd., London, 1960.
15. F.Basolo and R.G.Pearson, Mechanisms of Inorganic Reactions,Wiley, New York, 1967.
16. .J.D.Lee, Concise Inorganic Chemistry, 5th ed., Blackwell Science Ltd., 2005.
17. R.H. Crabtree, The Organometallic Chemistry of the Transition Metals, Wiley-Interscience, New york, 1988.
18. G.W.Parshall and S.D.Ittel, Homogeneous Catalysis, 2ndedition,John Wiley & sons, Inc., New York, 1992.
19. Gary O. Spessard and Gary L.Miessler, Organometallic Chemistry,Prentice-Hall, (1997).

20. .R.C.Mehrotra and A.Singh, Organometallic Chemistry-AUnifiedApproach, 2nd ed., New Age International Pvt.Ltd., 2000.
21. B.Douglas, D.H. McDaniel and J.J.Alexander, Concepts andModels of Inorganic Chmistry, 2nd edition, John Wiley &Sons,1983.
22. James E.Huheey, Inoganic Chemistry-Principles of structure and reactivity, edn Harper & Row Publishers (1972).
23. . F. A. Cotton, G. Wilkinson, C. Murillo and M.Bochmann,Advanced Inorganic Chemistry, 6th ed., John Wiley,
New York,1999.
24. F.A. Cotton and R.A.Walton, Multiple Bonds betweenMetalAtoms, 2nd edition, claranden Press, Oxford, 1993.
25. P.L. Soni, Vandana Soni ,Ane Books Pvt.,Ltd

| Course Code | Title | Credits |
|---|---|---|
| **RJSPGCHEI403** | **Paper - III**<br>**Instrumental methods in Inorganic Chemistry** | 4 |
| **Unit – I**<br>**Spectroscopy**<br>**(a) Infrared spectroscopy:** Fundamental modes of vibrations, selection rules, IR absorption bands of metal - donor atom, effect of complexation on the IR spectrum of ligands formations on the IR of ligands like $NH_3$, CN-, CO, olefins (C=C) and $C_2O_4^{2-}$ .<br>**(b)Raman spectroscopy:** Raman spectroscopy for diatomic molecules. Determination of molecular structures like diatomic and triatomic molecules.<br>**(c) Applications of Group theory in Infrared and Raman spectroscopy.**<br>Molecular Vibrations: Introduction; The Symmetry of Normal Vibrations; Determining the Symmetry Types of the Normal Modes; symmetry-based Selection Rules of IR and Raman; Interpretation of IR and Raman Spectra for molecules such as $H_2O$, $BF_3$, $N_2F_2$, $NH_3$and $CH_4$.<br>**(d) Nuclear Magnetic Resonance Spectroscopy:**<br>Introduction to basic principles and instrumentation. Use of 1H, 19F, 31P, 11B NMR spectra in structural elucidation of inorganic compounds; Spectra of paramagnetic materials: Contact shift, application of contact shift, lanthanide shift reagent. | | 1 |

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| **Unit II**<br>**Microscopy of Surface Chemistry-I**<br>Introduction to surface spectroscopy, Microscopy, problems of surface analysis, distinction of surface species, sputter etching and depth profile and chemical imaging, instrumentations, Ion Scattering Spectra (ISS), Secondary Ion Mass Spectroscopy (SIMS), Auger Emission Spectroscopy (AES). | 1 |
| **UNIT-III**<br>**Microscopy of Surface Chemistry-II**<br>**Instrumentation and applications of:**<br>Electron Spectroscopy for Chemical Analysis (ESCA), Scanning Electron Microscopy (SEM), Atomic force microscopy (AFM) and transmission electron microscopy (TEM). | 1 |
| **UNIT-IV**<br>**Thermal Methods**<br>**4.1 Application of TGA:** in Thermal characterization of polymers, quantitative analysis of mixture of oxalates, moisture content in coal, study of oxidation state of alloys etc.<br>**4.2 Application of DSC and DTA:** in determination of thermodynamic parameters such as heat capacity and standard enthalpy of formation of the compounds, investigation of phase transitions, thermal stability of polymeric materials, purity of pharmaceuticals samples, M.P. and B.P. of organic compounds etc.<br>**4.3** Basic principle, instrumentation and applications to other thermal methods like Thermomechanical Analysis (TMA) and evolved gas analysis (EGA). | 1 |

| M.Sc | Semester IV Theory<br>**Instrumental methods in Inorganic Chemistry** |
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| **RJSPGCHEI403**<br><br>**Paper- III**<br><br>**Instrumental methods in Inorganic Chemistry** | **Course Outcomes:**<br><br>Students learn Infrared (IR), Raman, NMR spectroscopy, for inorganic compounds and application of Group Theory to some selected molecules,<br><br>Students learn challenges in characterization of surfaces and advance spectroscopic techniques Viz.secondary ion mass spectrometry(SIMS), ion scatterind spectroscopy(ISS),And auger spectroscopy.<br><br>Students will be able to learn the instrumentation and applications of SEM, ESCA, AFM, and TEM.<br><br>Students will learn thermal methods such as TGA, DTA, DSC, TMA, and EGA for the characterization of materials<br>***Learning Outcomes:***<br>Students understand the application of IR spectroscopy for structural elucidation. Mutual exclusivity of IR and Raman techniques |

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| | NMR spectroscopy of proton, carbon, fluorine, phosphorous<br><br>Students understand basic concepts of SIMS, ISS, Auger spectroscopy, instrumentation, and application of the same for surface characterization.<br>Proper understanding of SEM, AFM, ESCA, and TEM will enable students to use these techniques for surface characterization in the field of metallurgy and microelectronics.<br>Proper understanding of thermal methods will enable students to select the appropriate thermal technique based on the type of analyte and the desired impurity level to characterize. |

**REFERENCES:**

1. G. H. Jeffery, J. Bassett, J. Mendham and R. C. Denney, Vogel'sTextbook of Quantitative Chemical Analysis Fifth edition,(1996),ELBS Publication. Chapter 2, 3, 11.
2. W.H. Zachariasen. Theory of X-Ray Diffration in Crystals.JohnWiley. New York. 1946.
3. B.D. Cality,, Elements of X-Ray Diffraction Procedures. JohnWiley and Sons.New York, 1954.
4. R. Reaching, Electron Diffraction, Methuen and Co. London. 19365. May and Leopold, An Introduction to MossbauerSpectroscopy,Plenum, New York, 1971.
6. H.H. Willard, L.L. Merrit, J.A. Dean and F.A. Settle, InstrumentalMethods of Analysis, C.B.S. Publishers and Distributors, NewDelhi, 1986.
7. P.J. Horne, Nuclear Magnetic Resonance. Oxford University Press,Oxford, 1995.
8. Reverts John D., Nuclear Magnetic Resonance, McGraw Hill,NewYork, 1959.
9. . H. Kambe and P.D.Garn. Thermal Analysis, Kondansha Ltd.Toyo,1974.
10. G.W. Ewing, Instrumental Methods, Of Analysis, 4th Ed. McFrawHill Ltd., 1970.
11. N.H. Ring, Inorganic Polymers, Academic Press, New York, 1978
12. H.G. Heal, The Inorganic Heterocyclic Chemistry of Sulphur,Nitrogen and Phosphorous, Academic Press, New York, 1980.
13. G.T. Seaborg, Man-made Transuranic Elements Preitce- Hall,1963.
14. M.T.R. Series, TheSuperheavy Elements.
15. Haissilsky, Nuclear Chemistry and its Application, 1962.
16. S. Glasstone, Sourcebook of Aomic Energy, East-WestPublisher,1969.
17. D.Harvey,Modern Analytical Chemistry, The McGraw-Hill Pub,1st Edition(2000);
18. John H. Block, E.B. Roche, T.P.Soine and Charles O.Wilson,Inorganic Medicinal and Pharmaceutical Chemistry, Lea andFebiger, 1974.
19. R. S. Drago, Physical Methods in Inorganic Chemistry, John-Wiley Pub.,1975
20. . M. Drescher an G. Jeschke,(Eds), EPR Spetroscopy: Applicationsin Chemistry and Biology, Springer-Verlag Berlin, Heidelberg2012
21. Graham Smith; David Keeble.Introduction to Modern EPRSpectroscopy CRC Press 2013.
22. C.N.R. Rao, Chemical Applications of Infrared SpectroscopyAcademic Pess,N.Y.(1963
23. K. Veera Reddy, Symmetry and Spectroscopy,
24. Paul Gabbott Principles and Applications of Thermal AnalysisWiley-Blackwell ; edition (2007)

25. . Richard Vernon Parish, NMR, NQR, EPR, and Mössbauer spectroscopy in inorganic chemistry, Publisher,E,.Horwood,(1990)

| Course Code | Title | Credits |
|---|---|---|
| **RJSPGCHEI404** | **Paper – IV**<br>**Intellectual Property Rights & Cheminformatics** | 4 |
| **Unit I:**<br>**Introduction to Intellectual Property:**<br>Historical Perspective, Different types of IP, Importance of protecting IP.<br>**Patents:**<br>Historical Perspective, Basic and associated right, WIPO, PCT system, Traditional Knowledge, Patents and Health care-balancing promoting innovation with public health, Software patents and their importance for India.<br>**Industrial Designs:**<br>Definition, How to obtain, features, International design registration.<br>**Copyrights:**<br>Introduction, How to obtain, Differences from Patents.<br>**Trade Marks:**<br>Introduction, How to obtain, Different types of marks – Collective marks, certification marks, service marks, trade names etc.<br>**Geographical Indications:**<br>Definition, rules for registration, prevention of illegal exploitation, importance to India. | | 1 |
| **Unit II:**<br>**Trade Secrets:**<br>Introduction and Historical Perspectives, Scope of Protection, Risks involved and legal aspects of Trade Secret Protection.<br>**IP Infringement issue and enforcement:**<br>Role of Judiciary, Role of law enforcement agencies – Police, Customs etc.<br>**Economic Value of Intellectual Property:**<br>Intangible assests and their valuation, Intellectual Property in the Indian context – Various Laws in India Licensing and Technology transfer.<br>**Different International agreements:**<br>**(a) World Trade Organization (WTO):**<br>(i) General Agreement on Tariffs and Trade (GATT), Trade Related Intellectual Property Rights (TRIPS) agreement | | 1 |

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| (ii) General Agreement on Trade Related Services (GATS) Madrid Protocol.<br>(iii) Berne Convention<br>(iv) Budapest Treaty<br>**(b) Paris Convention**<br>**WIPO** and **TRIPS, IPR** and Plant Breeders Rights, IPR and Biodiversity. | |
| **Unit III:**<br>**Introduction to Chem informatics:**<br>History and evolution of cheminformatics, Use of Cheminformatics, Prospects of cheminformatics, Molecular modeling and structure elucidation.<br><br>**Representation of molecules and chemical reactions:**<br>Nomenclature, Different types of notations, SMILES coding, Matrix representations, Structure of Molfiles and Sdfiles, Libraries and toolkits, Different electronic effects, Reaction classification.<br><br>**Searching Chemical Structures:**<br>Full structure search, sub-structure search, basic ideas, similarity search, three dimensional search methods, basics of computation of physical and chemical data and structure descriptors, data visualization. | 1 |
| **Unit IV:**<br>**Applications:**<br>Prediction of Properties of Compound, Linear Free Energy Relations, Quantitative Structure – Property Relations, Descriptor Analysis, Model Building, Modeling Toxicity, Structure – Spectra correlations, Prediction NMR, IR and Mass spectra, Computer Assisted Structure elucidations, Computer assisted Synthesis Design, Introduction to drug design, Target Identification and Validation, Lead Finding and Optimization, analysis of HTS data, Virtual Screening, Design of Combinatorial Libraries, Ligand based and Structure based Drug design, Application of Chem informatics in Drug Design. | 1 |

| M.Sc. | **Paper – IV**<br>**INTELLECTUAL PROPERTY RIGHTS & CHEMINFORMATICS** |
|---|---|
| **RJSPGCHEI404**<br><br>**Intellectual Property Rights & Cheminformatics** | Course outcomes:<br><br>1. To create awareness and understanding the terms like intellectual property, patents, copyright, industrial designs, trademarks, geographical indications etc.<br>2. To know trade secrets, IP infringement issues, economic value of intellectual property and study of various related international agreements.<br>3. To explore cheminformatics to facilitate molecular modeling and structure elucidations.<br>4. To apply the knowledge gained about various chemistry principles, techniques and tools in drug designing, target identification and validation, lead finding and optimization.<br><br>*Learning Outcomes:*<br>*After completing this course student will be able to:*<br>1. Apply for Patents, their related norms.<br>2. Obtain industrial design and trademarks.<br>3. Aware themselves about copyright rules.<br>4. Learn rules for registration, prevention of illegal exploitation, importance to India<br>5. understand Trade Secrets.<br>6. learn economic value of IPR.<br>7. learn history, evolution of nomenclature, different types of Notations.<br>8. Search chemical structure and data related to physical data of compounds.<br>9. Understand the application of cheminformatics in detail |

**REFERENCES:**

1. Andrew R. Leach & Valerie J. Gillet (2007) *An Introduction to Cheminformatics.* Springer: The Netherlands.
2. Gasteiger, J. & Engel, T. (2003) *Cheminformatics: A textbook*. Wiley–VCH

3. Gupta, S. P. *QSAR and Molecular Modeling.* Springer-Anamaya Pub.: New Delhi.

| Course Code | Practical Title | Credits |
|---|---|---|
| **RJSPGCHEPRI401** | **Practical – I (Properties of Inorganic Solids and Group Theory )** | 2 |

**Analysis of the following samples**

1. Electral powder for Na/K content flame photometrically.
2. Fasting salt for chloride content conductometrically.
3. Sea water for percentage salinity by Volhard's method.
4. Fertilizer for potassium content by flame photometry.

| M.Sc | Paper I Practical - I |
|---|---|
| **RJSPGCHEPRI401**<br>Practical I<br>**Properties of Inorganic Solids and Group Theory** | Course Outcomes:<br>Students learn instrumental techniques for estimation of elements such as K, Na, Cl.<br>A noninstrumental method such as the Volhard Method for estimation of chlorine is also studied.<br><br>*Learning Outcomes:*<br><br>Students understand the estimation of the amount of sodium and potassium from ORS and fertilizer respectively using Flame photometer, estimation of chlorine conductometrically, and by Volhard method. |

| Course Code | Practical Title | Credits |
|---|---|---|
| **RJSPGCHEPRI402** | **Practical – II (Organometallics and main group Chemistry)** | 2 |

**Coordination Chemistry**

1. Determination of Stability constant of $[Zn(NH_3)_4]^{2+}$ by potentiometry.
2. Determination of Stability constant of $[Ag(en)]^{+}$ by potentiometry.
3. Determination of Stability constant of $[Fe(SCN)]^{2+}$ by slope ratio method.
4. Determination of CFSE values of hexa-aqua complexes of $Ti^{3+}$ and $Cr^{3+}$.

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| 5. Determination of Racah parameters for $[Ni(H_2O)_6]^{2+}$ and $[Ni(en)_3]^{2+}$ |

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| M.Sc | Inorganic Chemistry, Paper II Practical |
| **RJSPGCHEPRI402**<br>Practical II<br>**Organometallics and main group Chemistry** | Course Outcomes:<br>Students learn to determine the stability constant of different coordination complexes using a potentiometer, CFSE values, and Racah parameter<br>*Learning Outcomes:*<br>Students could successfully determine the stability constants of zinc hexamine complex and silver ethylenediamine complex using a potentiometer, determine the CFSE value for Titanium and Chromium hexa aquo complexes, determine the Racah parameter for Nickel hexa aquo complex and tris- Nickel ethylenediamine complex. |

| Course Code | Practical Title | Credits |
|---|---|---|
| **RJSPGCHEPRI403** | **Practical – III (**Instrumental Methods in Inorganic Chemistry) | 2 |
| **Spectral Interpretation** | | |

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| M.Sc | Inorganic Chemistry, Paper III Practical |
| **RJSPGCHEPRI403**<br>Practical III<br>Instrumental Methods in Inorganic Chemistry | Course Outcomes:<br>Students will learn the interpretation of UV/VIS and FTIR spectra of Cu, Ni, V, and Co complexes and ligands.<br>*Learning Outcomes:*<br>Students will be capable to interpret spectra of any unknown inorganic complex which will help them to identify the structure of unknown complexes. |

| Course Code | Practical Title | Credits |
|---|---|---|
| **RJSPGCHEPRI404** | **Practical – IV (INTELLECTUAL PROPERTY RIGHTS & CHEMINFORMATICS)** | 2 |
| **Project Evaluation** | | |

| M.Sc | Inorganic Chemistry, Paper IV Practical |
|---|---|
| **RJSPGCHEPRI404**<br>Practical IV<br>**INTELLECTUAL PROPERTY RIGHTS & CHEMINFORMATICS** | Course Outcomes:<br>Students will learn to prepare PPT presentations on the project allotted to them and defense in viva -voce.<br>*Learning Outcomes:*<br>Students will understand the concept of different aspects of IPR during PPT presentation and use it for the presentation of their ideas in other projects. |

**Reference books for practicals**

1. A. I. Vogel, *Quantitative Inorganic Analysis.*
2. J. D. Woolins, *Inorganic Experiments.*
3. Palmer, *Inorganic Preparations.*
4. G. Raj, *Advanced Practical Inorganic Chemistry.*
5. J. E. House, Inorganic Chemistry, Academic press, 2nd edition, (2013).

Hindi Vidya Prachar Samiti's

# Ramniranjan Jhunjhunwala College

# of Arts, Science & Commerce

# (Autonomous College)

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## Syllabus for the M.Sc. Part – II

# Program: M.Sc. (Organic Chemistry)

# Program Code: RJSPGCHEO

# CBCS: 2020 -2021

## M.Sc. (Organic Chemistry) Semester – IV

| Course | Nomenclature | Credits | Topics |
|---|---|---|---|
| RJSPGCHEO401 | Paper I<br>Theoretical Organic Chemistry - II | 4 | 1. Physical organic chemistry<br>2. Supramolecular chemistry<br>3. Stereochemistry- II<br>4. Asymmetric synthesis |
| RJSPGCHEO402 | Paper II<br>Synthetic Organic Chemistry - II | 4 | 1. Designing Organic Synthesis-I<br>Protecting groups in Organic Synthesis<br>Concept of umpolung (Reversal of polarity).<br>Introduction to Retrosynthetic analysis and synthetic planning.<br>2. Designing Organic Synthesis-II<br>General strategy<br>One group C-C Disconnections.<br>Two group C-C Disconnections<br>3. Electro-organic chemistry and Selected methods of Organic synthesis.<br>4. Transition and rare earth metals in organic synthesis |
| RJSPGCHEO403 | Paper III<br>Natural Products and Heterocyclic Chemistry | 4 | 1. Natural products-III, Steroids.<br>2. Natural products-IV<br>Vitamins, Antibiotics.<br>Naturally occurring insecticides, Terpenoids.<br>3. Heterocyclic compounds-I<br>4. Heterocyclic compounds-II |
| RJSPGCHEO404 | Paper IV | 4 | 1. Introduction to Intellectual Property. |

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| | Intellectual Property Rights & Cheminformatics | | Patents, Industrial Designs, Copyrights, Trade Marks, Geographical Indications.<br>2. Trade Secrets<br>IP Infringement issue and enforcement.<br>Economic Value of Intellectual Property.<br>Different International agreements.<br>3. Introduction to Chem informatics<br>Representation of molecules and chemical<br>reactions, Searching Chemical Structures.<br>4. Applications |
| RJSPGCHEPRO401 | Practical - I | 8 | Theoretical Organic Chemistry – II |
| RJSPGCHEPRO402 | Practical - II | | Synthetic Organic Chemistry – II |
| RJSPGCHEPRO403 | Practical - III | | Natural Products And Heterocyclic Chemistry |
| RJSPGCHEPRO404 | Practical - IV | | Intellectual Property Rights & Cheminformatics |

| Course Code | Title | Credits |
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| **RJSPGCHEO401** | Paper - I<br>**Theoretical Organic Chemistry-II** | 4 |
| **Unit – I**<br><br>**Unit 1: Physical organic chemistry**<br>**1.1** Structural effects and reactivity**:** Linear free energy relationship (LFER) indetermination of organic reaction mechanism, The Hammett equation, substituent constants, theories of substituent effects, interpretation of σ-values, reaction constants ρ, Yukawa-Tsuno equation**.**<br>**1.2** Uses of Hammett equation, deviations from Hammett equation. Dual parameter correlations, Inductive substituent constants. The Taft model, $\sigma_I$ and $\sigma_R$ scales, steric parameters Es and β. Solvent effects, Okamoto-Brown equation, Swain-Scott equation, Edward and Ritchie correlations, Grunwald-Winstein equation, Dimroth's $E_T$ parameter, Solvatochromism, Z scale, Spectroscopic Correlations, Thermodynamic Implications. | | 1 |
| **Unit 2**<br><br>**Supramolecular chemistry**<br>**2.1** Principles of molecular associations and organizations as exemplified inbiological macromolecules like nucleic acids, proteins and enzymes.<br>**2.2** Synthetic molecular receptors: receptors with molecular cleft, molecular tweezers, receptors with multiple hydrogen sites.<br>**2.3** Structures and properties of crown ethers, cryptands, cyclophanes, calixarenes, rotaxanes and cyclodextrins. Synthesis of crown ethers, cryptands and calixarenes.<br><br>**2.4** Molecular recognition and catalysis, molecular self-assembly. Supramolecular Polymers, Gel sand Fibers . | | 1 |
| **UNIT-III**<br><br>**Stereochemistry- II**<br>**3.1** Racemization and resolution of racemates including conglomerates: Mechanism of racemization, methods of resolution: mechanical, chemical, kinetic and equilibrium asymmetric transformation and through inclusion compounds.<br><br>**3.2** Determination of enantiomer and diastereomer composition: enzymatic method, chromatographic methods. Methods based on NMR spectroscopy: use of chiral derivatizing agents (CDA), chiral solvating agents (CSA) and Lanthanide shift reagents (LSR). | | 1 |

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| **3.3** Correlative method for configurational assignment: chemical, optical rotation, and NMR spectroscopy.<br>**3.4** Molecular dissymmetry and chiroptical properties: Linearly and circularly polarized light. Circular birefringence and circular dichroism. ORD and CD curves. Cotton effect and its applications. The octant rule and the axial α–haloketone rule with applications. | |
| **UNIT-IV**<br>**Asymmetric synthesis**<br>**4.1** Principles of asymmetric synthesis: Introduction, the chiral pool in Nature, methods of asymmetric induction – substrate, reagent and catalyst controlled reactions.<br>**4.2** Synthesis of L-DOPA [Knowles's Mosanto process]. Asymmetric reactions with mechanism: Aldol and related reactions, Cram's rule, Felkin-Anhmodel, Sharpless enantioselective epoxidation, hydroxylation, amino hydroxylation, Diels-Alder reaction, reduction of prochiral carbonyl compounds and olefins.<br>**4.3** Use of chiral auxiliaries in diastereoselective reductions, asymmetric amplification. Use of chiral BINOLs, BINAPs and chiral oxazolines asymmetric transformations. | 1 |

| M.Sc. | **Paper – I**<br>**Theoretical Organic Chemistry-II** |
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| **RJSPGCHEO401 Theoretical Organic Chemistry-II** | Course outcomes:<br>1. To understand fundamental concepts of physical organic chemistry that governs various kinetic and thermodynamic aspects of organic reactions.<br>2. To study structure, properties, associations and organizations of organic macromolecules along with a typical synthesis of few of them.<br>3. To know the technique of resolution of racemates and to learn to determine the enantiomer and diastereomer composition.<br>2. To discuss principals involved in asymmetric synthesis and study of few selected similar organic name reactions<br><br>*Learning Outcomes:*<br>1. To learn various physical aspects of an organic reaction.<br>2. To study the synthesis and various properties of few macromolecules.<br>3. To be able to resolve the Racemic mixture.<br>4. To learn asymmetric synthesis. |

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| Course Code | Title | Credits |
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| **RJSPGCHEO402** | Paper – II<br>**Synthetic Organic Chemistry-II** | 4 |
| **Unit – I**<br><br>**Designing Organic Synthesis-I**<br>1.1 **Protecting groups in Organic Synthesis:** Protection and deprotection of the hydroxyl, carbonyl, amino and carboxyl functional groups and its applications.<br><br>1.2 **Concept of umpolung (Reversal of polarity):** Generation of acyl anion equivalent using 1,3-dithianes, methyl thiomethyl sulfoxides, cyanide ions, cyanohydrin ethers, nitro compounds and vinylated ethers.<br><br>1.3 **Introduction to Retrosynthetic analysis and synthetic planning:** Linear and convergent synthesis; Disconnection approach: An introduction to synthons, synthetic equivalents, disconnection approach, functional group interconversions (FGI), functional group addition (FGA), functional group removal (FGR) importance of order of events in organic synthesis, one and two group C-X disconnections (1,1; 1,2; 1,3 difunctionalized compounds),selective organic transformations: chemo selectivity, regioselectivity, stereo selectivity, enantio- selectivity. | | 1 |
| **Unit 2**<br><br>**Designing Organic Synthesis-II**<br>2.1 **General strategy:** choosing a disconnection-simplification, symmetry, high yielding steps, and recognizable starting material.<br><br>2.2 **One group C-C Disconnections:** Alcohols (including stereoselectivity), carbonyls (including regioselectivity), Alkene synthesis, use of acetylenes and aliphatic nitro compounds in organic synthesis.<br><br>2.3 **Two group C-C Disconnections:** 1,2- 1,3- 1,4- 1,5- and 1,6-difunctionalized compounds, Diels-Alder reactions, α, β-unsaturated compounds, control in carbonyl condensations, Michael addition and Robinson annellation. | | 1 |

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| **Unit 3**<br>**Electro-organic chemistry and Selected methods of Organic synthesis**<br>3.1 **Electro-organic chemistry:**<br>3.1.1 Introduction: Electrode potential, cell parameters, electrolyte, working electrode, choice of solvents, supporting electrolytes.<br><br>3.1.2 Cathodic reduction: Reduction of alkyl halides, aldehydes, ketones, nitrocompounds, olefins, arenes, electro-dimerization.<br>3.1.3 Anodic oxidation: Oxidation of alkylbezene, Kolbe reaction, non-Kolbe oxidation, Shono oxidation.<br><br>3.2 **Selected Methods of Organic synthesis**<br>Applications of the following in organic synthesis:<br>3.2.1 Crown ethers, cryptands, micelles, cyclodextrins, catenanes.<br>3.2.2 Organo catalysts: Proline, Imidazolidinone.<br>3.2.3 Pd catalyzed cycloaddition reactions: Stille reaction, Saeguse-Ito oxidation to enones, Negishi coupling.<br>3.2.4 Use of Sc(OTf), and Yb(OTf) as water tolerant Lewis acid catalyst in aldol condensation, Michael reaction, Diels-Alder reaction, Friedel – Crafts reaction. | 1 |
| **Unit 4**<br>**Transition and rare earth metals in organic synthesis**<br><br>4.1 **Introduction to basic concepts:** 18 electron rules, bonding in transition metal complexes, C-H activation, oxidative addition, reductive elimination, migratory insertion. [<br>4.2 **Palladium in organic synthesis:** $\pi$-bonding of Pd with olefins, applications in C-C bond formation, carbonylation, alkene isomerization, cross-coupling of organometallics and halides. Representative examples: Heck reaction, Suzuki-Miayura coupling, Sonogashira reaction and Wacker oxidation. Heteroatom coupling for bond formation between aryl/vinyl groups and N,S, or P atoms.<br>4.3 **Olefin metathesis** using Grubb's catalyst.<br><br>4.4 **Application of Ni, Co, Fe, Rh, and Cr carbonyls** in organic synthesis.<br><br>4.5 **Application of samarium iodide** including reduction of organic halides, aldehydes and ketones, α-functionalized carbonyl and nitro compounds.<br><br>4.6 **Application of Ce (IV)** in synthesis of heterocyclic quinoxaline derivatives and its role as a de-protecting agent**.** | 1 |

| M. Sc. | **Paper – II**<br>**Synthetic Organic Chemistry-II** |
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| **RJSPGCHEO402 Synthetic Organic Chemistry-II** | Course outcomes:<br><br>1. To find out the feasible pathways of organic synthesis of a target molecule by backward engineering based on comprehensive knowledge of reaction mechanism.<br>2. To incorporate well established organic name reactions in choosing appropriate starting material and designing high yielding steps for the required organic synthesis.<br>3. To know and understand the role of various electrochemical organic conversions in the field of organic synthesis.<br>4. To explore the possibilities of catalysis by different transition and rare earth metals and its compounds *Learning Outcomes:*<br><br>*Learning Outcome:*<br>1. To learn the name reactions and their applications in various organic synthesis to give high yields of the reaction steps.<br>2. To learn the retro synthesis.<br>3. To understand the different electrochemical reactions.<br>4. To learn the catalysis of various rare earth metals in organic synthesis. |

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▪ **Name Reactions,** Jie Jack Lie, 3rd Edn., Springer

▪ **Organic Electrochemistry,** H. Lund, and M. Baizer, 3rd Edn.,Marcel Dekker.

| Course Code | Title | Credits |
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| **RJSPGCHEO403** | Paper - III<br>**Natural Products And Heterocyclic Chemistry** | 4 |
| **Unit – I**<br><br>**Natural products-III**<br>1.1 **Steroids:** General structure, classification. Occurrence, biological role, important structural and stereochemical features of the following: corticosteroids, steroidal hormones, steroidal alkaloids, sterols and bile acids.<br><br>1.2 Synthesis of 16-DPA from cholesterol and plant sapogenin.<br><br>1.3 Synthesis of the following from 16-DPA: androsterone, testosterone, oestrone, oestriol, oestradiol and progesterone.<br><br>1.4 Synthesis of cinerolone, jasmolone, allethrolone, exaltone and muscone. | | 1 |
| **Unit 2**<br><br>**Natural products-IV**<br>2.1 **Vitamins:** Classification, sources and biological importance of vitamin $B_1$,$B_2$, $B_6$, folic acid, $B_{12}$, C, $D_1$, E (α-tocopherol), $K_1$, $K_2$, H (β- biotin).<br><br>Synthesis of the following:<br>Vitamin A from β-ionone and bromo ester moiety.<br>Vitamin $B_1$ including synthesis of pyrimidine and thiazole moieties<br>Vitamin $B_2$ from 3, 4-dimethylaniline and D(-)ribose<br>Vitamin $B_6$ from: 1) ethoxyacetylacetone and cyanoacetamide, 2) ethylester of N-formyl-DL-alanine (Harris synthesis)<br>Vitamin E (α-tocopherol) from trimethylquinol and phytyl bromide<br>Vitamin $K_1$ from 2-methyl-1, 4-naphthaquinone and phytol.<br>2.2 **Antibiotics:** Classification on the basis of activity. Structure elucidation,spectral data of penicillin-G, cephalosporin-C and chloramphenicol.Synthesis of chloramphenicol (from benzaldehyde and β-nitroethanol)penicillin-G and phenoxymethylpenicillin from D-penicillamine and t-butylphthalimidemalonaldehyde (synthesis of D-penicillamine and t-butylphthalimidemalonaldehyde expected).<br>2.3 **Naturally occurring insecticides:** Sources, structure and biologicalproperties of pyrethrums (pyrethrin I), rotenoids (rotenone). Synthesis ofpyrethrin I.<br><br>2.4 **Terpenoids**: Occurrence, classification, structure elucidation, stereochemistry, spectral data and synthesis of zingiberene . | | 1 |

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| **UNIT-III**<br>**Unit 3: Heterocyclic Compounds-I**<br>Heterocyclic compounds: Introduction, classification, Nomenclature of heterocyclic compounds of monocyclic (3-6 membered) (Common, systematic (Hantzsch-Widman) and replacement nomenclature) Structure, reactivity, synthesis and reactions of pyrazole, imidazole, oxazole, isoxazole, thiazole, isothiazole, pyridazines, pyrimidine, pyrazines and oxazines. | 1 |
| **UNIT-IV**<br>**Heterocyclic compounds-II**<br>Nomenclature of heterocyclic compounds of bicyclic/tricyclic (5-6Membered) fused heterocycles (up to three hetero atoms)**.** (Common, systematic (Hantzsch-Widman) and replacement nomenclature) Nucleophilic ring opening reactions of oxiranes, aziridines, oxetanes and azetidines. Structure, reactivity, synthesis and reactions of coumarins, quinoxalines, cinnolines, indole, benzimidazoles, benzoxazoles, benzothiazoles, Purines and acridines. | 1 |

| M.Sc. | **Paper –III**<br>**Natural Products and Heterocyclic Chemistry** |
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| **RJSPGCHEO403 Natural Products And Heterocyclic Chemistry** | Course outcomes:<br>1. To know the synthesis of some selected natural products and study of organic biomolecules like steroids.<br>2. To discuss the classification, sources, structure elucidation and biological importance of Vitamins and antibiotics.<br>3. To study classification, nomenclature and synthesis of hetero monocyclic compounds.<br>5. To study classification, labelling and preparation, reactivity of bi, tricyclic five and six membered heterocycles up to three heteroatoms.<br><br>*Learning Outcomes:*<br>1. To learn the natural products like steroids.<br>2. To learn the role of organic biomolecules like vitamins and antibiotics.<br>3. To understand and study various heteromonocycls.<br>4. To learn the classification, labelling and preparation, reactivity of bi, tricyclic five and six membered heterocycles up to three heteroatoms. |

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| Course Code | Title | Credits |
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| **RJSPGCHEO404** | **Paper – IV**<br>**Intellectual Property Rights & Cheminformatics** | 4 |
| **Unit I:**<br>**Introduction to Intellectual Property:**<br>Historical Perspective, Different types of IP, Importance of protecting IP.<br>**Patents:**<br>Historical Perspective, Basic and associated right, WIPO, PCT system, Traditional Knowledge, Patents and Health care-balancing promoting innovation with public health, Software patents and their importance for India.<br>**Industrial Designs:**<br>Definition, How to obtain, features, International design registration. | | 1 |

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| **Copyrights:**<br>Introduction, How to obtain, Differences from Patents.<br>**Trade Marks:**<br>Introduction, How to obtain, Different types of marks – Collective marks, certification marks, service marks, trade names etc.<br>**Geographical Indications:**<br>Definition, rules for registration, prevention of illegal exploitation, importance to India. | |
| **Unit II:**<br>**Trade Secrets:**<br>Introduction and Historical Perspectives, Scope of Protection, Risks involved and legal aspects of Trade Secret Protection.<br>**IP Infringement issue and enforcement:**<br>Role of Judiciary, Role of law enforcement agencies – Police, Customs etc.<br>**Economic Value of Intellectual Property:**<br>Intangible assests and their valuation, Intellectual Property in the Indian context – Various Laws in India Licensing and Technology transfer.<br>**Different International agreements:**<br>**(a) World Trade Organization (WTO):**<br>(i) General Agreement on Tariffs and Trade (GATT), Trade Related Intellectual Property Rights (TRIPS) agreement<br>(ii) General Agreement on Trade Related Services (GATS) Madrid Protocol.<br>(iii) Berne Convention<br>(iv) Budapest Treaty<br>**(b) Paris Convention**<br>**WIPO** and **TRIPS, IPR** and Plant Breeders Rights, IPR and Biodiversity. | 1 |
| **Unit III:**<br>**Introduction to Chem informatics:**<br>History and evolution of cheminformatics, Use of Cheminformatics, Prospects of cheminformatics, Molecular modeling and structure elucidation.<br>**Representation of molecules and chemical reactions:**<br>Nomenclature, Different types of notations, SMILES coding, Matrix representations, Structure of Molfiles and Sdfiles, Libraries and toolkits, Different electronic effects, Reaction classification.<br>**Searching Chemical Structures:** | 1 |

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| Full structure search, sub-structure search, basic ideas, similarity search, three dimensional search methods, basics of computation of physical and chemical data and structure descriptors, data visualization. | |
| **Unit IV:**<br>**Applications:**<br>Prediction of Properties of Compound, Linear Free Energy Relations, Quantitative Structure – Property Relations, Descriptor Analysis, Model Building, Modeling Toxicity, Structure – Spectra correlations, Prediction NMR, IR and Mass spectra, Computer Assisted Structure elucidations, Computer assisted Synthesis Design, Introduction to drug design, Target Identification and Validation, Lead Finding and Optimization, analysis of HTS data, Virtual Screening, Design of Combinatorial Libraries, Ligand based and Structure based Drug design, Application of Chem informatics in Drug Design. | 1 |

| M.Sc | **Paper – IV**<br>**Intellectual Property Rights & Cheminformatics** |
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| **RJSPGCHEO404 Intellectual Property Rights & Cheminformatics** | Course outcomes:<br>1. To create awareness and understanding the terms like intellectual property, patents, copyright, industrial designs, trademarks, geographical indications etc.<br>2. To know trade secrets, IP infringement issues, economic value of intellectual property and study of various related international agreements.<br>3. To explore cheminformatics to facilitate molecular modeling and structure elucidations.<br>4. To apply the knowledge gained about various chemistry principles, techniques and tools in drug designing, target identification and validation, lead finding and optimization.<br><br>*Learning Outcomes:*<br>*After completing this course student will be able to:* |

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| | 1. To learn the terms with their meaning such as intellectual property, patents, copyright, industrial designs, trademarks, geographical indications etc.<br>2. To understand various trades and their trade secrets.<br>3. To understand different IP infringement issues, economic value of intellectual property.<br>4. To learn the steps involved in drug designing and optimization. |

**REFERENCES:**

1. Andrew R. Leach & Valerie J. Gillet (2007) *An Introduction to Cheminformatics.* Springer: The Netherlands.
2. Gasteiger, J. & Engel, T. (2003) *Cheminformatics: A textbook*. Wiley–VCH

3. Gupta, S. P. *QSAR and Molecular Modeling.* Springer-Anamaya Pub.: New Delhi.

| Course Code | Practical Title | Credits |
|---|---|---|
| **RJSPGCHEPRO401** | **Practical – I (Theoretical Organic Chemistry-II)** | 2 |

**Separation of a solid-liquid / liquid-liquid ternary mixture using micro-scale technique**

1. Separation of solid components of a ternary mixture (solid-liquid / liquid-liquid) based upon differences in the physical and the chemical properties of the components.
2. Purification of the three components, measurement of their mass and determination of their physical constants.
3. Calculation of percentage yields of the individual components. (Identification of the components is not expected).

(**Minimum 6 mixtures**)

| M.Sc | Organic Chemistry, Paper I Practical |
|---|---|
| **RJSPGCHEPRO401**<br>Practical I<br>**Theoretical Organic Chemistry-II** | Course Outcomes:<br>1. To understand and employ concept of type determination and separation.<br>2. Purify (recrystalize/distill) the separated compounds.<br>3. Meticulously record physical constants<br><br>*Learning Outcomes:*<br>1. To be able to resolve the given solid/liquid ternary mixture into its components.<br>2. To be able to do the purification of separated components.<br>3. To be able to record the correct melting point of it |

| Course Code | Practical Title | Credits |
|---|---|---|
| **RJSPGCHEPRO402** | **Practical – II (Synthetic Organic Chemistry-II)** | 2 |

**Extraction / Estimation of natural products**

1. Extraction of clove oil from cloves.
2. Extraction of nicotine dipicrate from tobacco.
3. Estimation of proteins by Biuret method using spectrophotometer.
4. Estimation of glucose by Folin Wu method.
5. Estimation of citral using hydroxylamine hydrochloride.
6. Estimation of saponification value of oil.

| M.Sc | Organic Chemistry, Paper II Practical |
|---|---|
| **RJSPGCHEPRI402**<br>Practical II<br>**Synthetic Organic Chemistry-II** | Course Outcomes:<br>1. To develop the skill of extraction of natural products from various sources.<br>2. Purify (recrystalize/distill) the separated compounds.<br>3. To perform quantitative analysis of organic biomolecules<br><br>*Learning Outcomes:*<br>1. To be able to extract the natural products from their sources.<br>2. To know the various purification techniques.<br>3. To do the analysis of Biomolecules. |

| Course Code | Practical Title | Credits |
|---|---|---|
| **RJSPGCHEPRO403** | **Practical – III (Natural Products And Heterocyclic Chemistry)** | 2 |

**Techniques of purification and green methods of synthesis**

**Set I: Techniques of purification:**

1. Steam distillation
2. Vacuum distillation
3. Column chromatography

**Set II: Green methods of synthesis (microwave induced)**

1. Synthesis of Schiff's base from aniline and p-anisaldehyde in the presence of lime juice
2. Synthesis of coumarin by Knoevenagel reaction using salicylaldehyde, and ethyl acetate in presence of a base.
3. Synthesis of dihydropyrimidones- Biginelli reaction: acid-catalyzed three component reaction between vanillin, ethyl acetoacetate and thiourea.
4. Synthesis of acetanilide from aniline

| M.Sc. | Organic Chemistry, Paper III Practical |
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| **RJSPGCHEPRO403**<br>Practical III<br>**Natural Products And Heterocyclic Chemistry** | Course Outcomes:<br>**Set I:**<br>1. Students are expected to perform a purification technique using a known mass or volume of the given substance.<br>2. Check the purity of the purified compound by TLC, measure its mass and physical constant.<br>**Set II:**<br>Students are expected to purify the product by recrystallization, measure its mass, determine physical constant and calculate percentage yield<br>*Learning Outcomes:*<br>1. Set -1<br>To be able to apply different purification techniques to the given organic compound. 2.to be able to find the TLC and mass as well as physical constant of an organic compound.<br>2. Set -2<br>To be able to carry out certain green synthesis, and purify the product obtained quantitatively. |

| Course Code | Practical Title | Credits |
|---|---|---|
| **RJSPGCHEPRO404** | **Practical – IV (Intellectual Property Rights & Cheminformatics)** | 2 |

**Project evaluation**

1. The candidate is expected to submit a journal and project certified by the Head of the Department /institution at the time of the practical examination.
2. A candidate will not be allowed to appear for the practical examination unless he/she produces a certified journal or a certificate from the Head of the institution/department stating that the journal is lost and the candidate has performed the required number of experiments satisfactorily. The list of the experiments performed by the candidate should be attached with such certificate

| M.Sc | Organic Chemistry, Paper IVI Practical |
|---|---|
| **RJSPGCHEPRO404**<br>Practical IV<br>**Intellectual Property Rights & Cheminformatics** | Course Outcomes:<br>*Learning Outcomes:* |

**References for Practicals**

1. Comprehensive Practical Organic Chemistry: Preparation and Quantitative Analysis- V. K. Ahluwalia and Renu Aggarwal, Universities Press India Ltd., 2000
2. Advanced Practical Organic Chemistry – N. K. Vishnoi, Third Addition, Vikas Publishing House PVT Ltd
3. Systematic Laboratory Experiments in Organic Synthesis- A. Sethi, New Age International Publications
4. Systematic Identification of Organic compounds, 6th edition, R. L. Shriner, R. C. Fuson and D.Y. Curtin Wiley, New York.
5. Vogel's Textbook of Quantitative Analysis, revised, J. Bassett, R. C. Denney, G. H. Jeffery and J. Mendham, ELBS
6. Experiments and Techniques in Organic Chemistry, D. Pasto, C. Johnson and M. Miller, Prentice Hall
7. Macro-scale and Micro-scale Organic Experiments, K. L. Williamson, D. C. Heath.

8. Systematic Qualitative Organic Analysis, H. Middleton, Adward Arnold.
9. Handbook of Organic Analysis- Qualitative and Quantitative, H. Clark, Adward Arnold.
10. Vogel's Textbook of Practical Organic Chemistry, Fifth edition,2008, B.S.Furniss, A. J. Hannaford, P.
W. G. Smith, A. R. Tatchell, Pearson Education.
11. Laboratory Manual of Organic Chemistry, Fifth edition, R K Bansal, New Age Publishers.
12. Organic structures from spectra, L. D. Field, S. Sternhell, John R. Kalman, Wiley, 4$^{th}$ed., 2011.

Hindi Vidya Prachar Samiti's

# Ramniranjan Jhunjhunwala College

# of Arts, Science & Commerce

# (Autonomous College)

Affiliated to

# UNIVERSITY OF MUMBAI

## Proposed syllabus for the M.Sc. Part – II Sem IV

## Program: M.Sc. (Analytical Chemistry)

## Program Code: RJSPGCHEA

## CBCS: 2020 -2021

# M.Sc. (Analytical Chemistry) Semester – IV

| Course | Nomenclature | Credits | Topics |
|---|---|---|---|
| RJSPGCHEA401 | Quality In Analytical Chemistry | 4 | 1) Separation Science<br>2) Separation, Analysis and Standardization of Herbal based products.<br>3) Green Chemistry<br>4) Advanced Techniques |
| RJSPGCHEA402 | Advance Instrumental Techniques | 4 | 1) Spectral Methods III<br>2) Spectral Methods IV<br>3) Radiochemical And Thermal Methods<br>4) Hyphenated Techniques |
| RJSPGCHEA403 | Selected Topics in Analytical Chemistry | 4 | 1) Effluent Treatment<br>2) Solid Waste Management<br>3) Plastics and Polymers<br>4) Metallurgy |
| RJSPGCHEA404 | IPR & Cheminformatics | 4 | 1. Introduction to Intellectual Property. Patents, Industrial Designs, Copyrights, Trade Marks, Geographical Indications.<br>2. Trade Secrets<br>IP Infringement issue and enforcement. Economic Value of Intellectual Property. Different International agreements.<br>3. Introduction to Chem informatics<br>Representation of molecules and chemical reactions. Searching Chemical Structures.<br>4. Applications |
| RJSPGCHEA404 | Paper IV | 4 | 1) Print, journals, digital, information technology and library resources.<br>2) Data analysis.<br>3) Methods of scientific research and writing scientific papers.<br>4) Chemical safety & ethical handling of chemicals. |

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| RJSPGCHEPRA401 | Quality In Analytical Chemistry Practical | | Quality In Analytical Chemistry Practical |
| RJSPGCHEPRA402 | Advance Instrumental Techniques Practical | | Advance Instrumental Techniques Practical |
| RJSPGCHEPRA403 | Selected Topics In Analytical Chemistry Practical | 8 | Selected Topics in Analytical Chemistry Practical |
| RJSPGCHEPRA404 | IPR & Cheminformatics Practical | | IPR & Cheminformatics Practical |

| Course Code | Title | Credits |
|---|---|---|
| **RJSPGCHEA401** | Analytical Chemistry<br>**Quality in Analytical Chemistry** | 4 |
| **Unit – I**<br><br>**Separation Science**<br>1.1 Membrane separation processes: operating principles and applications of microfiltration, ultra-filtration, reverse osmosis, dialysis and electro-dialysis.<br>1.2 Applications of Solvent extraction in Analytical Chemistry recapitulation of solvent extraction, roles of solvent extraction in analytical chemistry, solvent extraction in sample preparation and pretreatment steps, solvent extraction as a means of analytical determination | | 1 |
| **Unit II**<br>**Separation, Analysis and Standardization of Herbal based products.**<br>2.1 Herbs as a raw material: Definition of herb, herbal medicine, herbal Medicinal products, herbal drug preparation. Sources of herbs. Selection, identification and authentication of herbal materials, drying and processing of herbal raw material.<br><br>2.2 Extraction of herbal materials: Choice of solvent for extraction, methods used for extraction and principles involved in extraction.<br><br>2.3 Standardization of herbal formulation and herbal extracts: Standardization of herbal extract as per WHO cGMP guidelines, Physical, Chemical, Spectral and toxilogical standardization, qualitative and quantitative estimations. | | 1 |
| **UNIT-III**<br><br>**Green Chemistry**<br><br>**3.1 Principle and concepts of green chemistry**: sustainable development and green chemistry, atom economy, examples of atom economic and atom uneconomic reactions, reducing toxicity<br>**3.2 Organic solvents:** environmentally benign solutions, solvent free systems, supercritical fluids (only introduction) Ionic liquids as catalysts and solvents<br><br>**3.3 Emerging Green Technologies:** photochemical reactions (advantages and challenges), examples. Chemistry using microwaves, sonochemistry and electrochemical synthesis.<br>**3.4 Designing Greener Processes:** Inherently Safer Designs (ISD), Process intensification (PI) in-process monitoring. | | 1 |

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| **UNIT-IV**<br>**Advanced Techniques**<br>**4.1 Electrophoresis:** introduction, factors affecting migration rate, supporting media (gel, paper, cellulose, acetate, starch, polyacrylamide, agarose, sephadex and thin layers)<br>**4.2 Techniques of Electrophoresis:** low and high voltage, sds-page, continuous electrophoresis, capillary electrophoresis, zone, gel, isoelectric focusing, isotachophoresis and micellar electrokinetic capillary chromatography, instrumentation, detection and applications.<br>**4.3 Introduction to Nanotechnology:** Analytical techniques in nanotechnology, consequences of the nanoscale, (nanoparticles morphology, electronic structure, optical properties) one dimensional nano materials (nanofilms, nanolayers), two dimensional nanomaterials (nanotubes, nanowires), three dimensional nanomaterials (nanoparticles and quantum dots). | 1 |

| M. Sc. | **Paper – I**<br>**Quality in Analytical Chemistry** |
|---|---|
| **RJSPGCHEA401 Quality in Analytical Chemistry** | Course outcomes:<br>1. understand the basic concept of Membrane separation processes<br>2. understand the concept of Applications of Solvent extraction in Analytical Chemistry.<br>1. implement good laboratory practiceswhile working in the laboratory.<br>2. understand the basic concept of Separation, Extraction,Analysis and Standardization of Herbal based products.<br>3. understand the basic concept of Principle and concepts of green chemistry,Emerging Green Technologies,Designing Greener Processes<br>4. understand the basic concept of **Advanced Techniques like** Electrophoresis,isotachophoresis ,Analytical techniques in nanotechnology<br>5. understand the basic concept of<br>*Learning Outcomes:*<br>**On successful completion of this course students will be able to** understand the basic concept of<br>1. Membrane separation processes<br>2. Applications of Solvent extraction in Analytical Chemistry.<br>3. Separation, Extraction,Analysis and Standardization of Herbal based products<br>4. .Principle and concepts of green chemistry,Emerging Green Technologies,Designing Greener Processes<br>5. **Advanced Techniques like** Electrophoresis,isotachophoresis ,Analytical techniques in nanotechnology |

**List of Books and references:**

1. Research Methodology: Methods & Techniques by C R Kothari, 2e, Wishwa Publication, New Delhi
2. Research Methodology by D K Bhattacharyya, 1 e, Excel Books, New Delhi, 2003
3. How to Research by Loraine Blaxter, Christina Hughes and Molcolm Tight, Viva Books Pvt.Ltd., New Delhi
4. Chemical methods of separation, J A Dean, Van Nostrand Reinhold, 1969
5. Solvent extraction and ion exchange, J Marcus and A. S. Kertes Wiley INC 1969.
6. Extraction Chromatography, T. Braun, G. Ghersene, Elsevier Publications 1978.
7. Super critical fluid extraction, Larry Taylor Wiley publishers N.Y. 1996
8. Ion exchange separation in analytical chemistry, O Samuelson John Wiley 2nd ed 1963
9. Ion exchange chromatography, Ed H.F Walton Howden, Hutchenson and Rossing 1976
10. Chromatographic and el ectrophoresis techniques, I Smith Menemann Interscience 1960
11. Green chemistry and catalyst, R. A. Sheldon, Isabella Arends, Ulf Hanefeld Wiley VCH verlag GmBH & co.
12. Sustainable residential development: planning and design for green neighborhoods. Avi Friedman, McGraw Hill professional.

| Course Code | Title | Credits |
|---|---|---|
| **RJSPGCHEA402** | Analytical Chemistry<br>**Advanced Instrumental Techniques** | 4 |
| **Unit – I**<br>**Spectral Methods: III**<br>NMR Spectroscopy<br>**1.1 Theory and Instrumentation:** recapitulation, FTNMR, 2D NMR-FID signal generation mechanism, Techniques in 2D NMR- homo nuclear correlation spectroscopy (COSY), total correlation spectroscopy (TOCSY), heteronuclear correlation (HETCOR)<br>**1.2 Radio waves in imaging:** Principle, instrumentation and applications of MRI.<br>**1.3 Application of NMR** to other nuclei $C^{13}$, $P^{31}$ and $F^{19}$ spectroscopy. | | 1 |
| **Unit-II**<br>**Spectral Methods: IV**<br>**2.1 Mass spectroscopy:** recapitulation, correlation of mass spectra with molecular structure- interpretation of mass spectra, analytical information derived from mass spectra- molecular identification, metastable peaks, Fragmentation Reactions<br>**2.2 Raman spectroscopy:** Principle theory, Instrumentation, techniques (SERS and Resonance Raman) and Applications of Raman spectroscopy. | | 1 |
| **UNIT-III**<br>**Radiochemical And Thermal Methods**<br>**3.1 Activation analysis:** NAA, radiometric titrations and radio-release methods<br>**3.2 Thermal analysis:** Principle, Interfacing, instrumentation and Applications of (a) Simultaneous Thermal Analysis- TG-DTA and TG-DSC (b) Evolved gas analysis(EGA)- TG-MS and TG-FTIR. | | 1 |
| **UNIT-IV**<br>**Hyphenated Techniques**<br>**4.1** Concept of hyphenation, need for hyphenation, possible hyphenations.<br>**4.2** Interfacing devices and applications of GC – MS, ICP -MS, GC - IR, Tandem Mass Spectrometry, LC – MS: HPLC-MS, CE-MS. | | 1 |

| M.Sc | **Paper – II**<br>**RJSPGCHEA402**<br>**Advanced Instrumental Techniques** |
|---|---|
| **RJSPGCHEA402 Advanced Instrumental Techniques** | Course outcomes:<br><br>**To understand the basic concept of :**<br>1. NMR Spectroscopy, its Theory and Instrumentation, applications of MRI<br>2. Raman spectroscopy in detail and interpretation of mass spectra, analytical information derived from mass spectra<br>3. Radiochemical method, NAA And Simultaneous Thermal Methods<br>4. hyphenation, and Interfacing devices and applications of Hyphenated Techniques<br>*Learning Outcomes:*<br>On successful completion of this course students will be able to:<br><br>1. understand the basic concept of NMR Spectroscopy, its Theory and Instrumentation, applications of MRI<br><br>2. the basic concept of Raman spectroscopy in detail and interpretation of mass spectra, analytical information derived from mass spectra<br><br>3. the basic concept of Radiochemical method NAA And Simultaneous Thermal Methods like TG-DTA, TG-DSC, TG-MS and TG-FTIR<br><br>4. the basic concept of hyphenation, and Interfacing devices and applications of GC – MS, ICP -MS, GC - IR, Tandem Mass Spectrometry, LC – MS: HPLC-MS, CE-MS. |

**List of Books and references:**

1. Analytical Chemistry, G. D. Christian, 4th Ed. John Wiley, New York (1986)
2. Fundamentals of Analytical Chemistry, D. A. Skoog and D. M. West and F. J Holler Holt- Saunders 6th
Edition (1998)
3. Principles of Instrumental Analysis, D. A. Skoog, F. J. Holler and J.A. Niemann 5th Ed.
4. Instrumental methods of Analysis, H. H. Willard, L. L. Merritt Jr, J. A. Dean and F. A.
5. Thermal methods of Analysis, P. J. Haines, Blackie Academic & Professional, London (1995)
6. Thermal Analysis, 3rd Edition W. W. Wendlandt, John Wiley, N.Y. (1986)
7. Principles and Practices of X-ray spectrometric Analysis, 2nd Ed E. P. Bertain, Plenum Press, NY, (1975)
8. Nuclear Analytical Chemistry, D. Bane, B. Forkman, B. Persson, Chartwell - Bratt Ltd (1984)
9. Standard Methods of Chemical Analysis, Eds. F. J. Welcher, Robert E. Krieger Publishing Company, A series of volumes
10. A Complete Introduction to Modern NMR Spectroscopy 1st Edition by Roger S. Macomber

11. Spectrometric Identification of Organic Compounds Hardcover – by Robert M.Silverstein Wiley
12 Tandem Techniques (Separation Science Series) 1st Edition by Raymond P. W. Scott John Wiley & Sons Ltd, 1997
13 Encyclopedia of Analytical Science, Editors-in-Chief: Paul Worsfold, Alan Townshend, and Colin Poole ISBN: 978-0-12-369397-6
14. Encyclopedia of Analytical Chemistry: Applications, Theory, and Instrumentation. Meyers Robert A Meyers
15. Introduction to Thermal Analysis Techniques and Applications Edited by Michael E. Brown
16 Principles and Applications of Thermal Analysis Edited by Paul Gabbott

| Course Code | Title | Credits |
|---|---|---|
| **RJSPGCHEA403** | Analytical Chemistry<br>**Selected Topics in Analytical Chemistry** | 4 |
| **Unit – I**<br><br>**Effluent Treatment**<br>**1.1** Effluent treatment plant general construction and process flow charts<br>**1.2** Treatment and disposal of Sewage.<br>**1.3.** Effluent parameters for metallurgical industry.<br>**1.4** Permissible limits for metal (example Cr, As, Pb, Cd etc.) traces in the effluent.<br>**1.5**Recovery of metals from effluent, modern methods-Electrodialysis, Electrodeposition and Ion Exchange etc.<br>**1.6** Recycle and reuse of process and treated (effluent) water. | | 1 |
| **Unit 2**<br><br>**Solid Waste Management**<br><br>**2.1** Solid waste management: objectives, concept of recycle, reuse and recovery<br><br>**2.2** Methods of solid waste disposal.<br><br>**2.3** Treatment and disposal of sludge / dry cake<br><br>**2.4** Managing non-decomposable solid wastes<br><br>**2.5 Biomedical waste:** Introduction, Classification and methods of disposal. | | 1 |
| **UNIT-III**<br><br>**Plastics and Polymers**<br>**3.1** Classification of plastic, determination of additives, molecular weight distribution, analysis of plastic and polymers based on styrene, vinyl chloride, ethylene, acrylic and cellulosic plastics.<br>**3.2** Metallic impurities in plastic and their determination,<br>**3.3** Impact of plastic on environment as pollutant.<br>**3.4** Paints and pigments: Types of paints pigments, determination of volatile and non - volatile components, Flash point (significance and method of determination), separation and analysis of pigments, binders and thinners.<br>**3.5** Role of organo silicones in paints and their impact on environment. | | 1 |

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| **UNIT-IV**<br>**Metallurgy**<br>**4.1 Ores and minerals:** Dressing of ores, pollution due to metallurgical processes (ore dressing, calcination, smelting)<br>**4.2 Chemical analysis of ores for principal constituents:** Galena, Pyrolusite, Bauxite, Hematite, Monazite.<br>**4.3 Alloys:** definition, analysis of Cupronickel, Magnalium , Steel And Stainless Steel, Bronze, Gun metal.<br>**4.4 Techniques of purification:** Zone refining, analysis of high purity materials like silicon, vacuum fusion and extraction techniques. | 1 |

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| M.Sc | **Paper – III** |
| **RJSPGCHEA403 Selected Topics in Analytical Chemistry** | **Course outcomes:**<br>To understand the basic concept of<br>1. Effluent Treatment, disposal of Sewage,Permissible limits for metal,Recovery of it,Recycle and reuse of process<br>2. Solid waste management,Methods,Treatment and disposal,Bio- medical waste<br>3. Plastics and Polymers,Classification of plastic, additives, analysis of plastic,Types of paints pigments<br>Metallurgy,Dressing of ores,Chemical analysis of ores,Techniques of purification.<br><br>***Learning Outcomes:***<br>On successful completion of this course students will be able to understand the basic concept of -<br>1. Effluent Treatment, disposal of Sewage, Permissible limits for metal, Recovery of it, Recycle and reuse of process.<br>2. Solid waste management, Methods, Treatment and disposal, Bio- medical waste.<br>3. Plastics and Polymers, Classification of plastic, additives, analysis of plastic, Types of paints pigments.<br>**4.** Metallurgy, Dressing of ores, Chemical analysis of ores, Techniques of |

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|---|---|
| | 5. the basic concept of Effluent Treatment, disposal of Sewage, Permissible limits for metal, Recovery of it, Recycle and reuse of process. |

**List of Books and References:**

1. Environmental Pollution Analysis, S. M. khopkar, New Age International publication (2011).
2. Water and water pollution (hand book) Ed., Seonard'l Ciacere, Vol I to IV, Marcel Dekker inc. N.Y.(1972)
3. Water pollution, Arvind kumar, APH publishing (2004)
4. Introduction to Potable Water Treatment Processes Simon Parsons, Bruce Jefferson, Paperback publication.
5. Solid waste management, K Sasikumar and Sanoop Gopi Krishna PHI publication (2009)
6. Solid waste management, Surendrakumar Northen Book Center (2009)
7. Handbook of chemical technology and pollution control 3rd Edn Martin Hocking AP Publication (2005).
8 Fundamental Concepts of Environmental Chemistry, Second Edition G. S. Sodhi , Alpha Science, 2005
9. Chemical analysis of metals ; Sampling and analysis of metal bearing ores: American Society for Testing and Materials 1980 - Technology & Engineering
10. Manual of Procedures for Chemical and Instrumental Analysis of Ores, Minerals, and Ore Dressing Products. Government of India Ministry of Steel & Mines, Indian Bureau of Mines, 1979.
11. Alloying: understanding the basics, edited by Joseph R. Davis, ASM International (2001).
**12.** Zone refining and allied techniques, Norman L. Parr, G. Newnes Technology & **Engineering (1960).**

| Course Code | Title | Credits |
|---|---|---|
| **RJSPGCHEA404** | **Paper – IV**<br>**Intellectual Property Rights & Cheminformatics** | 4 |
| **Unit I:**<br>**Introduction to Intellectual Property:**<br>Historical Perspective, Different types of IP, Importance of protecting IP.<br>**Patents:** | | 1 |

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| Historical Perspective, Basic and associated right, WIPO, PCT system, Traditional Knowledge, Patents and Health care-balancing promoting innovation with public health, Software patents and their importance for India.<br>**Industrial Designs:**<br>Definition, How to obtain, features, International design registration.<br>**Copyrights:**<br>Introduction, How to obtain, Differences from Patents.<br>**Trade Marks:**<br>Introduction, How to obtain, Different types of marks – Collective marks, certification marks, service marks, trade names etc.<br>**Geographical Indications:**<br>Definition, rules for registration, prevention of illegal exploitation, importance to India. | |
| **Unit II:**<br>**Trade Secrets:**<br>Introduction and Historical Perspectives, Scope of Protection, Risks involved and legal aspects of Trade Secret Protection.<br>**IP Infringement issue and enforcement:**<br>Role of Judiciary, Role of law enforcement agencies – Police, Customs etc.<br>**Economic Value of Intellectual Property:**<br>Intangible assests and their valuation, Intellectual Property in the Indian context – Various Laws in India Licensing and Technology transfer.<br>**Different International agreements:**<br>**(a) World Trade Organization (WTO):**<br>(i) General Agreement on Tariffs and Trade (GATT), Trade Related Intellectual Property Rights (TRIPS) agreement<br>(ii) General Agreement on Trade Related Services (GATS) Madrid Protocol.<br>(iii) Berne Convention<br>(iv) Budapest Treaty<br>**(b) Paris Convention**<br>**WIPO** and **TRIPS, IPR** and Plant Breeders Rights, IPR and Biodiversity. | 1 |

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| **Unit III:**<br>**Introduction to Chem informatics:**<br>History and evolution of cheminformatics, Use of Cheminformatics, Prospects of cheminformatics, Molecular modeling and structure elucidation.<br><br>**Representation of molecules and chemical reactions:**<br>Nomenclature, Different types of notations, SMILES coding, Matrix representations, Structure of Molfiles and Sdfiles, Libraries and toolkits, Different electronic effects, Reaction classification.<br><br>**Searching Chemical Structures:**<br>Full structure search, sub-structure search, basic ideas, similarity search, three dimensional search methods, basics of computation of physical and chemical data and structure descriptors, data visualization. | 1 |
| **Unit IV:**<br>**Applications:**<br>Prediction of Properties of Compound, Linear Free Energy Relations, Quantitative Structure – Property Relations, Descriptor Analysis, Model Building, Modeling Toxicity, Structure – Spectra correlations, Prediction NMR, IR and Mass spectra, Computer Assisted Structure elucidations, Computer assisted Synthesis Design, Introduction to drug design, Target Identification and Validation, Lead Finding and Optimization, analysis of HTS data, Virtual Screening, Design of Combinatorial Libraries, Ligand based and Structure based Drug design, Application of Chem informatics in Drug Design. | 1 |

| M.Sc | **Paper – IV**<br>**Intellectual Property Rights & Cheminformatics** |
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| **RJSPGCHEA404 Intellectual Property Rights & Cheminformatics** | Course outcomes:<br>1. To create awareness and understanding the terms like intellectual property, patents, copyright, industrial designs, trademarks, geographical indications etc.<br>2. To know trade secrets, IP infringement issues, economic value of intellectual property and study of various related international agreements.<br>3. To explore cheminformatics to facilitate molecular modeling and structure elucidations.<br>4. To apply the knowledge gained about various chemistry principles, techniques and tools in drug designing, target identification and validation, lead finding and optimization.<br><br>*Learning Outcomes:*<br>*After completing this course student will be able to:*<br>1. Apply for Patents, their related norms.<br>2. Obtain industrial design and trademarks.<br>3. Aware themselves about copyright rules.<br>4. Learn rules for registration, prevention of illegal exploitation, importance to India<br>5. understand Trade Secrets.<br>6. learn economic value of IPR.<br>7. learn history, evolution of nomenclature, different types of Notations.<br>8. Search chemical structure and data related to physical data of compounds.<br>9. Understand the application of cheminformatics in detail |

**REFERENCES:**

1. Andrew R. Leach & Valerie J. Gillet (2007) *An Introduction to Cheminformatics.* Springer: The Netherlands.
2. Gasteiger, J. & Engel, T. (2003) *Cheminformatics: A textbook*. Wiley–VCH
3. Gupta, S. P. *QSAR and Molecular Modeling.* Springer-Anamaya Pub.: New Delhi.

| Course Code | Title | Credits |
|---|---|---|
| **RJSPGCHEA404** | **Paper – IV**<br>**Research Methodology** | 4 |
| **Unit I:**<br>**Print:**<br>Primary, Secondary and Tertiary sources.<br>**Journals:**<br>Journal abbreviations, abstracts, current titles, reviews, monographs, dictionaries, text-books, current contents, Introduction to Chemical Abstracts and Beilstein, Subject Index, Substance Index, Author Index,<br>Formula Index, and other Indices with examples.<br>**Digital:**<br>Web sources, E-journals, Journal access, TOC alerts, Hot articles, Citation Index, Impact factor, H-index, E-consortium, UGC infonet, E-books, Internet discussion groups and communities, Blogs, preprint servers, Search engines, Scirus, Google Scholar, ChemIndustry, Wiki-databases, ChemSpider, Science Direct, SciFinder, Scopus.<br>**Information Technology and Library Resources:**<br>The Internet and World wide web, Internet resources for Chemistry, finding and citing published information. | | 1 |
| **Unit II:**<br>**DATA ANALYSIS**<br>**The Investigative Approach:**<br>Making and recording Measurements, SI units and their use, Scientific methods and design of experiments.<br>**Analysis and Presentation of Data:**<br>Descriptive statistics, choosing and using statistical tests, Chemometrics, Analysis of Variance (ANOVA), Correlation and regression, curve fitting, fitting of linear equations, simple linear cases, weighted linear case, analysis of residuals, general polynomial fitting, linearizing transformations, exponential function fit, r and its abuse, basic aspects of multiple linear regression analysis. | | 1 |
| **Unit III:**<br>**METHODS OF SCIENTIFIC RESEARCH AND WRITING SCIENTIFIC PAPERS**<br>Reporting practical and project work, Writing literature surveys and reviews, organizing a poster display, giving an oral presentation.<br>**Writing Scientific Papers:** | | 1 |

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|---|---|
| Justification for scientific contributions, bibliography, description of methods, conclusions, the need for illustration, style, publications of scientific work, writing ethics, avoiding plagiarism. | |
| **Unit IV:**<br>**CHEMICAL SAFETY & ETHICAL HANDLING OF CHEMICALS**<br>Safe working procedure and protective environment, protective apparel, emergency procedure, first aid, laboratory ventilation, safe storage and use of hazardous chemicals, procedure for working with substances that pose hazards, flammable or explosive hazards, procedures for working with gases at pressures above or below atmospheric pressur, safe storage and disposal of waste chemicals, recovery, recycling and reuse of laboratory chemicals, procedure for laboratory disposal of explosives, identification, verification and egregation of laboratory waste, disposal of chemicals in the sanitary sewer system, incineration and ransportation of hazardous chemicals. | 1 |

| M.Sc | **Paper – IV**<br>**Research Methodology** |
|---|---|
| **RJSPGCHEO404 Research Methodology** | Course outcomes:<br><br>*Learning Outcomes:* |

**REFERENCES:**

1. Dean, J. R., Jones, A. M., Holmes, D., Reed, R., Weyers, J., & Jones, A., (2011), *Practical skills in Chemistry,* 2nd Ed., Prentice Hall, Harlow.
2. Hibbert, D. B. & Gooding, J. J. (2006) *Data Analysis for Chemistry* Oxford University Press.
3. Topping, J., (1984) *Errors of Observation and their Treatment* 4th Ed., Chapman Hill, London.
4. Harris, D. C. (2007) *Quantative Chemical Analysis* 6th Ed., Freeman Chapters 3-5
5. Levie, R. De. (2001) *How to use Excel in Analytical Chemistryand in general scientific data analysis* Cambridge Universty Press.
6. Chemical Safety matters – IUPAC-IPCS, (1992) Cambridge University Press.
7. OSU Safety manual 1.01

| Course Code | Practical Title | Credits |
|---|---|---|
| RJSPGCHEPRA401 | **Quality In Analytical Chemistry Practical** | 2 |

**Group – A**:

1. Determination of pK value of $H_3PO_4$ potentimetrically
2. Estimation of Na+ in dairy whitener by flame photometry
3. Spectrophotometric determination of pH of buffer solution.
4. Simultaneous determination of $Ti^{3+}$ and $V^{5+}$ spectrophotometrically by $H_2O_2$ method
5. To analyze Bronze for Zn by complexometric method

| M.Sc | Physical Chemistry , Paper 1 Practical |
|---|---|
| **RJSPGCHEPRA401**<br>Practical I<br>**Quality In Analytical Chemistry Practical** | Course Outcomes:<br>1. To impart the knowledge of various ways of analyzing various commercial samples, and chemicals etc.<br><br>*Learning Outcomes:*<br>1. On successful completion of this course students will be able to understand the basic concept of to Have experience of handling various instruments and preparation of samples for it. |

| Course Code | Practical Title | Credits |
|---|---|---|
| RJSPGCHEPRA402 | **Advance Instrumental Techniques Practical** | 2 |

**Group – B:**

1. Analysis of drugs by non aqueous titration: Glycine , Sodium Benzoate
2. Analysis of detergents: Active detergent matter, alkalinity and Oxygen releasing capacity
3. Determination of the purity of crystal violet
4. Estimation of Ca in Ca-pentathonate/calcium lactate tablets
5. Canned food: Limits test for tin/zinc

| M.Sc | Analytical Chemistry , Paper II Practical |
|---|---|
| **RJSPGCHEPRA402**<br>Practical II<br><br>**Advance Instrumental Techniques Practical** | Course Outcomes:<br><br>*Learning Outcomes:* |

| Course Code | Practical Title | Credits |
|---|---|---|
| RJSPGCHEPRA403<br>**Selected Topics in Analytical Chemistry Practical** | **Selected Topics in Analytical Chemistry Practical** | 2 |
| 1. Analysis of Calcium, Iron and phosphorous in milk.<br>2. Determination of SAP value of oil.<br>3. Estimation of Aldehyde in lemon grass oil / Cinnamon oil<br>4. Estimation of Glucose by Folin-Wu method<br>5. Analysis of water sample : $Mn^{2+}$ by colorimetric method | | |

| RJSPGCHEPRA404 | **IPR & Cheminformatics Practical** | 2 |
|---|---|---|
| **Group – D:** Project Evaluation | | |

| M.Sc | Analytica Chemistry , Paper IV Practical |
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|---|---|
| **RJSPGCHEOPR404**<br>Practical IV<br>**IPR & Cheminformatics Practical** | Course Outcomes:<br><br>*Learning Outcomes:* |