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 (Physical Chemistry)

Program Code: RJSPGCHEP

CBCS : 2019 -2020

M.Sc. (Physical Chemistry) Semester – III

Course	Nomenclature	Credits	Topics
RJSPGCHEP301	Paper I	4	1. Polymer Chemistry-I 2. Modern Applications of SurfaceChemistry. 3. Photo Chemistry-I 4. Applications of Fluorescence Phenomena.
RJSPGCHEP302	Paper II	4	1. Nanochemistryof gold, cadmium, selenide. 2. Nano chemistry of silica and polydimethylsiloxane. 3. Statistical Mechanics. Thermodynamic probability. Partition functions. 4. Nuclear Chemistry
RJSPGCHEP303	Paper III	4	1. Atomic structure. 2. Atomic spectroscopy 3. Molecular Structure. 4. Molecular spectroscopy. Rotational Spectroscopy. Raman Spectroscopy. Electronic Spectra of molecules
RJSPGCHEP304	Paper IV	4	1. Spectral Methods 2. Electro-analytical Methods – I Principles, instrumentation and applications. 3. Radio-Analytical Methods 4. Pulse Polarography
RJSPGCHEPPR301 RJSPGCHEPPR302 RJSPGCHEPPR303 RJSPGCHEPPR304	Paper I Paper II Paper III Paper IV	16	

M.Sc. (Physical Chemistry) Semester – IV

Course	Nomenclature	Credits	Topics
RJSPGCHEP401	Paper I	4	1. Polymer Chemistry II 2. Polymer Chemistry-III. 3. Bio-physicalChemistry and Green Chemistry. 4. Photochemistry-II: Kinetics and Applications Photophysical Kinetics of bimolecular processes. Solar Cells.
RJSPGCHEP402	Paper II	4	1. Metals and alloys. 2. Mechanical properties of solid materials. 3. Lasers and superconductors. 4. Non-equilibrium thermodynamics
RJSPGCHEP403	Paper III	4	1. Symmetry in Chemistry. 2. N.M.R.Spectroscopy-I. 3. ESR and Mossbauer Spectroscopy. 4. ^{13}C N.M.R.Spectroscopy
RJSPGCHEP404	Paper IV	4	1. Introduction to Intellectual Property. Patents, Industrial Designs, Copyrights, Trade Marks, Geographical Indications. 2. Trade Secrets IP Infringement issue and enforcement. Economic Value of Intellectual Property. Different International agreements. 3. Introduction to Chem informatics Representation of molecules and chemical reactions . Searching Chemical Structures. 4. Applications
RJSPGCHEPPR401 RJSPGCHEPPR402 RJSPGCHEPPR403 RJSPGCHEPPR404	Paper I Paper II Paper III Paper IV	16	

M.Sc. (Physical Chemistry) Semester – III Paper – I

(Polymer, Surface & Photo Chemistry)

Paper Code: RJSPGCHEP301

Learning objective

1. To evaluate molar mass of polymers by different methods like end group analysis, viscometry, vapour phase osmometry and molecular weight distribution curve.
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, fullerens and nanomaterials.
3. To learn the principles of photo physical processes in electronically excited molecules and mechanism of their relaxation by fluorescence and phosphorescence.
4. To understand application of photochemical reactions in organic systems (conjugated olefins and aromatic compounds).

UNIT- I: Polymer Chemistry-I **(15L)**

1.1 Introduction: Polymer Science, fundamental terms, historical outline, classification based on: the origin (natural, semi-synthetic, synthetic etc.),the structure (linear, branched, network, hyper branched, dendrimer, ladder, cross linked, IPN),the type of atom in the main chain(homo chain,hetero chain),the formation (condensation, addition), homopolymers,copolymers(random,alternate,block,graft),the behavior onapplication of heat (thermoplastic and thermosetting),the form and application (plastics, fibre, elastomersandresins). **(05L)**

1.2 Molar Mass: Molecular weight averages, fractionation, molecular weight determination by GPC/SEC,end group analysis, viscometry, vapour phase osmometry, gradientelution, andmolecularweightdistributioncurve**.** **(05L)**

1.3 Types of polymerization: condensation, addition (cationic and anionic)andcopolymerization(withkinetics),chaintransferreactions. **(05L)**

Reference Books:

1. P. Bahadur and N. V. Sastry, Principles of Polymer Science, second edition,NarosaPublishingHouse,2005.
2. C. E. Carraher, Jr., Carraher's Polymer Chemistry, 8th edition, CRC Press, New York,2010.
3. Joel R.Fried,Polymer Science andTechnology,Prentice-HallofIndiaPvt.Ltd., 2000.
4. V.R.Gowarikar,H.V.Viswanathan and J.Sreedhar,PolymerScience.NewAge InternationalPvt.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, Prentice hall of India Pvt.Ltd.2000
8. F.J.Davis,Polymer Chemistry,Oxford UniversityPress,2000.
9. D.Walton & P.lotimer,Polymer,Oxford UniversityPress,2000.
10. R.Ypung, Introduction to Polymers,Chapman & Hall,reprint,989. 11V.Jain.Organic Polymer Chemistry,I V Y Publishing House,2003.
11. A.Singh,Polymer Chemistry,Campus Book International,2003.

UNIT-II Modern Applications of SurfaceChemistry (15L)

2.1 Surface active agents and micelle:

2.1.1 Surface active agents and their classification, hydrophile lipophile balance **(02L)**

2.1.2 Micellization: shape and structure of micelles , hydrophobic interaction, critical

Micelles concentration (cmc), factors affecting cmc of surfactants, counter ion binding to micelles,micelle catalysis, reverse micelles. **(04L)**

2.1.3 Emulsions: Solubilization,micro emulsions, characterization of micro emulsions, **(02L)**

2.2 Hydrogenstorage by Adsorption:

2.2.1 Hydrogen storage: fundamentals physisorption , temperature and pressure influence,chemisorption,adsorptionenergy,'Electrochemical'adsorption. **(03L)**

2.2.2. Practical adsorption: storage of hydrogen with carbon materials, activated carbon,graphitegraphene,carbonnanostructures,fullerene.Carbonnanofibres(CNF) and graphite nano fibers electrochemical storage of hydrogen in carbon materials. **(04L)**

Reference Books:

1. M. J. Rosen. Surfactants and Interfacial Phenomena (3rd edn.), John Wiley (2004).
2. Y. Moroi, Micelles: Theoretical and Applied Aspects, (1992) Plenum Press,New York
3. ArunK.Chattopadhyay,KashmiriLalMittal,SurfactantsinSolution,Volume64of Surfactant Science Series,Volume 64 of Lecture Notes in Pure and Applied Mathematics,illustrated,MarcelDekker,1996
4. K.L.Mittal,AmericanChemicalSociety,Micellization,solubilization,and microemulsions,Volume1
5. Micellization,Solubilization,andMicroemulsions,AmericanChemicalSociety, illustrated,PlenumPress,1977
6. DeepakThassu,MichelDeleers,YashwantPathak,NanoparticleDrugDelivery SystemsVolume166ofDrugsandthePharmaceuticalSciencesSeriesillustrated*,CRC Press,2007*
7. Tushar K. Ghosh, Energy Resources and Systems: Volume 2: Renewable Resources,Volume2ofEnergyResourcesandSystems,EnergyResourcesand Systems,SpringerLink:Bücher,Springer,2011
8. R. Str¨obel a, J. Garche b, P.T. Moseley c, L. J¨orissen b, G. Wolfd. "Review Hydrogen storage by carbon materials." Journal of Power Sources (WWW.Sciencedirect.com) 159 (June 2006): 781–801.
9. AgataGodula-Jopek,WalterJehle,Joerg Wellnitz,Hydrogen *Storage* Technologies:NewMaterials,Transport,andInfrastructure,JohnWiley&Sons, 2012
10. YuryGogotsi,CarbonNanomaterials,illustratedVolume1ofAdvancedMaterials Series,AdvancedMaterialsandTechnologiesSeries,CRCPress,2006
11. Robert A. Varin,Tomasz Czujko,Zbigniew S. Wronski,Nanomaterials for SolidStateHydrogenStorageFuelCellsandHydrogenEnergyillustratedSpringer,2009

UNIT-III Photo Chemistry-I **(15L)**

3.1 Photochemical principles: Environmental effect on absorption and emission spectra, properties of excited states, excited state acidity constants, dipole moments and redox properties, Importance of photochemistry, origin of life, **(04L)**

3.2 Photo physical processes in electronically excited molecules: types of photo physical pathways, types of radiation less transitions, fluorescence emission, fluorescence and structure. Triplet state and phosphorescence emission, delayed fluorescence–etypeandp-type delayed fluorescence. **(06L)**

3.3 Photochemical reactions:ketones,olefins conjugated olefins and aromatic compounds, photosynthesis. **(05L)**

Reference Books :

1 C.H.DePuy,O.L.Chapman,Molecularreactionsandphotochemistry,Prenticehall Of India PVT. LTD.1988.

2 K.K.Rohatgi-Mukherjee. Fundamentals of Photochemistry. Reprint 2002. NewAge International Publisher,1978.

UNIT-IV Applications of Fluorescence Phenomena **(15L)**

4.1 Fluorescence sensing: Mechanism of sensing; sensing techniques based on Coalitional quenching, energy transfer,electron transfer; examples of pH sensors glucose sensors and protein sensors. **(05L)**

4.2 Novel fluorophores: Quantum dots, lanthanides and long-lifetime Metal- ligand complexes. **(05L)**

4.3 Radiative decay engineering:metal enhanced fluorescence **(03L)**

4.4 DNA technology–sequencing. **(02L)**

Reference Books :

1. B. Valeur, Molecular Fluorescence: Principles and Applications, Wiley-VCH (2001).

2. J.R.Lakowicz,Principles of Fluorescence Spectroscopy,Springer(2006). Reference Book.

3. D.L.Andrews & A.A.Demidov,Resonance Energy Transfer, John Wiley & Sons (1999).

M.Sc. (Physical Chemistry) Semester – III Paper – II

(Nanochemistry, statistical mechanics & Nuclear chemistry)

Paper Code: RJSPGCHEP302

Learning objective

1. To introduce the nanochemistry of gold, cadamium and selenide and to understand optical and magnetic properties of nano material and how it varies with the shape, size and surface of nano particles.
2. To aware the learners about the diagnosis and treatment of diseases using nano particles.
3. To learn the concept of distribution and thermodynamic probability and to evaluate most probable distribution state for all type of statics i.e. for Maxwell- Boltzmann, Fermi dirac and Bose –Einstein statistics.
4. To understand the concept of partition function, its physical significance and calculation of molar and atomic partition function
5. To determine the age of minerals, rocks, earth and solar system employing the nuclear chemistry and to discuss the application of radiochemistry in medical, industrial and agricultural field.

UNIT-I: Nanochemistryof gold, cadmium, selenide.

1.1 Variation of optical and magnetic properties of non material with size,shape,surface characteristics and impurities **(04L)**
1.2 Relationship between size and shape of nanomaterials **(03L)**
1.3 Nano architecture:self assembly and template methods **(03L)**
1.4 Diagnosis and treatment of diseases using nanoparticles **(03L)**
1.5 Safety and ethics of use of nanoparticles **(02L)**

UNIT-II Nano chemistry of silica and polydimethylsiloxane:

2.1 Variation of optical and magnetic properties of nanomaterials with size, shape, surface characteristics and impurities **(04L)**
2.2 Relationship between size and shape of nanomaterials. **(03L)**
2.3 Nano architecture:self assembly and template methods. **(04L)**
2.4 Diagnosis and treatment of diseases using nanoparticles **(04L)**

Reference Books:

1. Ludovico Cademartiri and Geoffrey A.Ozin,ConceptsofNanochemistry,Wiley–VCH Verlag Gmb H & co,2009
2. C.Bréchignac,P.Houdy,MarcelLahmani,NanomaterialsandNanochemistry, Springer,2007
3. C.N.R.Rao,Achim Müller,Anthony K.Cheetham,Nanomaterials Chemistry,John Wiley & Sons, 2007
4.Geoffrey A. Ozin,André C. Arsenault,Ludovico Cademartiri,Nanochemistry: AChemical Approach to Nanomaterials ,Royal Society of Chemistry (GreatBritain)2, illustrated, Royal Society of Chemistry,2009

Unit- III Statistical Mechanics

3.1 Thermodynamic probability: Combinatral problems, Stiriling apporoximation**,** Lagranges method, macro and microstates,ensembles,Boltzmann distribution law. **(03L)**

3.2 Partition functions:Translational,rotational,vibrational,electronic and nuclear partition functions, Expressions for thermodynamic functions in terms of partition function -Internal energy, heat capacity, the Helmholtz and Gibbs functions, Enthalpy, entropy and equilibrium constants. Sackur –Tetrode equation for the entropy of a mono atomic gas. Molecular partition function. **(07L)**

3.3 Maxwell-Boltzmann,Bose-Einstein and Fermi-Diracstatistics. **(03L)**

3.4 Debye and Einstein theory of specific heat of solids. **(02L)**

Reference Books:

1. AtkinsP.W,PhysicalChemistry,OxfordUniversityPress,6thedition,1998
2. John M.Seddon & Julian D.Gale,Thermodynamics and statistical mechanics, Tutorial Chemistry Text series,Vol.10,Royalsocietyof Chemistry,2001.
3. SilbeyRJ&AlbertyRA,Physical Chemistry,3rd edition,JohnWileyandsons, Inc.2002.
4. Laidler K.J. and Meiser J.H., Physical Chemistry, 2nd edition, CBS publishers & distributors,1999.
5. B.K.Agarwal and M.Eisner,Statistical Mechanics,(1988)Wiley Eastern,New Delhi.
6. D.A.McQuarrie,Statistical mechanics,(1976)Harper and Row Publishers, New York.

UNIT—IV Nuclear Chemistry

4.1Charged particle accelerator- linear accelerator, cyclotron, Betatron, Synchro-cyclotron,synchrotron **(04L)**

4.2 Nuclear forces-characteristics and Meson field theory of nuclear forces **(02L)**

4.3 Nuclear Models-Liquid drop model**,** Fermi Gas Model, Shell Model, Collective Model, Optical Model. **(04L)**

4.4 Applications of Nuclear radiations-geological applications of radioactivity, age of minerals and rocks, age of earth and solar system, medical, industrial and agricultural applications of radiochemistry, positron emission tomography,Radio immune assay. **(05L)**

Reference Books:

1. G.Fried lander,J.W.Kennedy.Nuclear andRadiochemistry.Third.JohnWiley and sons,,1981.
2. H.J.Arnikar,EssentialsofNuclearChemistry.second.Wiley Eastern Ltd., 1989.

M.Sc. (Physical Chemistry) Semester – III Paper – III

(Atomic and Molecular: Structure and Spectroscopy)

Paper Code: RJSPGCHEP303

Learning objective:

1. To discuss the variation and perturbation theory and its application to Helium atom. To introduce term symbol for multi electron atoms, exchange of interactions and multiplicity of states.
2. To evaluate hydrogen molecule using valence bond method.
3. To apply molecular spectroscopy on spherical top, symmetrical top and asymmetrical top molecules.

UNIT-I:Atomic structure

1.1 Introduction to approximate methods inQuantum Mechanics- **(09L)**

1.1.1 Variation Theorem, linear and non linear variation functions.

1.1.2 Perturbation Theory,Non degenerate Perturbation Theory, first order wave function correction, first order and second order energy correction.

1.1.3 Application of variation and perturbation theory to ground state of Helium Atom.

1.2 Multi –electron atoms:Antisymmetry and Pauli principle, Slater determinants, Hartree. –Fock and configuration interaction wave functions, Slater type orbitals, Gaussian orbitals, orbitals plots,Basis sets. Density functional theory. **(06L)**

UNIT-II Atomic spectroscopy

2.1 Angular momentum, orbital and spin,total angular momentum, total angular momentum(J) of many electron atoms, Russell Saunders(L-S) coupling and J-Jcoupling, **(04L)**

2.2 Term symbols,term symbols for multi electron atoms like He,Li,Be, B etc. **(04L)**

2.3 Exchange of interactions and multiplicity of states. **(02L)**

2.4 Anomalous Zeeman Effect and Paschen Back effect. **(02L)**

2.5 Atomic spectra and selection rules, energy level diagram of atomic sodium. **(03L)**

UNIT-III: Molecular Structure

3.1 The Born–Oppenheimer approximation **(01L)**

3.2 LCAO method-molecular orbital formation **(01L)**

3.3 Calculation of energy of hydrogen molecule ion using **(05L)**

3.3.1 Valence bond method

3.3.2 Heitler-London treatment

3.3.3 Improvements in Heitler-London treatment

3.4 Electronic structure of polyatomic molecules **(08L)**

3.4.1 Valence bond method for BeH_2,H_2O,NH_3,BH_3,CH_4

3.4.2 Huckel molecular orbital's Theory for–ethylene, Allyl system, cyclopropenyl system. And cyclobutadiene.

UNIT-IV: Molecular spectroscopy

4.1 Rotational Spectroscopy: Einstein coefficients, classification of polyatomic molecules spherical top, symmetric top and asymmetric top molecules, rotational spectra of polyatomic molecules Stark modulated microwave spectrometer. **(03L)**

4.2 Raman Spectroscopy-Classical theory of molecular polarizability, pure rotational, vibrational and vibration-rotation spectra of diatomic and polyatomic molecules polarization and depolarization of Raman lines correlation between IR and Raman spectroscopy instrumentation. **(05L)**

4.3 Electronic Spectra of molecules: Term symbols for line and molecules, selection rules characteristics of electronic transitions-Franck-C on don principle, types of electronic transitions-d-d, vibronic, charge transfer, π-π^*,n-π^* transitions, fate of electronically excited states, fluorescence, phosphorescence, dissociation and pre-dissociation **(07L)**

Reference Books:

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, NewAge InternationalPublishers,2001.
3. H.S.Randhawa, Modern Molecular Spectroscopy,McMillan IndiaLtd.,2003
4. G.Aruldas,Molecular Structure and Spectroscopy,Prentice-HallofIndia,2001.
5. J.Michael Hollas, Modern Spectroscopy,4thEd.,JohnWileyandSons,2004.
6. Laidler and Miser,PhysicalChemistry,2nd edition, CBS publishers, New Delhi.(chapters11-14)
7. SilbeyandAlberty,PhysicalChemistry,3rd edition, John Wiley and sons,2000.(Part two quantum chemistry)
8. Atkins P.W, Physical Chemistry, Oxford UniversityPress,6th edition,1998.
9. William Kemp,Organic spectroscopy,3rd Edition,ELBS,1996.
10. R. K. Prasad, Quantum Chemistry,3rd Ed., New AgeInternationalPublishers,2006.
11. James E. House, Fundamentals of Quantum Chemistry,Second Ed.,AcademicPress,2005.
12. T.A. Little field and N. Thorley , Atomic and Nuclear Physics- InIntroduction,VanNostrand,1979.

M.Sc. (Physical Chemistry) Semester – III Paper – IV
(Advanced Instrumental Techniques)
Paper Code: RJSPGCHEP304

UNIT-I Spectral Methods

Principle, instrumentation and applications of the following

1.1 Reflectance spectroscopy **(03L)**

1.2 Photo-acousticspectroscopy **(03L)**

1.3 Polarimetry :ORD,CD **(04L)**

1.4 Chemiluminescence method **(02L)**

1.5 Nuclear quadrapole resonance spectroscopy, ENDOR,ELDOR,EWDOR **(03L)**

UNIT-II Electro-analytical Methods – I

Principles, instrumentation and applications

2.1 Ion selective field effect transistors,bio-catalytic membrane electrodes, disposable multi Layer Ionsystems,screen–print ed electrodes. **(08L)**

2.2 Chronopotentiometry and chronoamperometry **(05L)**

2.3 Fused salt electrolysis **(02L)**

Reference Books:

1. A.J.Bardand L.R.Faulkner,Electrochemical Methods,2nd Ed, John Wiley and sons, Asia Pvt. Ltd, (2004).
2. J.J.Lingane,Electro-analyticalChemistry,2nd Ed, Inter science Publishers, Inc., New York (1958)
3. A.M.Bond,Modern Polarographic Methods in Analytical Chemistry, Marcel Dekker Publishers, Inc., NewYork,(1980)
4. A.J.Bard (Ed),Electro-analytical Chemistry,Marcel Dekkre Inc.,NewYork(A series of volumes).
5. Donald T.Sawyer,A.Sobkowiakand,J.L.Roberts,Jr.,Electrochemistry for Chemists,2nd Ed., John Wiley and Sons, Inc., NewYork.,(1995).
6. D.A.Skoog,F.J.Holler, J.A.Nieman,Principles of Instrumental analysis, 6th Ed.
7. R.D.Braun.introduction to Instrumental Analysis,MacGraw hill,1987.
8. H.A. Willard, L.L.Merritt, J.A.Dean & F.A.Settle, Instrumental methods of analysis, 5th Ed. CBS, 1986.
9. M.noel,K.J.Vasu, Cyclic Voltammetry and Frontiers of electrochemistry,IBH, NewDelhi,1990.
10. P.T.Kissinger,W.R.heinman, Laboratoty Techniques in electroanalytical Chemistry, Dekkar, NY. 1984.

UNIT-III Radio-Analytical Methods

3.1 Activation analysis-basic principles, fast neutron activation analysis, radio-chemical method inactivation analysis **(04L)**

3.2 Isotopic dilution method-principle and applications. **(02L)**

3.3 Auto, x-ray and gamma radiography **(04L)**

3.4 RadiometricTitrations **(03L)**

3.5 Applications of radio-analytical techniques. **(02L)**

References Books:

1. J.Ruticka and J.Stary, Substoichiometry in Radiochemical Analysis, Pergamon Press,(1968)
2. R.A.FairesandG.G.J.Boswell,RadioisotopeLaboratoryTechnique,4th Ed, Rutterworths; London, (1981)
3. D.Brune,B.Forkman,B.Person,Nuclear Analytical Chemistry, Chartwell- Bratt Ltd.,(1984)
4. Maheshwar Sharon and Madhuri Sharon,Nuclear Chemistry,Ane Books Pvt. Ltd.(2009)
5. Nuclear Chemistry By Arnikar

UNIT-IV Pulse Polarography:

4.1 Normal pulse polarography(NPP), Differential pulse polarography(DPP), Double differential pulse polarography(DDPP), **(08L)**

4.2 Sinusoidal AC polarography,Square wave polarography **(05L)**

4.3 Applications of electrochemical methods in Organic synthesis**.** **(02L)**

References Books:

1. M.NoelandKI.Vasu,CyclicVoltammetry and the frontiers of Electrochemistry, IBH, New Delhi,(1990)
2. A.M.Bond, Modern Polarographic Methods in Analytical Chemistry, Marcel Dekker Publishers,Inc.,NewYork,1980.
3. A. J. Bard and Faulkner, Electrochemical Methods, 2nd Ed, John Wiley and Sons (Asia) Pvt. Ltd., 2004.

M.Sc. (Physical Chemistry) Semester – III Practicals

Learning Objectives:

1. To understand the standard operating procedure of various instruments.
2. To learn complex formation by instrumental and non-instrumental methods.
3. To determine transport number by Hittorf's method.
4. To learn various physical parameters by instrumental and non- instrumental methods.

Paper I

Paper Code: RJSPGCHEPPR301

1. To determine of the formula of the copper (II) ammonia complex by partition method.
2. To determine the transport no. of copper (II)ions by Hittorf's method.
3. To determine the isoelectric point of gelatin by viscosity measurement.

Paper II

Paper Code: RJSPGCHEPPR302

1. To determine the mean ionic activity coefficient of zinc chloride by emf method.
2. To construct the phase diagram for a two component system forming a simple eutectic.

Non instrumental

1. To determine the equilibrium constant for the reaction

$$CaSO_4\ (s) + 2Ag^{+}\ (aq) = Ag_2SO_4(s) + Ca^{+2}\ (aq)$$

2. To determine the partial molar volume of ethanol.

Paper III

Paper Code: RJSPGCHEPPR303

1. Determination of the energy of activation and other thermodynamic parameters of activation for the acid catalyzed hydrolysis of methyl acetate.
2. To determine the proton ligand stability constant of an organic acid and metal ligand stability constant of its complex by pH measurement.

Conductometry

1. To determine the molar conductance of a weak electrolyte at infinite dilution hence to determine its dissociation constant.
2. To titrate potassium ferrocyanide with zinc sulphate and hence to determine the formula of the complex.

Potentiometry

1. To determine the E^0 of the quinhydrone electrode.
2. To determine the formula of the zinc(II)ferrocyanide complex by titration of Zn(II) sulphate with potassium ferrocyanide.

pH metry

1. To estimate the amount of hydrochloric acid and acetic acid in a mixture by titration with an alkali using a pH meter.
2. To determine hydrolysis constant and degree of hydrolysis of ammonium chloride and hence to estimate the dissociation constant of the base.

Paper IV

Paper Code: RJSPGCHEPPR304

1. To determine the molar mass of a nonvolatile solute by cryoscopic method.

Colorimetry & spectrophotometry

2. To determine the ionization constant of bromophenol blue
3. To study complex formation between nickel(II)with o-phenanthroline.
4. To determine the rate constant and the order of the reaction between persulphate and iodide ions.

M.Sc. (Physical Chemistry) Semester – IV Paper – I

(Polymer, Green, Biophysical and Applied)

Paper Code: RJSPGCHEP401

Learning objectives

1. To understand properties of polymers in solid state, characterization of polymers and chemical analysis by spectral methods and.
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, fullerens and nanomaterials.
3. To learn the principles of photo physical processes in electronically excited molecules and mechanism of their relaxation by fluorescence and phosphorescence.
4. To understand application of photochemical reactions in organic systems (conjugated olefins and aromatic compounds).

Unit I: Polymer Chemistry II **(15L)**

1.1 Polymers in solid state – Transitions (glass transition and crystalline melting temperature),crystalline behaviour,factors affecting crystallinity,polymer blends and Alloys.**(03L)**

1.2 Identification and characterization of polymers:Chemical analysis- End group analysis; Physicalanalysis by Spectral methods: IR, UV, Ramam, NMR, X-ray diffraction analysis, Microscopic methods: SEM, TEM, Thermal analysis-TGA,DTA, DSC. **(06L)**

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, **(04L)**

1.4 Polymer degradation and stabilization: Oxidative, thermal, radiation, Biodegradation **(02L)**

Unit II: Polymer Chemistry-III **(15L)**

2.1 Techniques of polymerization: Bulk polymerization, solution polymerization, suspension polymerization, emulsion polymerizations, **(03L)**

2.2 Thermodynamics of polymer solutions:Solubility parameter, thermodynamics of mixing**,** theta temperature **(02L)**

2.3 Polymer technology: **(05L)**

2.3.1 Polymer auxiliaries,plasticizers,heat Stabilizers,colorants,flame retardants. fillers,rein forcements,

2.3.2 Elastomers:Introduction,Processing,RubberTypes,Vulcanization,Properties, Reclaiming.

2.3.3 Fibers:introduction,production,Fiberspinning,Textilefibers,Industrialfibers, recycling.

2.3.4 Filmssheets:Introduction and processing techniques(injection and blow Moulding extrusion), Recycling of plastics.

2.4 Properties and applications of some commercially important polymers.Carbo chain 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, sulphurcontainingpolymers **(05L)**

Reference Books:

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, 8thedition, 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, 3rdedition, 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.

UNIT-III Bio-physicalChemistry and Green Chemistry **(15L)**

3.1 BiophysicalChemistry

3.1.1 Introduction to Complex Biomolecules: Proteins, enzymes, DNA, RNA, polysaccharidesand lipids. chirality and pH dependence of biomolecules. **(02L)**

3.1.2 Biosensors : Enzyme based, Electrochemical, immunosensor, fluorescence, optical, Piezoelectric Biosensors **(02L)**

3.1.3 Electrophoresis (Technique for bio-molecular study): Principle and factors affectingelectro-phoreticmobility,zoneelectrophoresis–Paperelectrophoresis,cellules acetate electrophoresis, Gel electrophoresis. capillary Electrophoresis, Application of electrophoresis. **(04L)**

3.2 Green Chemistry:

3.2.1 Recapitulation of principles of green chemistry, Waste minimization techniques. **(01L)**

3.2.2 Catalysis and Green Chemistry: Phase transfer catalysts, biocatalyst, photo catalysis. **(02L)**

3.2.3 Organic solvents, solvent free system, supercritical fluid, ionic liquid, their characteristics,use as catalyst and solvents. **(02L)**

3.2.4 Alternative energy sources for initiation and execution of chemical reaction: Microwave and sono chemistry. **(02L)**

Reference Books:

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.

UNIT-IV Photochemistry-II: Kinetics and Applications **(15L)**

4.1: Photophysical Kinetics of bimolecular processes. **(10L)**

4.1.1: Mechanism of fluorescence quenching.

4.1.2: Collisionsin solutions

4.1.3: Kinetics of collisional quenching and Stern-Volmer equation and deviations from Stern Volmer equation,

4.1.4: Concentration dependence of quenching and excimer formation

4.1.5: Quenching by added substances–charge transfer mechanism and energy transfer mechanism.

4.2: Solar Cells: photovoltaic and photo galvaniccells;photoelectron chemistry; prospects of solar energy conversion and storage, organic solar cells. **(05L)**

Reference Book:

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

M.Sc. (Physical Chemistry) Semester – IV Paper – II
(Material Science, network and irreversible thermodynamics)
Paper Code: RJSPGCHEP402

UNIT-I Metals and alloys: **(15L)**

1.1 Solidification of metals and alloys-homogeneous and heterogeneous nucleationGrowth of crystals, growth of silicon single crystal. **(04L)**

1.2 Metallic solid solutions-substitutional and interstitial solid solutions. **(03L)**

1.3 Crystalline imperfections-point, line and boundary defects **(04L)**

1.4 Atomic diffusions in solids-diffusion mechanisms, steady state and non-steady state diffusions,-impurity diffusion into silicon wafers for integrated circuits. **(04L)**

UNIT-II Mechanical properties of solid materials **(15L)**

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. **(05L)**

2.2 Hardness and hardness testing ,plastic deformations of metals in single crystals ,plastic deformation of polycrystalline metals ,solid solution strengthening of metals. **(05L)**

2.3 Fracture of metals-ductile and brittle fracture ,toughness and impact testing, fatigue of metals, the creep test ,creep-rupture test. **(05L)**

Reference Books :

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.

Unit III Lasers and superconductors **(15L)**

3.1 Lasers in chemistry **(10L)**

3.1.1 General principles of LASER action-Population Inversion, cavity and mode characteristics,Q-switching,Modelocking. **(02L)**

3.1.2 Practicallasers-Solidstatelasers-Ruby,neodymium,gas lasers-He-Ne,Ar,Kr, Carbon dioxide, Chemical and exciplexLasers,Dye lasers LED and Semiconductor Lasers**.** **(05L)**

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**.** **(03L)**

3.2 Superconducting solid materials **(05L)**

Band theory of electrical conductivity, Bardeen-Cooper-Schriffer Theory of super conductivity, the super conducting state,High critical temperature superconductors, magnetic properties of superconductors

Reference Book:

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

Unit IV Non-equilibrium thermodynamics **(15L)**

4.1.1 Features of non-equilibrium thermodynamics, second law of thermodynamics, uncompensated heat and its relation to thermodynamics function. **(02L)**

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. **(04L)**

4.1.3 Onsagers theory: Reciprocal relation, principle of microscopic reversibility. Coupled and uncoupled reactions and their condition. **(05L)**

4.1.4 Transport phenomena across membranes. Electro kinetic effect and thermo mechanical effects.**(04L)**

Reference Books:

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.

M.Sc. (Physical Chemistry) Semester – IV Paper – III
(Symmetry & Spectroscopy)
Paper Code: RJSPGCHEP403

UNIT-I: Symmetry in Chemistry **(15L)**

1.1 Recapitulation: point groups, character tables **(02L)**
1.2 Reduction formula, application of reduction formula to vibrational modes of water molecule**.** **(02L)**
1.3 Application in vibrational spectroscopy, selection rules for IR spectroscopy for molecules such as H_2O, CO_2,HF,H_2 **(03L)**
1.4 Application to Raman spectra,selection rules,comparison of IR and Raman selection rules, general approach to vibrational spectroscopy. **(02L)**
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. **(06L)**

Reference Books :

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.

UNIT-II N.M.R.Spectroscopy-I **(15L)**

2.1 A review of one dimensional NMR spectroscopy. **(01L)**
2.2 Spin-relaxation.Nuclear Over hauser Effect(NOE).polarization transfer. **(03L)**
2.3 Two-dimensional NMR.Correlated spectroscopy(COSY) **(03L)**
2.4 Nuclear Over hauser effect Spectroscopy(NOESY) **(02L)**
2.5 Heteronuclear correlation Spectroscopy(HETCOR) **(02L)**
2.6 Solid-state NMR **(02L)**
2.7 Magnetic Resonance Imaging(MRI) **(02L)**

UNIT-III ESR and Mossbauer Spectroscopy **(15L)**
3.1 Electron spin Resonance Spectroscopy- **(10L)**
3.1.1 Basic principle,hyper fine splitting(isotropic systems); **(02L)**

3.2.2 G-value and the factors affecting thereof; interactions affecting electron energies in paramagnetic complexes (Zero-field splitting and Kramer's degeneracy); **(03L)**

3.3.3 Anisotropic effects(the g-value and the hyper fine couplings);The EPR of triplet states; Structural applications to transition metal complexes. **(02L)**

3.4.3 Fundamentals and hyperfine splitting, application to study of free radicals spin densities McConnell relationship Zero field splitting. **(03L)**

3.2 Mossbauer Spectroscopy: **(05L)**

Principles, Recoilless emission and absorption of γ-rays,experimental methods, isomer shift, hyperfine structure (quadrupole interaction), magnetic hyper fine interaction,applications.

Reference Books:

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.

UNIT-IV ^{13}C N.M.R.Spectroscopy **(15L)**

4.1 Elementary ideas, instrumental difficulties, FT technique advantages and disadvantages. proton noised ecoupling technique advantages and disadvantages, off-resonance technique. **(05L)**

4.2 Chemical shifts of solvents, factors affecting chemical shifts, analogy with ^{1}H NMR. **(03L)**

4.3 Calculations of chemical shift of hydrocarbons, effect of substituent's on chemical shifts, different types of carbons(alkene,alkyne and allene). **(03L)**

4.4 Chemical shift of aromatic carbon sand effect of substituent. **(02L)**

4.5 Chemical shifts of carbonyl, nitrile and oxime carbons. **(02L)**

Reference Books:

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.

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

(INTELLECTUAL PROPERTY RIGHTS &CHEMINFORMATICS)

Paper Code: RJSPGCHEP404

Learning Objective:

1. To create awareness and understanding the terms like intellectual property, patents, copyright, industrial designs, trademarks, geographical indications etc.
2. To know trade secrets, IP infringement issues, economic value of intellectual property and study of various related international agreements.
3. To explore cheminformatics to facilitate molecular modeling and structure elucidations.
4. To apply the knowledge gained about various chemistry principals, techniques and tools in drug designing, target identification and validation, lead finding and optimization.

Unit I: **[15L]**

Introduction to Intellectual Property: **[2L]**

Historical Perspective, Different types of IP, Importance of protecting IP.

Patents: **[5L]**

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.

Industrial Designs: **[2L]**

Definition, How to obtain, features, International design registration.

Copyrights: **[2L]**

Introduction, How to obtain, Differences from Patents.

Trade Marks: **[2L]**

Introduction, How to obtain, Different types of marks – Collective marks, certification marks, service marks, trade names etc.

Geographical Indications: **[2L]**

Definition, rules for registration, prevention of illegal exploitation, importance to India.

Unit II: **[15L]**

Trade Secrets: **[2L]**

Introduction and Historical Perspectives, Scope of Protection, Risks involved and legal aspects of Trade Secret Protection.

IP Infringement issue and enforcement: **[2L]**

Role of Judiciary, Role of law enforcement agencies – Police, Customs etc.

Economic Value of Intellectual Property: **[5L]**

Intangible assests and their valuation, Intellectual Property in the Indian context – Various Laws in India Licensing and Technology transfer.

Different International agreements:

(a) World Trade Organization (WTO): **[5L]**

(i) General Agreement on Tariffs and Trade (GATT), Trade Related Intellectual Property Rights (TRIPS) agreement

(ii) General Agreement on Trade Related Services (GATS) Madrid Protocol.

(iii) Berne Convention

(iv) Budapest Treaty

(b) Paris Convention **[1L]**

WIPO and **TRIPS, IPR** and Plant Breeders Rights, IPR and Biodiversity.

Unit III: **[15L]**

Introduction to Chem informatics: **[5L]**

History and evolution of cheminformatics, Use of Cheminformatics, Prospects of cheminformatics, Molecular modeling and structure elucidation.

Representation of molecules and chemical reactions: **[5L]**

Nomenclature, Different types of notations, SMILES coding, Matrix representations, Structure of Molfiles and Sdfiles, Libraries and toolkits, Different electronic effects, Reaction classification.

Searching Chemical Structures: **[5L]**

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: **[15L]**

Applications:

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.

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.

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

Learning Objectives:

1. To learn complex formation by instrumental and non-instrumental methods.
2. To determine transport number by Hittorf's method.
3. To learn various physical parameters by instrumental and non- instrumental methods.
4. To learn interpretation of spectra and analysis of data.

Paper I

Paper Code: RJSPGCHEPPR401

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, $\Delta H$and ΔS of dissolution of a sparingly soluble salt by conductometry.

pHmetry

1. To determine K_1 and K_2 of a dibasic acid by titration with a base.

2. To determine dissociation constant of p-nitro phenol.

Paper II

Paper Code: RJSPGCHEPPR402

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

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

Paper III

Paper Code: RJSPGCHEPPR403

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 Mössbauer spectra.
6. Analysisof XRD pattern of cubic system
7. Interpretation of DTA, TG, and DTG curves

Paper IV

Paper Code: RJSPGCHEPPR404

Project Evaluation

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.

M.Sc. (Physical Chemistry) Semester – III & IV

Paper Pattern

Internal Exam

1. Class Test : 20 marks
2. Presentation : 20 marks

Paper Pattern for Semester End Examination

Maximum Mark: 60 Duration : 2Hrs

There will be 5 questions each of 12 marks.

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

The pattern for above questions is as follows:

- Each question will have five sub questions of 4 marks each.
- Learners have to attempt any 3 questions out of 5.

Q. 5 will have 8 sub questions of 3 marks each (2 questions will be from each unit).

Learners have to attempt any 4 questions out of 8.

Practical Exam

Practical exam will be of 50 marks.

- Experiment : 40 marks
- Journal : 5 marks
- Viva : 5 marks

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 : 2019 -2020

M.Sc. (Inorganic Chemistry) Semester – III

Course	Nomenclature	Credits	Topics
RJSPGCHEI301	Paper I	4	1. Descriptive Crystal Chemistry Simple structures Linked Polyhedra 2. Imperfection in crystals and Non- Stoichiometry. Point defects. Line defects. Surface Defects. 3. Methods of Preparations 4. Behaviour of Inorganic Solids Diffusion in Solids. Solid state reactions. Liquid Crystals.
RJSPGCHEI302	Paper II	4	1. Bioinorganic Chemistry 2. Reactivity of Chemical Species –I 3. Reactivity of Chemical Species –II Pourbaix Diagrams. 4. Structure, Bonding, and Stereochemistry ofCoordination Compounds
RJSPGCHEI303	Paper III	4	1. Diffraction Methods –I 2. Diffraction Methods –II Electron Diffraction Neutron Diffraction 3. Electron Spin Resonance Spectroscopy. 4. Mossbauer Spectroscopy
RJSPGCHEI304	Paper IV	4	1. Inorganic Materials Classification, manufacture and applications. Preparation, properties and uses of industrially important chemicals. 2. Nuclear Chemistry and Inorganic Pharmaceuticals. 3. Advances in Nanomaterials 4. Some Selected Topics i) Isopoly and Hetropoly acids, ii) Supramolecular chemistry iii) Inorganic pesticides, and iv) Intercalation compounds
RJSPGCHEIPR301 RJSPGCHEIPR302 RJSPGCHEIPR303 RJSPGCHEIPR304	Paper I Paper II Paper III Paper IV	16	

M.Sc. (Inorganic Chemistry) Semester – IV

Course	Nomenclature	Credits	Topics
RJSPGCHEI401	Paper I	4	1. Electrical Properties 2. Magnetic Properties 3. Thermal and Optical Properties. 4. Applications of group theory to –Electronic structures
RJSPGCHEI402	Paper II	4	1. Organometallic Chemistry 2. Applications of Organometallic Compounds 3. Inorganic cluster and cage compounds. 4. Inorganic ring and chain compounds
RJSPGCHEI403	Paper III	4	1. Spectroscopy Infrared spectroscopy. Raman spectroscopy. Applications of Group theory in Infrared and Raman spectroscopy. Nuclear Magnetic Resonance Spectroscopy. 2. Microscopy of Surface Chemistry-I 3. Microscopy of Surface Chemistry-II 4. Thermal Methods
RJSPGCHEI404	Paper IV	4	1. Introduction to Intellectual Property. Patents, Industrial Designs, Copyrights, Trade Marks, Geographical Indications. 2. Trade Secrets IP Infringement issue and enforcement. Economic Value of Intellectual Property. Different International agreements. 3. Introduction to Chem informatics Representation of molecules and chemical reactions . Searching Chemical Structures. 4. Applications
RJSPGCHEIPR401 RJSPGCHEIPR402 RJSPGCHEIPR403 RJSPGCHEIPR404	Paper I Paper II Paper III Paper IV	16	

M.Sc. (Inorganic Chemistry) Semester – III Paper – I

(Chemistry of Inorganic Solids)

Paper Code: RJSPGCHEI301

Learning Objective:

1. The topic helps the student gain knowledge about the structures of simple compoundsand linked polyhedral units.
2. To understand the imperfections and non-stoichiometry in crystal structures so as to design and develop various inorganic compounds with desired properties.
3. To study the different methods of synthesis of crystal structures, their reactions and properties.
4. To study the above crystal structures using x-ray diffraction and density measurements.
5. To discuss properties like Laws of diffusion, Kirkendal effect, polymorphism in liquid crystals, optical properties etc.

Unit I Descriptive Crystal Chemistry (15 Lectures)

(a) Simple structures

Structures of **AB** type compounds (PbO and CuO), **AB_2** type (β cristobalite, CaC_2 and Cs_2O), **A_2B_3** type (Cr_2O_3 and Bi_2O_3), AB_3 (ReO_3, Li_3N), **ABO_3** type, relation between ReO_3 and perovskite $BaTiO_3$ and its polymorphmic forms, Oxide bronzes, ilmenite structure, **AB_2O_4** type, normal, inverse, and random spinel structures.

(b) Linked Polyhedra

(i) Corner sharing: tetrahedral structure (Silicates) and octahedral structure (ReO_3) and rotation of ReO_3 resulting in VF_3, RhF_3 and calcite type structures.

(ii) Edge sharing: tetrahedral structures (SiS_2) and octahedral structures (BiI_3 and $AlCl_3$). pyrochlores, octahedral tunnel structures and lamellar structures

Unit II Imperfection in crystals and Non- Stoichiometry (15 Lectures)

(a) Point defects: Point defects in metals and ionic Crystal – Frenkel defect and Schottky defect. Thermodynamics formation of these defects (mathematical derivation to find defect concentration); Defects in non- Stoiochiometric compounds, colour centres.

(b) Line defects: Edge and Screw Dislocations. Mechanical Properties and Reactivity of Solids.

(c) Surface Defects: Grain Boundary and Stacking Fault. Dislocation and Grain Boundaries, Vacancies and Interstitial Space in Non-Stoichiometric Crystals, Defect Clusters, Interchangeable Atoms and Extended Atom Defects.

Unit III Methods of Preparations (15 Lectures)

(a) Methods of Synthesis: Chemical Method, High Pressure Method, Arc Technique and Skull Method (with examples).

(b) Different methods for single crystal growth:

(i) Crystal Growth from Melt–: Bridgman and Stockbargar, Czochralski and Vernuil methods.

(ii) Crystal growth from liquid solution: Flux growth and temperature gradient methods

(iii) Crystal growth from vapor phase: – Epitaxial growth methods.

(c) Thin film preparation: Physical and Chemical methods.

(d) Solid Solutions: Formation of Substitutional, Interstitial and Complex Solid Solutions; Mechanistic Approach; Study of Solid solutions by X-ray Powder Diffraction and Density Measurement. **IV**

Unit IV Behaviour of Inorganic Solids (15 Lectures)

(a) Diffusion in Solids: Fick's Laws of Diffusion; KirkendalEffect;Wagner mechanism,Diffusion and Ionic Conductivity; Applications of Diffusion in Carburizing and non-Carburizing Processes in Steel Making.

(b) Solid state reactions: General principles and factors influencing reactions of solids, Reactivity of solids.

(c) Liquid Crystals: Introduction and classification of thermotropic liquid crystals, Polymorphism in liquid crystal, Properties and applications of liquid crystals.

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

M.Sc. (Inorganic Chemistry) Semester – III Paper – II
(Bioinorganic and Coordination Chemistry)
Paper Code: RJSPGCHEI302

Learning Objective:

1. On completion of this topic, student will be able to understand the geometry and functions of various co-ordination metal complexes in the biological system.
2. To learn the different methods of determining the stability constant of co-ordination compounds that helps them to understand the reactive nature of the compounds.
3. To study the structure and bonding involved in the metal complexes.
4. To understand the photochemical properties and stereo chemistry of these complexes.
5. To make students familiarise with Latimer, Pourbaix and Frost diagram thereby helping them to understand various redox reactions taking place in aqueous, non-aqueous and solvent free media.

Unit I Bioinorganic Chemistry (15 Lectures)

(i)Coordination geometry of the metal ion and functions.

(ii)Zn in biological systems: Carbonic anhydrase,protolytic enzymes, e.g. carboxy peptidase,Zinc finger.

(iii)Role of metal ions in biological electron transfer processes: ironsulphur proteins,

(iv)Less common ions in biology e.g. Mn (arginase; structure andreactivity), Ni (urease ; structure and reactivity)

(v) Biomineralization

Unit II Reactivity of Chemical Species –I (15Lectures)

2.1 Recapitulation of the definition of Lewis acids and bases,Classification of Lewis acids and bases based on frontier Molecular orbitaltopology, Reactivity matrix of Lewis acids and bases.

2.2 Group Characteristic of Lewis acids (Gp-1,13-17).

2.3 Pauling rules to determine the strength of oxoacids; classification andStructural anomalies.

Unit III Reactivity of Chemical Species –II (15Lectures)

3.1 Pourbaix Diagrams.

3.2Amphoteric behavior, Periodic trends in amphoteric propertiesof p-block and d-block elements

3.3 Oxoanions and Oxocations.

3.4 Measures of hardness and Softness of Acids and Bases, Dragowaylandequations

3.5 Applications of acid-base Chemistry: Super acids and Superbases, heterogeneous acid-base reactions.

Unit IV Structure, Bonding, and Stereochemistry ofCoordination Compounds (15 Lectures)

(a) Structure and Bonding.

i) Molecular Orbital Theory for Complexeswith Coordination Number 4 and 5 for thecentral ion (sigma as well as Pi bonding)

(ii) Angular Overlap Model for octahedral and tetrahedral complexes forsigma and pi bond.

(b) Stereochemistry of CoordinationCompounds.

(i) Chirality and Fluxionality of CoordinationCompounds with Higher Coordination Numbers.

(ii) Geometries of Coordination compounds from Coordination number 6to 9.

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 InorganicReactions,Wiley, New York, 1967.
16. .J.D.Lee, Concise Inorganic Chemistry, 5th ed., BlackwellScienceLtd., 2005.
17. R.H. Crabtree, The Organometallic Chemistry of the TransitionMetals, 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, OrganometallicChemistry,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.
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M.Sc. (Inorganic Chemistry) Semester – III Paper – III

(Spectral Methods in Inorganic Chemistry)
Paper Code: RJSPGCHEI303

Learning Objective:

1. To explain structural techniques based on different physical phenomenon such as diffraction of X-rays, electron and neutron waves and resonance with monochromatic radiation and electron spin resonance (ESR) and Mossbauer spectroscopy.

Unit I Diffraction Methods –I **(15 Lectures)**

X-Ray Diffraction: Bragg Condition; MillerIndices; Laue Method; Bragg Method; DebyeScherrer Method of X-Ray Structural Analysis of Crystals.

Unit II Diffraction Methods –II **(15 Lectures)**

(**a) Electron Diffraction:** Scattering of electrons, Scattering Intensityversus Scattering Angle, Weirl Measurement Technique, Elucidation ofStructures of Simple gas Phase Molecules.

(b) Neutron Diffraction: Scattering of Neutrons: Scattering of neutronsby Solids and Liquids, Magnetic Scattering, Measurement Technique.

Unit III Electron Spin Resonance Spectroscopy **(15 Lectures)**

(a) Electron behaviour, interaction between electron spin and magneticfield.

(b) Instrumentation : Source, Sample cavity. Magnet and Modulation coils,Microwave Bridge, Sensitivity.

(c) Relaxation processes and Line width inESR transitions:

(i) ESR relaxation and chemical bonding.

(ii) Interaction between nuclear spin andelectron spin (hyperfine coupling)

(iii) Spin polarization for atoms and transitionmetal ions,

(iv) Spin-orbit coupling and significance of gtensors,

(v) Application to transition metal complexes

(having one unpaired electron)

Unit IV Mossbauer Spectroscopy **(15 Lectures)**

Mössbauer Spectroscopy:

4.1 Basic principle, recoil energy and Doppler shift.

4.2 Instrumentation: sources and absorber; motion devices, detection,reference substances and calibration,

4.3 Isomer shift, quadrupole interaction, magnetic interaction,electronegativity and chemical shift.

4.4 Applications: *Iron compounds*- low spin and high spin Fe(II) andFe(III) compounds and complexes, effect of pi-bonding, mono and polynuclear Iron complexes, spinel oxides and iron-sulphur proteins; *Tincompounds*- tin halides and tin oxides, organotin compounds; *Iodinecompounds*- I2 and alkali metal iodide compounds.

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M.Sc. (Inorganic Chemistry) Semester – III Paper – IV

(Applied Chemistry)

Paper Code: RJSPGCHEI304

Learning Objective:

1. To learn about inorganic fibers and inorganic fillers, their classification based on shape, size, properties economic importance and applications.
2. To understand the coordinate polymers as (MOF) metal-organic frame works, their ordered structures, synthesis and application as building blocks.
3. Preparation, properties and uses of some widely used compounds.
4. Application of radiopharmaceuticals containing Tc and Bi.
5. Application of some compounds as gastrointestinal agents and as topical agents.
6. To know the growing importance of nanomaterials.
7. Concept of supramolecules, types of forces present in supramolecules, classification and applications of supramolecules.
8. To caution the students about adverse effects of pesticide on environment.

Unit I Inorganic Materials **(15 Lectures)**

(a) Classification, manufacture and applications :

(i) Inorganic fibers, and

(ii) Inorganic fillers.

Study of

(i) Condensed phosphates, and

(ii)Coordination polymers.

(b) Preparation, properties and uses of industrially important chemicals – potassium permanganate, sodium thiosulphate, bleaching powder, hydrogen peroxide, potassiumdichromate

Unit II Nuclear Chemistry and Inorganic Pharmaceuticals **(15 Lectures)**

(a) Nuclear Chemistry :

Introduction to of nuclear fuels and separation of fission products from spent fuel rods by PUREX process. Super heavy element, discovery,preparation, position in the periodic table.

(b) Inorganic Pharmaceuticals :

Radiopharmaceuticals containing Tc and Bi, contrast agents for X-ray and NMR imaging. Gasrtrointestinal agents viz. (i) antacids(aluminium hydroxide, milk of magnesia, sodium bicarbonate and (ii)Cathratics(magnesium sulphate and sodium phosphate).Topical agents viz.(i) protectives and adsorbents (talc,calamine), (ii)antimicrobial agents(potassium permanganate, tincture iodine, boric acid)and astringents(potash alum) .

Unit III Advances in Nanomaterials: (15 Lectures)

(a) Types of nanomaterials, e.g. nanotubes,nanorods, solid spheres, core-shell Inanoparticles, mesoporous materials; isolation of nano materials

(b) Some important properties of nanomaterials: optical properties of metal and semiconductor nanoparticles, magnetic properties.

(c) Some special nanomaterials: Carbon nanotubes: Types, synthesis using various methods, growth mechanism, electronic structure; Porous silicon: Preparation and mechanism of porous silicon formation, Factors affecting porous structure, properties of porous silicon; Aerogels: Types of aerogels, Properties and applications of aerogels.

(d) Applications of nanomaterials in

electronics, energy, automobiles, sports and toys, textile, cosmetics, medicine, space and defense. Environmental effects of nanotechnology

Unit IV Some Selected Topics (15 Lectures)

i) Isopoly and Hetropoly acids,

ii) Supramolecular chemistry

iii) Inorganic pesticides, and

iv) Intercalation compounds

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1. G.M.Masters, Introduction to Environmental Engineering and Science, Prentice-Hall of India Pvt. Ltd. New Delhi, 1995.

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M.Sc. (Inorganic Chemistry) Semester – III Practicals

Learning Objective:

1. To dissolve the given alloy by suitable acid treatment followed by estimating the metal content present in it quantitatively by gravimetric or volumetric method.
2. To make students understand the process of solvent extraction by making them separate the metals from their mixtures by using a suitable solvent and to estimate the separated metal quantitatively.
3. To study preparation of some co-ordination complexes.
4. To analyze metal contents in some commercial samples.

Paper I
Paper Code: RJSPGCHEIPR301

Analysis of alloys/ores

1. Analysis of Brass alloy:
   (i) Cu content by iodometric method.
   (ii) Zn content by complexometric method.
2. Analysis of Bronze alloy:
   (i) Cu content by complexometric method,
   (ii) Sn content by gravimetric method.
3. Analysis of galena ore:
   (i) Pb content as $PbCrO_4$ by gravimetric method using 5% potassium chromate.
   (ii) Fe content by colorimetrically using 1,10- phenonthroline.
4. Analysis of Zinc blend ore:
   (i) Zn content by complexometric method.
   (ii) Fe content by colorimetric method(Azide method).

Paper II
Paper Code: RJSPGCHEIPR302

Solvent Extraction

1. Separation of Co and Ni using n-butyl alcohol and estimation of Co.
2. Separation of U and Fe using 8-hydroxyquinoline in chloroform and estimation of U.
3. Separation of Fe and Mo using isoamyl alcohol and estimation of Mo.
4. Separation of Cu and Fe using n-butyl acetate and estimation of Cu.

Paper III
Paper Code: RJSPGCHEIPR303

Inorganic Preparations

1. Preparation of $Co(\alpha\text{-nitroso-}\beta\text{-naphthol})_3$
2. Preparation of $Ni(salicylaldoxime)_2$
3. Hexaamine cobalt (III) chloride
4. Preparation of Trans-bis (glycinato)Cu(II)

Paper IV
Paper Code: RJSPGCHEIPR304

Analysis of the following samples

1. Calcium tablet for its calcium content by complexometric titration.
2. Bleaching powder for its available chlorine content by iodometric method.
3. Iron tablet for its iron content colorimetrically by using 1,10-phenonthroline.
4. Nycil powder for its Zn content complexometrically.

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).

M.Sc. (Inorganic Chemistry) Semester – IV Paper – I

(Properties of Inorganic Solids and Group Theory)

Paper Code: RJSPGCHEI401

Learning Objective:

1. The topic provides a vivid description of the properties of inorganic materials which includes electrical, thermal and magnetic properties.
2. To extend the above study to a wide range of inorganic materials such as alloys, metals, metal oxides, spinels, ilmenites, Perovskites and Magneto Plumbites.
3. To apply molecular orbital theory to understand the structure of cage and cluster compounds and metal sandwich compounds.
4. To apply group theory to study the symmetry of molecular vibrations which help students to understand the vibrational transitions and to interpret IR and Raman spectra.

Unit I Electrical Properties- **(15 Lectures)**

(**a) Electrical properties of solids:**

(i) Conductivity: Solid Electrolytes; Fast IonConductors; Mechanism of Conductivity;Hopping Conduction.

(b) Other Electrical Properties: Thomson andSeebeck Effects; Thermocouples and theirApplications; Hall Effect; Dielectric, Ferroelectric, Piezoelectric andPyrroelectricMaterials and their Inter-relationships andApplications

Unit II Magnetic Properties. **(15 Lectures)**

(a) Behaviour of substances in magnetic field, mechanism offerromagnetic and antiferromagnetic ordering , superexchange,Hysteresis, Hard and soft magnets, structures and magnetic PropertiesofMetals and Alloys; Transition metal Oxides; Spinels; garnets, Ilmenites;Perovskite and Magneto plumbites, Application in transformer cores,information storage, magnetic bubble memory devices and aspermanent magnets.

Unit III Thermal and Optical Properties **(15 Lectures)**

a) Thermal Properties: Introduction, HeatCapacitiy and its Temperature Dependance;Thermal Expansion of Metals; Ceramics and Polymers and Thermal Stresses.

(b) Optical properties: Color Centres andBirefringence; Luminescent and PhosphorMaterials; Coordinate Model; PhosphorModel; Anti Stokes Phosphor; Ruby Laser;Neodymium Laser

Unit IV Applications of group theory to –Electronic structures (15Lectures)

(a) Recapitulation of Points groups and Character tables.

(b) Transformation Properties of Atomic Orbitals;

(c) Sigma and pi- molecular orbitals for AB4 (tetrahedral) and AB6(octahedral) molecules;

(d) **Ligand Field Theory :** Electronic structures of free atoms and ions;Splitting of levels and terms in a chemical environment; Construction ofenergy level diagrams; Direct product ; Correlation diagrams for d2 ions inoctahedral and tetrahedral ligand field; Methods of Ascending andDescending Symmetry; Hole formalism.

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

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

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M.Sc. (Inorganic Chemistry) Semester – IV Paper – II

(Organometallics and main group Chemistry)

Paper Code: RJSPGCHEI402

Learning Objective:

1. The purpose of learning this topic is to provideknowledge about the fundamental principles involved in bonding inOrgano-metallic compounds of f-block elements.
2. To provide students with some basic ideas on synthesis and applications of organo palladium and platinum compounds.
3. To make students familiar about the structure and bonding involved in inorganic cage, cluster, ring and chain compounds.
4. To study the use of organo metallic compounds as catalyst in several organic homogenous and heterogeneous reactions.

Unit I Organometallic Chemistry **(15 Lectures)**

(a) Metal-Metal Bonding and Metal Clusters,

(b) Electron Count and Structures of Clusters,,

(c) Isolobal Analogy.

(d)Organo Palladium and Organo Platinum Complexes (preparations,properties and applications.)

Unit II Applications of Organometallic Compounds **(15 Lectures)**

(a) Catalysis-Homogenous and HeterogenousCatalysis: Comparison, Fundamental ReactionSteps.

(b) Organometallics as Catalysts in OrganicReactions:

(i)Hydrosilation, (ii)Hydroborationn.(iii) Water gas Shifts Reaction (iv) Wacker process(Oxidation of alkenes)

(v)Alcohol corbonylation

(c)Coupling reactions :(i) Heck's reaction (ii) Suzuki reaction

Unit III Inorganic cluster and cage compounds **(15 Lectures)**

(i) Introduction, (ii) Bonding in boranes, (iii)Heteroboranes, (iv) Carboranes, (v) clustercompounds, (vi) electron precise compoundsand their relation to clusters.

Unit IV Inorganic ring and chain compounds **(15 Lectures)**

(a) Silicates, polysilicates and aluminosilicates,

(b) Phosphazenes, phosphazene polymers

(c) Polyanionic and polycationic compounds

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1. Gary Wulfsberg, Inorganic Chemistry ; Viva Books PA Ltd., NewDelhi; 2002.
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M.Sc. (Inorganic Chemistry) Semester – IV Paper – III

(Instrumental methods in Inorganic Chemistry)

Paper Code: RJSPGCHEI403

Learning Objective:

1. Learn to interpretation of IR and Raman spectra of inorganic molecules.
2. Understanding the need and challenges in characterization of surfaces.
3. To learn instrumentation of various electron microscopic techniques.
4. Ability to choose the appropriate thermal technique based on the type of analyte and the desired qualitative and quantitative analytical information.

Unit I Spectroscopy (15 Lectures)

(a) Infrared spectroscopy: Fundamental modes of vibrations, selectionrules, IR absorption bands of metal - donor atom, effect of complexationon the IR spectrum of ligands formations on the IR of ligands like NH_3,CN-, CO, olefins (C=C) and $C_2O_4^{2-}$.

(b) Raman spectroscopy: Raman spectroscopy for diatomicmolecules.Determination of molecular structures like diatomic andtriatomic molecules.

(c) Applications of Group theory in Infrared and Raman spectroscopy.
Molecular Vibrations: Introduction; The Symmetry of NormalVibrations; 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.

(d) Nuclear Magnetic Resonance Spectroscopy :
Introduction to basic principles and instrumentation. Use of 1H, 19F, 31P, 11B NMRspectra in structural elucidation of inorganic compounds; Spectra of paramagneticmaterials: Contact shift, application of contact shift, lanthanide shift reagent.

Unit II Microscopy of Surface Chemistry-I (15 Lectures)
Introduction to surface spectroscopy, Microscopy, problems of surfaceanalysis, distinction of surface species, sputter etching and depth profileand chemical imaging,instrumentations, Ion Scattering Spectra (ISS),Secondary Ion Mass Spectroscopy (SIMS),Auger Emission Spectroscopy(AES),

Unit III Microscopy of Surface Chemistry-II (15 Lectures)
ESCA, Scanning Electron Microscopy (SEM),Atomic force microscopy(AFM) andtransmission electron microscopy (TEM):Instrumentation and applications.

Unit IV Thermal Methods (15 Lectures)

4.1 Application of TGA in Thermal characterization of polymers, quantitative analysis of mixture of oxalates, moisture content in coal, studyof oxidation state of alloys etc.

4.2 Application of DSC and DTA in determination of thermodynamicparameters such as heat capacity and standard enthalpy of formation of thecompounds, investigation of phase transitions, thermal stability ofpolymeric materials, purity of pharmaceuticals samples, M.P. and B.P. oforganic compounds etc.
4.3 Basic principle, instrumentation and applications to other thermalmethods like Thermomechanical analysis (TMA) and evolved gas analysis(EGA).

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

(INTELLECTUAL PROPERTY RIGHTS &CHEMINFORMATICS)

Paper Code: RJSPGCHEI404

Learning Objective:

1. To create awareness and understanding the terms like intellectual property, patents, copyright, industrial designs, trademarks, geographical indications etc.
2. To know trade secrets, IP infringement issues, economic value of intellectual property and study of various related international agreements.
3. To explore cheminformatics to facilitate molecular modeling and structure elucidations.
4. To apply the knowledge gained about various chemistry principals, techniques and tools in drug designing, target identification and validation, lead finding and optimization.

Unit I: **[15L]**

Introduction to Intellectual Property: **[2L]**

Historical Perspective, Different types of IP, Importance of protecting IP.

Patents: **[5L]**

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.

Industrial Designs: **[2L]**

Definition, How to obtain, features, International design registration.

Copyrights: **[2L]**

Introduction, How to obtain, Differences from Patents.

Trade Marks: **[2L]**

Introduction, How to obtain, Different types of marks – Collective marks, certification marks, service marks, trade names etc.

Geographical Indications: **[2L]**

Definition, rules for registration, prevention of illegal exploitation, importance to India.

Unit II: **[15L]**

Trade Secrets: **[2L]**

Introduction and Historical Perspectives, Scope of Protection, Risks involved and legal aspects of Trade Secret Protection.

IP Infringement issue and enforcement: **[2L]**

Role of Judiciary, Role of law enforcement agencies – Police, Customs etc.

Economic Value of Intellectual Property: **[5L]**

Intangible assests and their valuation, Intellectual Property in the Indian context – Various Laws in India Licensing and Technology transfer.

Different International agreements:

(a) World Trade Organization (WTO): [5L]

(i) General Agreement on Tariffs and Trade (GATT), Trade Related Intellectual Property Rights (TRIPS) agreement

(ii) General Agreement on Trade Related Services (GATS) Madrid Protocol.

(iii) Berne Convention

(iv) Budapest Treaty

(b) Paris Convention [1L]

WIPO and **TRIPS, IPR** and Plant Breeders Rights, IPR and Biodiversity.

Unit III: [15L]

Introduction to Chem informatics: [5L]

History and evolution of cheminformatics, Use of Cheminformatics, Prospects of cheminformatics, Molecular modeling and structure elucidation.

Representation of molecules and chemical reactions: [5L]

Nomenclature, Different types of notations, SMILES coding, Matrix representations, Structure of Molfiles and Sdfiles, Libraries and toolkits, Different electronic effects, Reaction classification.

Searching Chemical Structures: [5L]

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: [15L]

Applications:

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.

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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.

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

Learning Objective:

1. To make students learn the technique of opening the ore using suitable acid followed by estimating the metal quantitatively by gravimetric or volumetric or colorimetric technique.
2. To understand the method for determining the stability constant of zinc and silver complexes using potentiometer.
3. To calculate the CFSE of titanium and chromium complexes and Racah parameter of nickel complexes from spectral data using spectrophotometer.
4. To analyze the alkali metal content in electral powder and fertilizer sample, salinity of sea water and chloride content in fasting salt.
5. To understand the interpretation of structure of complexes using spectral Techniques.

Paper I

Paper Code: RJSPGCHEIPR401

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.

Paper II

Paper Code: RJSPGCHEIPR402

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

Paper III

Paper Code: RJSPGCHEIPR403

Spectral Interpretation

Paper IV

Paper Code: RJSPGCHEIPR404

Project Evaluation

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).

M.Sc. (Inorganic Chemistry) Semester – III & IV

Paper Pattern

Internal Exam

1. Class Test : 20 marks
2. Presentation : 20 marks

Paper Pattern for Semester End Examination

Maximum Mark: 60 Duration : 2Hrs

There will be 5 questions each of 12 marks.

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

The pattern for above questions is as follows:

- Each question will have five sub questions of 4 marks each.
- Learners have to attempt any 3 questions out of 5.

Q. 5 will have 8 sub questions of 3 marks each (2 questions will be from each unit).

Learners have to attempt any 4 questions out of 8.

Practical Exam

Practical exam will be of 50 marks.

- Experiment : 40 marks
- Journal : 5 marks
- Viva : 5 marks

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 (Organic Chemistry)

Program Code: RJSPGCHEO

CBCS : 2019 -2020

M.Sc. (Organic Chemistry) Semester – III

Course	Nomenclature	Credits	Topics
RJSPGCHEO301	Paper I	4	1. Organic reaction mechanisms 2. Pericyclic reactions 3. Stereochemistry-I 4. Photochemistry
RJSPGCHEO302	Paper II	4	1. Name reactions with mechanism and application. 2. Radicals in organic synthesis 3. Enamines, Ylides and α-C-H functionalization. 4. Metals / Non-metals in organic synthesis
RJSPGCHEO303	Paper III	4	1. Natural products-I Carbohydrates Natural pigments Insect pheromones Alkaloids 2. Natural products-II Multi-step synthesis of natural products. Prostaglandins. Lipids. Insect growth regulators. Plant growth regulators. 3. Advanced spectroscopic techniques-I Proton NMR spectroscopy 13C –NMR spectroscopy 4. Advanced spectroscopic techniques-II
RJSPGCHEO304	Paper IV	4	1. Drug discovery, design and development. 2. Drug design, development and synthesis. 3. Biogenesis and biosynthesis of natural products. 4. Green chemistry
RJSPGCHEOPR301 RJSPGCHEOPR302 RJSPGCHEOPR303 RJSPGCHEOPR304	Paper I Paper II Paper III Paper IV	16	

M.Sc. (Organic Chemistry) Semester – IV

Course	Nomenclature	Credits	Topics
RJSPGCHEO401	Paper I	4	1. Physical organic chemistry 2. Supramolecular chemistry 3. Stereochemistry- II 4. Asymmetric synthesis
RJSPGCHEO402	Paper II	4	1. Designing Organic Synthesis-I Protecting groups in Organic Synthesis Concept of umpolung (Reversal of polarity). Introduction to Retrosynthetic analysis and synthetic planning. 2. Designing Organic Synthesis-II General strategy One group C-C Disconnections. Two group C-C Disconnections 3. Electro-organic chemistry and Selected methods of Organic synthesis. 4. Transition and rare earth metals in organic synthesis
RJSPGCHEO403	Paper III	4	1. Natural products-III Steroids. 2. Natural products-IV Vitamins. Antibiotics. Naturally occurring insecticides Terpenoids. 3. Heterocyclic compounds-I 4. Heterocyclic compounds-II
RJSPGCHEO404	Paper IV	4	1. Introduction to Intellectual Property. Patents, Industrial Designs, Copyrights, Trade Marks, Geographical Indications. 2. Trade Secrets IP Infringement issue and enforcement. Economic Value of Intellectual Property. Different International agreements. 3. Introduction to Chem informatics Representation of molecules and chemical reactions, Searching Chemical Structures. 4. Applications
RJSPGCHEOPR401 RJSPGCHEOPR402 RJSPGCHEOPR403 RJSPGCHEOPR404	Paper I Paper II Paper III Paper IV	16	

M.Sc. (Organic Chemistry) Semester – III Paper – I

(Theoretical organic chemistry-I)

Paper Code: RJSPGCHEO301

Learning Objective:

1. To predict the major and minor products of a variety of organic reactions with appropriate stereochemistry and regiochemistry.
2. Understanding of concerted reactions (Pericyclic Reaction): Principle, reactions, and applications.
3. To understand the conformational analysis of medium ring and fused ring compounds.
4. To understand the principle, reactions, and applications of photochemistry.

Unit 1 Organic reaction mechanisms **[15L]**

1.1 Organic reactive intermediates, methods of generation, structure, stability and important reactions involving carbocations, nitrenes, carbenes, arynes and ketenes**.** **[5L]**

1.2 Neighbouring group participation**:** Mechanism and effects of anchimeric assistance, NGP by unshared/ lone pair electrons, π-electrons, aromatic rings, σ-bonds with special reference to norbornyl and **bicyclo[2.2.2]octyl cation** systems (formation of non-classical carbocation) **[3L]**

1.3 Role of FMOs in organic reactivity**:** Reactions involving hard and soft electrophiles and nucleophiles, ambident nucleophiles, ambident electrophiles, the α effect. **[2L]**

1.4 Pericyclic reactions: Classification of pericyclic reactions; thermal and photochemical reactions. Three approaches: Evidence for the concertedness of bond making and breaking Symmetry-Allowed and ymmetry-Forbidden Reactions –

- The Woodward-Hoffmann Rules-Class by Class
- The generalised Woodward-Hoffmann Rule Explanations for Woodward-Hoffmann Rules
- The Aromatic Transition structures [Huckel and Mobius]
- Frontier Orbitals
- Correlation Diagrams, FMO and PMO approach Molecular orbital symmetry, Frontier orbital of ethylene, 1,3 butadiene, 1,3,5 hexatriene and allyl system. **[5L]**

Unit 2 Pericyclic reactions **[15L]**

2.1 Cycloaddition reactions: Supra and antra facial additions, 4n and 4n+2 systems, 2+2 additions of ketenes. Diels-Alder reactions, 1, 3-Dipolar cycloaddition and cheletropic reactions, ene reaction, retro-Diels-Alder reaction, regioselectivity, periselectivity, torquoselectivity, site selectivity and effect of substituents in Diels-Alder reactions. **Other Cycloaddition Reactions- [**4+6] Cycloadditions, Ketene Cycloaddition, Allene Cycloadditions, Carbene Cycloaddition, Epoxidation and Related Cycloadditions. Other Pericyclic reactions: Sigmatropic Rearrangements, Electrocyclic Reactions, Alder 'Ene' Reactions. **[7L]**

2.2 Electrocyclic reactions: Conrotatory and disrotatary motions, 4nπ and (4n+2)π electron and allyl systems. **[3L]**

2.3 Sigmatropic rearrangements: H-shifts and C-shifts, supra and antarafacial migrations, retention and inversion of configurations. Cope (including oxy- Cope and aza-Cope) and Claisen rearrangements. Formation of Vitamin D from 7-dehydrocholesterol, synthesis of citral using pericyclic reaction, conversion of Endiandric acid E to Endiandric acid A. **[5L]**

Unit 3: Stereochemistry-I **[15L]**

3.1 Classification of point groups based on symmetry elements with examples(nonmathematical treatment). **[2L]**

3.2 Conformational analysis of medium rings: Eight **to** ten membered rings andtheir unusual properties**,** I-strain, transannular reactions. **[3L]**

3.3 Stereochemistry of fused ring and bridged ring compounds: decalins,hydrindanes,**perhydroanthracenes**, steroids, and Bredt's rule. **[5L]**

3.4 Anancomeric systems, Effect of conformation on reactivity of cyclohexanederivatives in thefollowing reactions (including mechanism): electrophilicaddition, elimination, molecular rearrangements, reduction ofcyclohexanones **(with $LiAlH_4$, selectride and MPV reduction)** andoxidation ofcyclohexanols**.** **[5L]**

Unit 4 Photochemistry **[15L]**

4.1 Principles of photochemistry: quantum yield, electronic states andtransitions, selection rules, modes of dissipation of energy (Jablonskidiagram), electronic energy transfer: photosensitization and quenchingprocess. **[3L]**

4.2 Photochemistry of carbonyl compounds:$\pi \rightarrow \acute{\pi}^*$, $n \rightarrow \acute{\pi}^*$ transitions,Norrish- I and Norrish-II cleavages, Paterno-Buchi reaction.Photoreduction, calculation of quantum yield, photochemistry of enones,photochemical rearrangements of α, β-unsaturated ketones andcyclohexadienones. Photo Fries rearrangement, Barton reaction. **[8L]**

4.3 Photochemistry of olefins: cis-trans isomerizations, dimerizations, hydrogenabstraction, addition and Di-π- methane rearrangement including aza-di- π-methane. Photochemical Cross-Coupling of Alkenes, Photodimerisation ofalkenes. **[2L]**

4.4 Photochemistry of arenes**:** 1, 2- , 1, 3- and 1, 4- additions.Photocycloadditions of aromatic Rings.**[1L]**

4.5 Singlet oxygen and photo-oxygenation reactions. Photochemically inducedRadical Reactions. Chemiluminescence. **[1L]**

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3 Advanced Organic Chemistry: Reaction Mechanisms, R. Bruckner,Academic Press (2002).

4 Mechanism and theory in Organic Chemistry, T. H. Lowry and K.C. Richardson, Harper and Row.

5 Organic Reaction Mechanism, 4th edition, V. K. Ahluvalia, R. K.Parashar, Narosa Publication.

6 Reaction Mechanism in Organic Chemistry, S.M. Mukherji, S.P.Singh, Macmillan Publishers, India.

7 Organic Chemistry, Part A and B, Fifth edition,2007, Francis A.Carey and Richard J. Sundberg, Springer.

8 Carbenes, Nitrenes and Arynes. Von T. L. Gilchrist, C. W. Rees. Th.Nelson and Sons Ltd., London 1969.

9 Organic reactive intermediates, Samuel P. MacManus, AcademicPress.

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12 Organic reactions & their mechanisms, third revised edition, P.S.Kalsi, New Age International Publishers.
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19 Organic chemistry, 8th edition, John McMurry
20 Modern methods of Organic Synthesis, 4th Edition W. Carruthersand Iain Coldham, Cambridge University Press 2004
21 Modern physical chemistry, Eric V Anslyn, Dennis A. Dougherty,University science books,2006
22 Physical Organic Chemistry, N. S. Isaacs, ELBS/Longman
23 Stereochemistry of Carbon Compounds: Principles andApplications, D, Nasipuri, 3rd edition, New Age International Ltd.
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25 Stereochemistry, P. S. Kalsi, 4th edition, New Age International Ltd
26 Organic Stereochemistry, M. J. T. Robinson, Oxford UniversityPress, New Delhi, India edition, 2005
27 Bioorganic, Bioinorganic and Supramolecular chemistry, P.S. Kalsiand J.P. Kalsi. New Age International Publishers
28 Supramolecular Chemistry; Concepts and Perspectives, J. M. Lehn,VCH.
29 Crown ethers and analogous compounds, M. Hiraoka, Elsevier,1992.
30 Large ring compounds, J.A.Semlyen, Wiley-VCH, 1997.
31 Fundamentals of Photochemistry, K. K. Rohtagi-Mukherji, Wiley-Eastern
32 Essentials of Molecular Photochemistry, A. Gilbert and J. Baggott,Blackwell Sciertific Publication.
33 Molecular Photochemistry, N. J. Turro, W. A. Benjamin.
34 Introductory Photochemistry, A. Cox and T. Camp, McGraw-Hill
35 Photochemistry, R. P. Kundall and A. Gilbert, Thomson Nelson.
36 Organic Photochemistry, J. Coxon and B. Halton, CambridgeUniversity Press.
37 Molecular Orbitals and Organic Chemical Reactions by Ian Fleming
(Wiley – A john Wiley and Sons, Ltd., Publication)

M.Sc. (Organic Chemistry) Semester – III Paper – II

(Synthetic Organic Chemistry-I)

Paper Code: RJSPGCHEO302

Learning Objective:

1. To discuss mechanistic aspects of some multicomponent reactions.
2. To explore the importance of radicals in organic synthesis with relevant application.
3. To understand the reactions and applications of enamines and ylieds in organic synthesis.
4. To discuss the importance of reaction, mechanism, andregiochemistry of metals and non-metals in synthetic organic chemistry with illustration.

Unit 1: Name reactions with mechanism and application [15L]

1.1 Mukaiyama esterification, Mitsonobu reaction, Darzen'sGlycidic Estersyntheis, Ritter reaction, Yamaguchi esterification, Peterson olefination. **[5L]**

1.2 Domino reactions: Characteristics; Nazerov cyclization **[3L]**

1.3 Multicomponent reactions: Strecker Synthesis, Ugi 4CC, Biginellisynthesis, Hantzsch synthesis, Pictet-Spengler synthesis **[5L]**

1.4 Click Reactions: Characteristics; Huisgen 1,3-Dipolar Cycloaddition **[2L]**

Unit 2: Radicals in organic synthesis [15L]

2.1 **Introduction:** Generation, stability, reactivity and structural andstereochemical properties of free radicals, Persistent and charged radicals,Electrophilic and nucleophilic radicals. **[3L]**

2.2 **Radical Initiators**: azobisisobutyronitrile (AIBN) and dibenzoyl peroxide. **[1 L]**

2.3 **Characteristic reactions** - Free radical substitution, addition to multiplebonds. Radical chain reactions, Radical halogenation of hydrocarbons(Regioselectivity),radicalcyclizations, autoxidations: synthesis of cumenehydroperoxide from cumene. **[4L]**

2.4 **Radicals in synthesis**: Inter and intra molecular C-C bond formation viamercuric hydride, tin hydride, thiol donors. Cleavage of C-X, C-Sn, C-Co,C-S, O-O bonds. Oxidative coupling, C-C bond formation in aromatics:S_{RN}Ar reactions. **[4L]**

2.5 Hunsdiecker reaction, Pinacol coupling, McMurry coupling, Sandmeyerreaction, Acyloin condensation. **[3L]**

Unit 3: Enamines, Ylides and α-C-H functionalization [15]

3.1 **Enamines:** Generation & application in organic synthesis with mechanisticpathways, Stork enamine reaction. Reactivity, comparison betweenenamines and enolates. Synthetic reactions of enamines includingasymmetric reactions of chiral enamines derived from chiral secondaryamines. **[4L]**

3.2 **Phosphorus, Sulfur and Nitrogen Ylides:** Preparation and their syntheticapplications along with their stereochemical aspects. Wittig reaction,Horner-Wadsworth-Emmons Reaction, Barton-Kellogg olefination. **[6L]**

3.3 **α-C-H functionalization:** By nitro, sulfoxide, sulfone and phosphonategroups: generation of carbanions by strong bases (LDA/n-butyl lithium) andapplications in C-C bond formation. Bamford-Stevens reaction, Juliaolefination and its modification, Seyferth–Gilbert homologation, Steven'srearrangement. **[5L]**

Unit 4: Metals / Non-metals in organic synthesis **[15]**

4.1 **Mercury in organic synthesis:** Mechanism and regiochemistry ofoxymercuration and demercuration of alkenes, mercuration of aromatics,transformation of aryl mercurials to aryl halides. Organomercurials ascarbene transfer reagents. **[3L]**

4.2 **Organoboron compounds:** Mechanism and regiochemistry ofhydroboration of alkenes and alkynes, asymmetric hydroboration usingchiral boron reagents, 9-BBN hydroboration, oxazaborolidine (CBScatalyst) and functional group reduction by diborane. **[3L]**

4.3 **Organosilicons:** Salient features of silicon governing the reactivity oforganosilicons, preparation and important bond-forming reactions of alkylsilanes, alkenyl silanes, aryl silanes and allyl silanes. β-silyl cations asintermediates. Iodotrimethylsilane in organic synthesis. **[3L]**

4.4 **Silyl enol ethers**: Application: As nucleophiles (Michael reaction,Mukaiyama aldol reaction), in ring contraction reactions. **[2L]**

4.5 **Organotin compounds**: Preparation of alkenyl and allyl tin compounds;application in C-C bond formation, in replacement of halogen by H at thesame C atom. **[2L]**

4.6 **Selenium in organic synthesis:** Preparation of selenols/selenoxide,selenoxide elimination to create unsaturation, selenoxide and selenoacetalsas α-C-H activating groups **[2L]**

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- **Name Reactions and Reagents in Organic Synthesis,** 2nd Edn.,Bradford P. Mundy, Michael G. Ellard, and Frank Favoloro, Jr.,Wiley-Interscience
- **Name Reactions,** Jie Jack Lie, 3rd Edn., Springer
- **Organic Electrochemistry,** H. Lund, and M. Baizer, 3rd Edn.,Marcel Dekker.

M.Sc. (Organic Chemistry) Semester – III Paper – III

(Natural products and Spectroscopy)

Paper Code: RJSPGCHEO303

Learning Objective:

1. To give the students an overview of biomolecules.
2. Recognize the structures and functions of biomolecules that form the basis of what we understand to be living organisms.
3. Learn basic principles of structure and applications of carbohydrates, natural pigments, insect pheromones, and alkaloids.
4. Understanding the use of nuclear magnetic resonance spectroscopy and advance nuclear magnetic resonance spectroscopy in diverse area of organic chemistry.
5. Understanding multi-step synthesis of natural products with respect to reagents used, stereochemistry and functional group transformations.
6. Understand general idea, structure, biological importance and application of prostaglandins, lipids, insect and plant growth regulators

Unit 1: Natural products-I **[15L]**

1.1 **Carbohydrates:** Introduction to naturally occurring sugars: Deoxysugars,aminosugars, branched sugars. Structure elucidation of lactose and Dglucosamine(synthesis not expected).Structural features and applications ofinositol, starch, cellulose, chitin and heparin**.** **[5L]**

1.2 **Natural pigments:** General structural features, occurrence, biologicalimportance and applications of: carotenoids, anthocyanins, quinones,flavones, pterins and porphyrins (chlorophyll). Structure elucidation of β-carotene and Cyanin (with synthesis).Synthesis of ubiquinone from 3, 4, 5-trimethoxyacetophenone. **[5L]**

1.3 **Insect pheromones:** General structural features and importance. Types ofpheromones (aggregation, alarm, releaser, primer, territorial, trail, sexpheromones etc.), advantage of pheromones over conventional pesticides.Synthesis of bombykol from acetylene, disparlure from 6-methylhept-1-ene,grandisol from 2-methyl-1, 3-butadiene**.** **[3L]**

1.4 **Alkaloids:** Occurrence and physiological importance of morphine andatropine. Structure elucidation, spectral data and synthesis of coniine. **[2L]**

Unit 2: Natural products-II **[15L]**

2.1 **Multi-step synthesis of natural products:** Synthesis of the followingnatural products with special reference to reagents used, stereochemistryand functional group transformations: [8L]

a) Woodward synthesis of Reserpine from benzoquinone
b) Corey synthesis of Longifoline from resorcinol
c) Gilbert-Stork synthesis of Griseofulvin from phloroglucinol
d) Corey's Synthesis of Caryophyllene from 2-Cyclohexenone andIsobutylene
e) Synthesis of Juvabione from Limonene
f) Synthesis of Taxol.

2.2 **Prostaglandins:** Classification, general structure and biologicalimportance. Structure elucidation of **PGE_1**. [2L]

2.3 **Lipids:** Classification, role of lipids, Fatty acids and glycerol derived fromoils and fats. [2L]

2.4 **Insect growth regulators:** General idea, structures of JH_2 and JH_3 . [1L]
2.5 **Plant growth regulators:** Structural features and applications of arylaceticacids, gibberellic acids and triacontanol. Synthesis of triacontanol (synthesisof stearyl magnesium bromide and 12-bromo-1-tetrahydropyranyloxydodecane expected). [2L]

Unit 3: Advanced spectroscopic techniques-I [15L]
3.1 **Proton NMR spectroscopy:** Recapitulation, chemical and magneticequivalence of protons, First order, second order, Spin system notations(A_2, AB, AX, AB_2, AX_2, AMX and A_2B_2-A_2X_2 spin systems with suitableexamples). Long range coupling (Allylic coupling, 'W' coupling andCoupling in aromatic and heteroaromatic systems), Temperature effects,Simplification of complex spectra, nuclear magnetic double resonance,chemical shift reagents. [7L]
3.2 **^{13}C –NMR spectroscopy:** Recapitulation, equivalent and non-equivalentcarbons (examples of aliphatic and aromatic compounds), **^{13}**C- chemicalshifts, calculation of ^{13}C- chemical shifts of aromatic carbons, heteronuclearcoupling of carbon to ^{19}F and **^{31}**P. [4L]
3.3 Spectral problems based on UV, IR, ^{1}HNMR and ^{13}CNMR and Massspectroscopy . [4L]

Unit 4: Advanced spectroscopic techniques-II [15L]
4.1 **Advanced NMR techniques:** DEPT experiment, determining number ofattached hydrogens (Methyl/methylene/methine and quaternary carbons),two dimensional spectroscopic techniques, COSY and HETCOR spectra,NOE and NOESY techniques. [10L]
4.2 Spectral problems based on UV, IR, ^{1}HNMR, ^{13}CNMR (Including 2Dtechnique) and Mass spectroscopy [5L]

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M.Sc. (Organic Chemistry) Semester – III Paper – IV

(Medicinal, Biogenesis and green chemistry)

Paper Code: RJSPGCHEO304

Learning Objective:

1. To familiarize students with drug discovery, design, and development.
2. To understand the uses of QSAR, computer in design, development, and synthesis of drugs.
3. To study the synthesis and application of different drugs
4. Students will learn about biogenesis, the nature of a variety of metabolic pathways, the regulation of these pathways and the mechanisms by which regulation is accomplished.
5. To familiarize the student with basic principle and application of green chemistry with suitable examples of reagents, catalyst, solvent and modern reaction methods.

Unit 1: Drug discovery, design and development [15L]

1.1 Introduction, important terms used in medicinal chemistry: receptor,therapeutic index, bioavailability, drug assay and drug potency. Generalidea of factors affecting bioactivity: Resonance, inductive effect,bioisosterism, spatial considerations. Basic pharmacokinetics: drugabsorption, distribution, metabolism (biotransformation) and elimination.Physical and chemical parameters like solubility, lipophilicity, ionization,pH, redox potential, H-bonding, partition coefficient and isomerism in drugdistribution and drug-receptor binding. [7L]

1.2 Procedures in drug design: Drug discovery without a lead: Penicillin,Librium. Lead discovery: random screening, non-random (or targeted)screening. Lead modification: Identification of the pharmacophore,Functional group modification. Structure-activity relationship, Structuremodification to increase potency and therapeutic index: Homologation,chain branching, ring-chain transformation, bioisosterism, combinatiorialsynthesis (basic idea). [8L]

Unit 2: Drug design, development and synthesis [15L]

2.1 Introduction to quantitative structure activity relationship studies. QSARparameters: - steric effects: The Taft and other equations; Methods used tocorrelate regression parameters with biological activity: Hansch analysis- Alinear multiple regression analysis. [5L]

2.2 Introduction to modern methods of drug design and synthesis- computeraidedmolecular graphics based drug design, drug design via enzymeinhibition (reversible and irreversible), bioinformatics and drug design. [3L]

2.3 Concept of prodrugs and soft drugs. (a) Prodrugs: Prodrug design, types ofprodrugs, functional groups in prodrugs, advantages of prodrug use. (b) Softdrugs: concept and properties. [3L]

2.4 Synthesis and application of the following drugs: Fluoxetine, cetrizine,esomeprazole, fluconazole, zidovudine, methotrexate, diclofenac, labetalol,fenofibrate. [4L]

Unit 3: Biogenesis and biosynthesis of natural products [15L]

3.1Primary and secondary metabolites and the building blocks, generalpathway of amino acid biosynthesis. [3L]

3.2Acetate pathway: Biosynthesis of malonylCoA, saturated fatty acids,prostaglandins from arachidonic acid, aromatic polyketides. [4L]

3.3Shikimic Acid pathway: Biosynthesis of shikimic acid, aromatic aminoacids, cinnamic acid and its derivatives, lignin and lignans, benzoic acid andits derivatives, flavonoids and isofalvonoids. [4L]
3.4Mevalonate pathway: Biosynthesis of mevalonic acid, monoterpenes –geranyl cation and its derivatives, sesquiterpenes – farnesyl cation and itsderivatives and diterpenes. [4L]

Unit 4: Green chemistry [15L]
4.1Introduction, basic principles of green chemistry. Designing a greensynthesis: Green starting materials, green reagents, green solvents andreaction conditions, green catalysts. [1L]
4.2Use of the following in green synthesis with suitable examples: [9L]
a) Green reagents: dimethylcarbonate, polymer supported reagents.
b) Green catalysts: Acid catalysts, oxidation catalysts, basic catalysts, phasetransfer catalysts [Aliquat 336, benzyltrimethyl ammonium chloride(TMBA), Tetra-n-butyl ammonium chloride, crown ethers], biocatalysts.
c) Green solvents: water, ionic liquids, deep eutectic solvents, supercriticalcarbon dioxide.
d) Solid state reactions: solid phase synthesis, solid supported synthesis
e) Microwave assisted synthesis: reactions in water, reactions in organicsolvents, solvent free reactions.
f) Ultrasound assisted reactions.
4.3Comparison of traditional processes versus green processes in the synthesesof ibuprofen, adipic acid, 4-aminodiphenylamine, p-bromotoluene andbenzimidazole. [3L]
4.4Green Catayst s :Nanocatalyst, Types of nanoctalysts, Advantages andDisadvantages of Nanocatalysts, Idea of Magnetically separablenanocatalysts. [2L]

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M.Sc. (Organic Chemistry) Semester – III Practicals

Learning Objective:

1. Students are expected to know the planning of synthesis, effect of reaction parameters including stoichiometry, and safety aspects including MSDS
2. Students are expected to purify the product by recrystallization, measure its mass, check the purity by TLC, determine physical constant and calculate percentage yield.
3. Students are expected to perform a purification technique using a known mass or volume of the given substance.
4. Check the purity of the purified compound by TLC, measure its mass and physical constant. Students are expected to purify the product by recrystallization, measure its mass, determine physical constant and calculate percentage yield.

Paper I
Paper Code: RJSPGCHEOPR301

Separation of a ternary mixture of organic compounds and identification including derivative preparations using micro-scale technique

1. Separation of a ternary mixture (S-S-S, S-S-L, S-L-L and L-L-L) (for solid mixture: water insoluble/ soluble including carbohydrates) based upon differences in the physical and the chemical properties of the components.
2. Identification of the two components (indicated by the examiner) using micro-scale technique.
3. Preparation of derivatives (any one of separated compound).

(**Minimum 8 experiments**)

Paper II
Paper Code: RJSPGCHEOPR302

Single step organic preparation(1.0 g scale) involving purification by Steam distillation / Vacuum distillation or Column chromatography.

1. Preparation of acetanilide from aniline and acetic acid using Zn dust. (Purification by column chromatography)
2. Preparation of 1-nitronaphthalene from naphthalene. (Purification by steam distillation)
3. Preparation of acetyl ferrocene from ferrocene. (Purification by column chromatography)
4. Preparation of 3-nitroaniline from 1,3-dinitrobenzene. (Purification by column chromatography)
5. Preparation of benzyl alcohol from benzaldehyde. (Purification by vacuum distillation).
6. Preparation of methyl salicylate from salicylic acid. (Purification by vacuum distillation).
7. Preparation of 4-methylacetophenone from toluene. (Purification by vacuum distillation).
8. Preparation of phenyl acetate from phenol. (Purification by vacuum distillation)
9. Preparation of 2-chlorotoluene from *o*-toluidine. (Purification by steam distillation)
10. Preparation of 4-nitrophenol from phenol. (Purification by steam distillation/ column chromatography)
11. Preparation of fluorenone from fluorene. (Purification by column chromatography)
12. Preparation of dimethylphthalate from phthalic anhydride. (Purification by vacuum distillation)

(Minimum 8 experiments)

Note:

1. Students are expected to know (i) the planning of synthesis, effect of reaction parameters including stoichiometry, and **safety aspects including MSDS** (ii) the possible mechanism, expected spectral data (IR and NMR) of the starting material and final product.
2. Students are expected to purify the product by Steam distillation / Vacuum distillation or Column chromatography, measure its mass or volume, check the purity by TLC, determine physical constant and calculate percentage yield.

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M.Sc. (Organic Chemistry) Semester – IV Paper – I

(Theoretical organic chemistry-II)

Paper Code: RJSPGCHEO401

Learning Objective:

1. To understand fundamental concepts of physical organic chemistry that governs various kinetic and thermodynamic aspects of organic reactions.
2. To study structure, properties, associations and organisations of organic macromolecules along with a typical synthesis of few of them.
3. To know the technique of resolution of racemates and to learn to determine the enantiomer and diastereomer composition.
4. To discuss principals involved in asymmetric synthesis and study of few selected similar organic name reactions.

Unit 1: Physical organic chemistry **[15L]**

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**.** **[7L]**

1.2 Uses of Hammett equation, deviations from Hammett equation. Dualparameter correlations, Inductive substituent constants. The Taft model, $\sigma_I$and $\sigma_R$scales, steric parameters Es and β. Solvent effects, Okamoto-Brownequation, Swain-Scott equation, Edward and Ritchie correlations,Grunwald-Winstein equation, Dimroth's E_T parameter, SolvatochromismZscale,Spectroscopic Correlations, Thermodynamic Implications. **[8L]**

Unit 2 Supramolecular chemistry **[15L]**

2.1 Principles of molecular associations and organizations as exemplified inbiological macromolecules like nucleic acids, proteins and enzymes. **[3L]**

2.2 Synthetic molecular receptors: receptors with molecular cleft, moleculartweezers, receptors with multiple hydrogen sites. **[3L]**

2.3 Structures and properties of crown ethers, cryptands, cyclophanes,calixarenes, rotaxanes and cyclodextrins. Synthesis of crown ethers,cryptands and calixarenes. **[5L]**

2.4 Molecular recognition and catalysis, molecular selfassembly.Supramolecular Polymers, GelsandFibres. **[4L]**

Unit 3 Stereochemistry- II **[15L]**

3.1 Racemisation and resolution of racemates including conglomerates:Mechanism of racemisation, methods of resolution: mechanical, chemical,kinetic and equilibrium asymmetric transformation and through inclusioncompounds. **[3L]**
3.2 Determination of enantiomer and diastereomer composition: enzymaticmethod, chromatographic methods. Methods based on NMR spectroscopy:use of chiral derivatising agents (CDA), chiral solvating agents (CSA) andLanthanide shift reagents (LSR). **[3L]**

3.3 Correlative method for configurational assignment: chemical, opticalrotation, and NMR spectroscopy. **[4L]**
3.4 Molecular dissymmetry and chiroptical properties: Linearly and circularlypolarized light. Circular birefringence and circular dichroism.ORD and CDcurves.Cotton effect and its applications. The octant rule and the axial α–haloketone rule with applications. **[5L]**

Unit 4: Asymmetric synthesis **[15L]**

4.1 Principles of asymmetric synthesis: Introduction, the chiral pool in Nature,methods of asymmetric induction – substrate, reagent and catalystcontrolled reactions. **[3L]**

4.2 Synthesis of L-DOPA [Knowles's Mosanto process]. Asymmetric reactionswith mechanism: Aldol and related reactions, Cram's rule, Felkin-Anhmodel, Sharpless enantioselective epoxidation, hydroxylation,aminohydroxylation, Diels-Alder reaction, reduction of prochiral carbonylcompounds and olefins. **[9L]**

4.3 Use of chiral auxiliaries in diastereoselective reductions, asymmetricamplification. Use of chiral BINOLs, BINAPs and chiral oxazolinesasymmetric transformations. **[3L]**

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M.Sc. (Organic Chemistry) Semester – IV Paper – II

(Synthetic organic chemistry-II)

Paper Code: RJSPGCHEO402

Learning Objective:

1. To find out the feasible pathways of organic synthesis of a target molecule by backward engineering based on comprehensive knowledge of reaction mechanism.
2. To incorporate well established organic name reactions in choosing appropriate starting material and designing high yielding steps for the required organic synthesis.
3. To know and understand the role ofvarious electrochemical organic conversions in the field of organic synthesis.
4. To explore the possibilities of catalysis by different transition and rare earth metals and its compounds.

Unit 1: Designing Organic Synthesis-I [15L]

1.1 **Protecting groups in Organic Synthesis:** Protection and deprotection ofthe hydroxyl, carbonyl, amino and carboxyl functional groups and itsapplications. [3L]

1.2 **Concept of umpolung (Reversal of polarity):** Generation of acyl anionequivalent using 1,3-dithianes, methyl thiomethyl sulfoxides, cyanide ions,cyanohydrin ethers, nitro compounds and vinylated ethers. [3L]

1.3 **Introduction to Retrosynthetic analysis and synthetic planning:** Linearand convergent synthesis; Disconnection approach: An introduction tosynthons, synthetic equivalents, disconnection approach, functional groupinterconversions (FGI), functional group addition (FGA), functional groupremoval (FGR) importance of order of events in organic synthesis, one andtwo group C-X disconnections (1,1; 1,2; 1,3 difunctionalized compounds),selective organic transformations: chemoselectivity, regioselectivity,stereoselectivity, enantioselectivity. [9L]

Unit 2: Designing Organic Synthesis-II [15L]

2.1 **General strategy:** choosing a disconnection-simplification, symmetry, highyielding steps, and recognisable starting material. [3L]

2.2 **One group C-C Disconnections:** Alcohols (including stereoslectivity),carbonyls (including regioselectivity), Alkene synthesis, use of acetylenesand aliphatic nitro compounds in organic synthesis. [6L]

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-unsaturatedcompounds, control in carbonyl condensations, Michael addition andRobinson annelation. [6L]

Unit 3: Electro-organic chemistry and Selected methods of Organic synthesis [15L]

3.1 **Electro-organic chemistry:** [7L]

3.1.1 Introduction: Electrode potential, cell parameters, electrolyte, workingelectrode, choice of solvents, supporting electrolytes.

3.1.2 Cathodic reduction: Reduction of alkyl halides, aldehydes, ketones, nitrocompounds, olefins, arenes, electro-dimerization.

3.1.3 Anodic oxidation: Oxidation of alkylbezene, Kolbe reaction, Non-Kolbeoxidation, Shono oxidation.

3.2 **Selected Methods of Organic synthesis** [8L]
Applications of the following in organic synthesis:

3.2.1 Crown ethers, cryptands, micelles, cyclodextrins, catenanes.

3.2.2 Organocatalysts: Proline, Imidazolidinone.

3.2.3 Pdcatalysed cycloaddition reactions: Stille reaction, Saeguse-Ito oxidationto enones, Negishi coupling.

3.2.4 Use of Sc(OTf), and Yb(OTf) as water tolerant Lewis acid catalyst in aldolcondensation, Michael reaction, Diels-Alder reaction, Friedel – Craftsreaction.

Unit 4: Transition and rare earth metals in organic synthesis [15L]

4.1 **Introduction to basic concepts:** 18 electron rule, bonding in transitionmetal complexes, C-H activation, oxidative addition, reductive elimination,migratory insertion. [3L]

4.2 **Palladium in organic synthesis:** π-bonding of Pd with olefins, applicationsin C-C bond formation, carbonylation, alkene isomerisation, cross-couplingof 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. [5L]

4.3 **Olefin metathesis** using Grubb's catalyst. [1L]

4.4 **Application of Ni, Co, Fe, Rh, and Cr carbonyls** in organic synthesis. [4L]

4.5 **Application of samarium iodide** including reduction of organic halides,aldehydes and ketones, α-functionalised carbonyl and nitro compounds. [1L]

4.6 **Application of Ce(IV)** in synthesis of heterocyclic quinoxaline derivativesand its role as a de-protecting agent**.** [1L]

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M.Sc. (Organic Chemistry) Semester – IV Paper – III

(Natural products and heterocyclic chemistry)

Paper Code: RJSPGCHEO403

Learning Objective:

1. To know the synthesis of some selected natural products and study of organic biomolecules like steroids.
2. To discuss the classification, sources, structure elucidation and biological importanceof Vitamins and antibiotics.
3. To study classification, nomenclature and synthesis of hetero monocyclic compounds.
4. To study classification, labelling and preparation, reactivity of bi, tricyclic five and six membered heterocycles up to three heteroatoms.

Unit 1: Natural products-III **[15L]**

1.1 **Steroids:** General structure, classification. Occurrence, biological role, important structural and stereochemical features of the following:corticosteroids, steroidal hormones, steroidal alkaloids, sterols and bileacids. [5L]

1.2 Synthesis of 16-DPA from cholesterol and plant sapogenin. [2L]

1.3 Synthesis of the following from 16-DPA: androsterone, testosterone, oestrone, oestriol, oestradiol and progesterone. [5L]

1.4 Synthesis of cinerolone, jasmolone, allethrolone, exaltone and muscone. [3 L]

Unit 2: Natural products-IV **[15L]**

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). [5L]
Synthesis of the following:
Vitamin A from β-ionone and bromoester moiety.
Vitamin B_1 including synthesis of pyrimidine and thiazole moieties
Vitamin B_2 from 3, 4-dimethylaniline and D(-)ribose
Vitamin B_6 from: 1) ethoxyacetylacetone and cyanoacetamide, 2) ethylester of N-formyl-DL-alanine (Harris synthesis)
Vitamin E (α-tocopherol) from trimethylquinol and phytyl bromide
Vitamin K_1 from 2-methyl-1, 4-naphthaquinone and phytol.

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). [6L]

2.3 **Naturally occurring insecticides:** Sources, structure and biologicalproperties of pyrethrums (pyrethrin I), rotenoids (rotenone). Synthesis ofpyrethrin I. [2L]
2.4 **3.4 Terpenoids**: Occurrence, classification, structure elucidation, stereochemistry, spectral data and synthesis of zingiberene . [2L]

Unit 3: Heterocyclic compounds-I [15L]
Heterocyclic compounds: Introduction, classification, Nomenclature ofheterocyclic 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, pyrazinesand oxazines.

Unit 4: Heterocyclic compounds-II [15L]
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 andazetidines.Structure, reactivity, synthesis and reactions of coumarins, quinoxalines,cinnolines, indole, benzimidazoles, benzoxazoles, benzothiazoles, Purinesand acridines.

REFERENCES:
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3. Organic Chemistry Natural Products Volume-II, O. P. Agarwal,Krishna Prakashan, 2011.
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18. Introduction to Flavonoids, B.A. Bohm, Harwood AcademicPublishers, 1998.
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22. Total. Synthesis of Longifolene, J. Am. Chem. Soc. 1961, 83, 1251.
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27. Synthesis of (±)-4-demethoxydaunomycinone,A. V. Rama Rao ,G. Venkatswamy , S. M. Javeed M. , V. H. Deshpande, B.Ramamohan Rao, J. Org. Chem., 1983, 48 (9), 1552.
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33. Total synthesis of Natural Products, J. Apsimon, John Wileyand Sons.
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37. Applications of Absorption Spectroscopy of Organic compounds, J.R. Dyer, Prentice Hall of India, 1987.
38. Spectrometric Identification of Organic compounds, R.M.Silverstein and others, John Wiley and Sons Inc., 5th ed., 1991
39. Absorption spectroscopy of organic Molecules, V.M. Parikh, 1974.
40. Spectroscopic methods in organic chemistry, Williams and Fleming,Tata McGraw Hill, 4th ed, 1989.
41. Organic spectroscopy, William Kemp, ELBS, 3rd ed., 1987.
42. Organic structures from spectra, L. D. Field, S. Sternhell, John R.Kalman, Wiley, 4th ed., . 3122
43. Introduction to spectroscopy, Donald L. Pavia, Gary M. Lampman,George S. Kriz, James R. Vyvyan, 4th ed., 2009.
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47. Biotransformations in Organic Chemistry, 5thEdition, Kurt Faber,Springer
48. Structure Determination of Organic Compounds, EPretsch, P.Buhlmann, C.Affolter, Springer

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

(INTELLECTUAL PROPERTY RIGHTS & CHEMINFORMATICS)

Paper Code: RJSPGCHEO404

Learning Objective:

1. To create awareness and understanding the terms like intellectual property, patents, copyright, industrial designs, trademarks, geographical indications etc.
2. To know trade secrets, IP infringement issues, economic value of intellectual property and study of various related international agreements.
3. To explore cheminformatics to facilitate molecular modeling and structure elucidations.
4. To apply the knowledge gained about various chemistry principals, techniques and tools in drug designing, target identification and validation, lead finding and optimization.

Unit I: **[15L]**

Introduction to Intellectual Property: **[2L]**

Historical Perspective, Different types of IP, Importance of protecting IP.

Patents: **[5L]**

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.

Industrial Designs: **[2L]**

Definition, How to obtain, features, International design registration.

Copyrights: **[2L]**

Introduction, How to obtain, Differences from Patents.

Trade Marks: **[2L]**

Introduction, How to obtain, Different types of marks – Collective marks, certification marks, service marks, trade names etc.

Geographical Indications: **[2L]**

Definition, rules for registration, prevention of illegal exploitation, importance to India.

Unit II: **[15L]**

Trade Secrets: **[2L]**

Introduction and Historical Perspectives, Scope of Protection, Risks involved and legal aspects of Trade Secret Protection.

IP Infringement issue and enforcement: **[2L]**

Role of Judiciary, Role of law enforcement agencies – Police, Customs etc.

Economic Value of Intellectual Property: **[5L]**

Intangible assests and their valuation, Intellectual Property in the Indian context – Various Laws in India Licensing and Technology transfer.

Different International agreements:

(a) World Trade Organization (WTO): **[5L]**

(i) General Agreement on Tariffs and Trade (GATT), Trade Related Intellectual Property Rights (TRIPS) agreement

(ii) General Agreement on Trade Related Services (GATS) Madrid Protocol.

(iii) Berne Convention

(iv) Budapest Treaty

(b) Paris Convention **[1L]**

WIPO and **TRIPS, IPR** and Plant Breeders Rights, IPR and Biodiversity.

Unit III: **[15L]**

Introduction to Chem informatics: **[5L]**

History and evolution of cheminformatics, Use of Cheminformatics, Prospects of cheminformatics, Molecular modeling and structure elucidation.

Representation of molecules and chemical reactions: **[5L]**

Nomenclature, Different types of notations, SMILES coding, Matrix representations, Structure of Molfiles and Sdfiles, Libraries and toolkits, Different electronic effects, Reaction classification.

Searching Chemical Structures: **[5L]**

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: **[15L]**

Applications:

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.

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.

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

Learning Objective:

1. To learn the technique of separation of ternary mixture.
2. To identify bifunctional organic compounds.
3. To learn Instrumental and non-instrumental methods of estimation of organic compounds.
4. To learn interpretation of structure of organic compounds by spectral methods.

Paper I
Paper Code: RJSPGCHEOPR401

Two steps preparations

1. Acetophenone → Acetophenone phenyl hydrazine → 2-phenyl indole.
2. 2-naphthol → 1-phenyl azo-2-naphthol → 1-amino-2-naphthol.
3. Cyclohexanone → cyclohexanone oxime → Caprolactum.
4. Hydroquinone → hydroquinone diacetate → 2,5-dihydroxyacetophenone.
5. 4-nitrotoluene → 4-nitrobenzoic acid → 4-aminobenzoic acid.
6. *o*-nitroaniline → *o*-phenylene diamine → Benzimidazole.
7. Benzophenone → benzophenone oxime → benzanilide.
8. *o*-chlorobenzoic acid → N-phenyl anthranilic acid → acridone.
9. Benzoin → benzil → benzilic acid.
10. Phthalic acid → phthalimide → anthranilic acid.
11. Resorcinol → 4-methyl-7-hydroxy coumarin → 4-methyl-7-acetoxy coumarin.
12. Anthracene → anthraquinone → anthrone.

(Minimum 8 experiments)

Note:

1. Students are expected to know (i) the planning of synthesis, effect of reaction parameters including stoichiometry, and **safety aspects including MSDS** (ii) the possible mechanism, expected spectral data (IR and NMR) of the starting material and final product.
2. Students are expected to purify the product by recryllization, measure its mass or volume, check the purity by TLC, determine physical constant and calculate percentage yield.

Paper II
Paper Code: RJSPGCHEOPR402

Session-I: Combined spectral identification: Interpretation of spectral data of organic compounds (UV, IR, PMR, CMR and Mass spectra).

A student will be given UV, IR, PMR, CMR, and Mass spectra of a compound from which preliminary information should be reported within first half an hour of the examination without referring to any book/reference material. The complete structure of the compound may then be elucidated by referring to any standard text-book/reference material etc
(**Minimum 8 spectral analysis).**

Session-II: 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.
3. Use of non-programmable calculator is allowed both at the theory and the practical examination.

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, 4thed., 2011.

M.Sc. (Organic Chemistry) Semester – III & IV

Paper Pattern

Internal Exam

1. Class Test : 20 marks
2. Presentation : 20 marks

Paper Pattern for Semester End Examination

Maximum Mark: 60 Duration : 2Hrs

There will be 5 questions each of 12 marks.

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

The pattern for above questions is as follows:

- Each question will have five sub questions of 4 marks each.
- Learners have to attempt any 3 questions out of 5.

Q. 5 will have 8 sub questions of 3 marks each (2 questions will be from each unit).

Learners have to attempt any 4 questions out of 8.

Practical Exam

Practical exam will be of 50 marks.

- Experiment : 40 marks
- Journal : 5 marks
- Viva : 5 marks

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 III & Sem IV

Program: M.Sc (Analytical Chemistry)

Program Code: RJSPGCHEA

CBCS : 2019 -2020

M.Sc. (Analytical Chemistry) Semester – III

Course	Nomenclature	Credits	Topics
RJSPGCHEA301	Paper I	4	1) Quality In Analytical Chemistry – I 2) Quality In Analytical Chemistry – II 3) Chromatographic Techniques –I 4) Chromatographic Techniques -II
RJSPGCHEA302	Paper II	4	1) Spectral Methods I 2) Spectral Methods – II 3) Electroanalytical Methods 4) Miscellaneous Techniques
RJSPGCHEA303	Paper III	4	1) Bioanalytical chemistry 2) Immunological Methods 3) Food Analysis – I 4) Food Analysis - II
RJSPGCHEA304	Paper IV	4	1) Air Pollution 2) Water Quality Standards 3) Other Types Of Pollution 4) Industrial Materials
RJSPGCHEA304	Paper IV	4	1) Pharmaceutical Analysis 2) Drugs 3) Forensic Science 4) Cosmetic Analysis
RJSPGCHEAPR301 RJSPGCHEAPR302 RJSPGCHEAPR303 RJSPGCHEAPR304	Paper I Paper II Paper III Paper IV	16	

M.Sc. (Analytical Chemistry) Semester – IV

Course	Nomenclature	Credits	Topics
RJSPGCHEA401	Paper I	4	1) Separation Science 2) Separation, Analysis and Standardization of Herbal based products. 3) Green Chemistry 4) Advanced Techniques
RJSPGCHEA402	Paper II	4	1) Spectral Methods III 2) Spectral Methods IV 3) Radiochemical And Thermal Methods 4) Hyphenated Techniques
RJSPGCHEA403	Paper III	4	1) Effluent Treatment 2) Solid Waste Management 3) Plastics and Polymers 4) Metallurgy
RJSPGCHEA404	Paper IV	4	5. Introduction to Intellectual Property. Patents, Industrial Designs, Copyrights, Trade Marks, Geographical Indications. 6. Trade Secrets IP Infringement issue and enforcement. Economic Value of Intellectual Property. Different International agreements. 7. Introduction to Chem informatics Representation of molecules and chemical reactions . Searching Chemical Structures. 8. Applications
RJSPGCHEA404	Paper IV	4	1) Print, journals, digital, information technology and library resources. 2) Data analysis. 3) Methods of scientific research and writing scientific papers. 4) Chemical safety & ethical handling of chemicals.
RJSPGCHEAPR401 RJSPGCHEAPR402 RJSPGCHEAPR403 RJSPGCHEAPR404	Paper I Paper II Paper III Paper IV	16	

M.Sc. ANALYTICAL CHEMISTRY
SEMESTER – III
RJSPGCHEA301
QUALITY IN ANALYTICAL CHEMISTRY

UNIT I Quality In Analytical Chemistry - I **15**

1.1 Sampling: Definition, types of sample, sampling plan, quality of sample, subsampling, Sampling of raw materials, intermediates and finished products.Sample preparations – dissolution technology and decomposition, storage ofsamples.Pre-treatment of samples: soil, food and cosmetics. (8L)

1.2 Selection of the Method: sources of methods, factors to consider when selecting a method, performance criteria for methods used, reasons for incorrect analytical results, method validation, and quality by design (PAT). (7L)

UNIT II Quality In Analytical Chemistry - II **15**

2.1 Measurement of uncertainty: Definition and evaluation of uncertainty, putting uncertainty to use, interpretation of results and improving the quality of results. (4L)

2.2 Signal to noise: Signal to noise ratio, sources of noise in instrumental analysis. Signal to noise enhancement, hardware devices for noise reduction, software methods for noise reduction. (6L)

2.3 Pharmaceutical Legislation: introduction to drug acts, drug rules (schedules), concept of regulatory affairs in pharmaceuticals, review of GLP and GMP and their regulations for analytical labs, roles and responsibilities of personnel, appropriate design and placement of laboratory equipment, requirements for maintenance and calibration. (5L)

UNIT III Chromatographic Techniques -I **15**

3.1 Ion exchange chromatography: Ion exchange equilibria, breakthrough capacity, inorganic ion exchangers, synthetic ion exchangers, chelating resins and their applications for separation of inorganic and organic compounds. (8L)

3.2 Ion chromatography: Principle, instrumentation with special reference to separation and suppressor columns, applications. (2L)

3.3 Exclusion chromatography : Theory, instrumentation and applications of gel permeation chromatography, retention behavior, inorganic molecular sieves, determination of molecular weight of polymers, (5L)

UNIT IV Chromatographic Techniques -II **15**

4.1 Supercritical fluid Chromatography: Theory, concept of critical state of matter and supercritical state, types of supercritical fluids, instrumentation, applications to environmental, food, pharmaceuticals and polymeric analysis. (8L)

4.2 Affinity Chromatography: principle, instrumentation and applications (4l)

4.3 Optimum pressure liquid chromatography (OPLC) (3L)

List of books and references:

1. Quality in the analytical chemistry laboratory, E Prichard, John Wiley and sons N.Y 1997.
2. Quality assurance in analytical Chemistry, W Funk, V Dammann, G. Donnevert VCH Weinheim1995.
3. Amit S. Patil *et. al.*,Quality by Design (QbD) : A new concept for development of Quality pharmaceuticals, International Journal of Pharmaceutical Quality Assurance; 4(2); 13-19.
4. Lalit Singh and Vijay Sharma, Quality by Design (QbD) Approach in Pharmaceuticals: Status, Challenges and Next Steps, Drug Delivery Letters, 2015, 5, 2-8. Quality in the analytical chemistry laboratory, E Prichard, John Wiley and sons N.Y 1997

5. Fundamentals of Analytical Chemistry, D. A. Skoog and D. M. West, Saonders, College publication.
6. Chemical methods of separation, J A Dean, Van Nostrand Reinhold, 1969
7. Solvent extraction and ion exchange, J Marcus and A. S. Kertes Wiley INC 1969.
8. Analytical Chemistry, G. D. Christain, Wiley
9. Extraction Chromatography T. Braun, G. Ghersene, Elsevier Publications 1978.
10 Supercritical Fluid Extraction, Larry Taylor Wiley publishers N.Y. 1996
11. Ion exchange separation in analytical chemistry O Samuelson John Wiley 2 nd ed 1963
12 Ion exchange chromatography Ed H.F Walton Howden, Hutchenson and Rossing 1976
13. Chromatographic and electrophoresis techniques I Smith Menemann Interscience 1960

SEMESTER-III

RJSPGCHEA302

Advance Instrumental Techniques

UNIT I Spectral Methods I **15**

1.1 Surface Analytical Techniques: Preparation of the surface, difficulties involved in the surface analysis. (1L)

1.2 Principle, instrumentation and applications of the following:

a. Secondary Ion mass spectroscopy. (4L)
b. Particle-Induced X-Ray Emission (5L)
c. Low-Energy Ion Scattering and Rutherford Backscattering (5L)

UNIT II Spectral Methods – II **15**

Principle, Instrumentation, and Applications of

2.1 Electron Spin Resonance Spectroscopy (ESR) (5L)
2.2 Mossbauer's Spectroscopy (5L)
2.3 Atomic Emission Spectroscopy- based on plasma and electrical discharge sources (5L)

UNIT III Electroanalytical Methods **15**

Advanced Electroanalytical Techniques:-

3.1 Current Sampled (TAST) Polarography, Normal and Differential Pulse Polarography (3L)
3.2 Potential Sweep methods- Linear Sweep Voltammetry and Cyclic voltammetry. (3L)
3.3 Potential Step method- Chronoamperomertry (2L)
3.4 Controlled potential technique- Chronopotentiometry (2L)
3.5 Stripping Voltammetry- anodic, cathodic, and adsorption (2L)
3. 6 Chemically and electrolytically modified electrodes and ultramicroelectrodes in voltammetry (3L)

UNIT IV Miscellaneous Techniques **15**

Principle, Instrumentation and Applications of:

4.1 Chemiluminesescence techniques (3L)
4.2 Chirooptical Methods : ORD, CD (5L)
4.3 Photoacoustic spectroscopy (3L)
4.4 Spectroelectrochemistry (4L)

List of books and references:

1. Analytical Chemistry, G. D. Christian, 4thEd. John Wiley, New York (1986)
2. Fundamentals of Analytical Chemistry, D .A. Skoog and D. M. West and F. J. HollerHolt- Saunders 6th Edition (1992)

3. Principles of Instrumental Analysis, D. A. Skoog, F. J. Holler and J.A. Niemann,5th Edition (1998)
4. Instrumental Methods of Analysis, H. H. Willard, L. L. Merritt, Jr. J. A. Dean and F.A. Settle Jr 6th Ed CBS (1986)
5. Instrumental Methods of Analysis, H. H. Willard, L. L. Merritt Jr, J. A. Dean and F. A.Settle Jr 7th Ed CBS (1986)
6. Introduction to Instrumental Analysis, R. D. Braun, Mc Graw Hill (1987)
7. Electrochemical Methods, A. J. Bard and L.R. Faulkner, John Wiley, New York,(1980)
8. Electroanalytical Chemistry, J.J . Lingane, 2nd Ed Interscience, New York (1958)
9. Modern Polarographic Methods in Analytical Chemistry, A. M. Bond, Marcel Dekker,New York, 1980.
10. Electroanalytical Chemistry, Ed A. J. Bard and Marcel Dekker, New York, (A series of volumes)
11. Techniques and mechanism of electrochemistry, P. A. Christian and A. Hamnett, Blachie Academic and Professional (1994)
12. Wilson and Wilson's Comprehensive Analytical Chemistry, Ed. G. Svehla. (A series of Volumes)
13. Treatise on Analytical Chemistry, Eds. I. M. Kolthoff and Others, Interscience Pub. (A series of volumes).
14. Standard Methods of Chemical Analysis, Eds. F. J. Welcher, Robert E. Krieger Publishing Company, (A series of volumes)
15. Polarographic Methods in Analytical Chemistry, M. G. Arora, Anmol Publications Pvt Ltd
16 Surface Analysis –The Principal Techniques, 2nd Edition Edited by John C. Vickerman and Ian S. Gilmore 009 John Wiley & Sons, Ltd. ISBN: 978-0-470-01763-0
17. NMR, NQR, EPR, and Mössbauer Spectroscopy in Inorganic Chemistry *R. V. Parish*. Ellis Horwood, Chichester

SEMESTER – III

RJSPGCHEA303

Bioanalytical Chemistry and Food Analysis

UNIT I Bioanalytical chemistry **15**

1.1 Body Fluids

1.1.1 Composition of body fluids and detection of abnormal levels of glucose, creatinine, uric acid in blood, protein, ketone bodies and bilirubin in urine leading to diagnosis of diseases. (5L)

1.1.2 Physiological and nutritional significance of vitamins (water soluble and fat soluble) and minerals.(5L)

1.1.3 Analytical techniques (including microbiological techniques) for vitamins. (5L)

UNIT II Immunological Methods **15**

2.1 General processes of immune response, antigen-antibody reactions, precipitation reactions, radio, enzyme and fluoro-immuno assays. (8L)

2.2 Human Nutrition: Biological values and estimation of enzymes, carbohydrates, proteins, essential amino acids and lipids. (7L)

UNIT III Food Analysis - I **15**

3.1 Fuel value of food and importance of food nutrients (2L)

3.2 Food Additives – General idea about Food processing and preservation, Chemical preservatives, fortifying agents, emulsifiers, texturizing agents, flavours, colours, artificial sweeteners, enzymes. Analysis of food products for flavoring agents and colour. (5L)

3.3 Food Contaminants– Trace metals and pesticide residues, contaminants from industrial wastes (polychlorinated polyphenols, dioxins), toxicants formed during food processing (aromatic hydrocarbons, nitrosamines), veterinary drug residues and melamine contaminants. (8L)

UNIT IV Food Analysis - II **15**

4.1 4.1.1 Food packaging – Introduction, types of packing materials, properties and industrial requirements. (2L)

4.1. 2 Processing and Quality requirements of Milk and milk products (cheese, butter and ice cream), vegetables and fruits, meat and meat products. (6L)

4.2 Analysis of Milk – Fat content, proteins, acidity, bacteriological quality and milk adulterants. (2L)

4.3 Analysis of Oils and Fats – acid value, sap value, iodine value. Determination of rancidity and antioxidants. (2L)

4.4 Analysis of spices (cloves, cinnamon, pepper, mustard) Determination of volatile oils and fixed oils.(3L)

List of books and References:

1. General, organic and biological chemistry, H. Stephen Stoker, Cengage Learning.
2. Advance dairy chemistry, vol 3, P. F. Fox, P. L. H. McSweeney Springer.
3. Physiological fluid dynamics vol 3, Nanjanagud Venkatanarayanasastry Chandrasekhara Swamy Narosa Pub. House, 1992
4. Molecular Biological and Immunological Techniques and Applications for food, edited by Bert Popping, Carmen Diaz-Amigo, Katrin Hoenicke, John Wiley & sons.
5. Food Analysis: Theory and practice, Yeshajahu Pomeranz, Clifton E. Meloan, Springer.
6. Principles of package development, Gribbin et al
7. Modern packaging Encyclopedia and planning guide, Macgra Wreyco.
8. Food Analysis, Edited by S. Suzanne Nielsen, Springer
9. Analytical Biochemistry, D, J. Homes and H. Peck, Longman (1983)
10. Bioanalytical Chemistry, S. R. Mikkelesen and E. Corton, John Wiley and sons 2004 Analysis of food and beverages, George Charalanbous, Accademic press 1978

SEMESTER-III

RJSPGCHEA304

Environmental and Certain Industrially Important Matrials

UNIT I Air Pollution **15**

1.1 Sources, classification, pollutants and permissible limits. (2L)

1.2 Sampling methods for air, flew gas, Industrial Exhaust, stag samples etc. (2L)

1.3 Importance of automobile exhaust control and its limits (2L)

1.4 Sampling and analysis of: Particulate matter, aerosols, ammonia and organic vapors. (3L)

1.5 Carbon credit and global issues related to air pollution. (3L)

1.6 Greenhouse gases and their substitutes. (1L)

1.7 Environmental Legislation: role of pollution control boards, article 48A and 51A, Motor Vehicle Act and method of analysis with respect to PUC. (2L)

UNIT II Water Quality Standards **15**

2.1 Water: quality and requirements of potable water, direct and indirect pollutants for potable water reservoirs, quality of potable water from natural sources. (6L)

2.2 Bore well water quality and analytical parameters. Quality of bottled mineral water (3L)

2.3 Process of purification of bore well water to bottled mineral water. (2L)

2.4 Regulatory requirements for packaged drinking water (4L)

UNIT III Other Types Of Pollution **15**

3.1 Soil pollution and Soil Analysis : sources of soil pollution and their control, sampling of soil, determination of water holding capacity, determination total nitrogen, ammonia and nitrates, fertility of soil and effect of pollution on it, synthetic fertilizers and their long term effect on soil quality. (6L)

3.2 Noise Pollution : sources, effects, methods of measurements and control measures. (2L)

3.3 Thermal Pollution: definition, source, impact, control measures, working of cooling towers and cooling ponds, involved economy. (3L)

3.4 Radioactive pollutants: source, exposure hazards, precautions in handling and safety, Long term effects. (2L)

3.5 Environmental Audits: concept of audit, authorities, evaluation methodology, benefits and certification (2L)

UNIT IV Industrial Materials **15**

4.1 Insecticides, Pesticides: definition, classification of insecticides pesticides. Biodegradation of insecticides and pesticides (5L)

4.2 Soaps and Detergents: classification and composition, qualitative analysis, quantitative analysis of detergents- alkalinity, active ingredients and oxygen releasing capacity. Biodegradable detergents (5L)

4.3 Petrochemical products: crude oils, fuels, and calorific values, fractional distillation process and fractions, properties of fuel, composition of fuel, flashpoint, fire point, corrosion test, carbon residue and impact on environment. (5L)

List of Books and References:

1. Environmental Chemistry, A. K. De, 2nd ED. Wiley (1989).
2. Environmental Pollution Analysis, S. M. Khopkar, John Wiely (1993).
3. Air Pollution Sampling And Analysis, Sharad Gokhale, IIT Guwahati, May 2009.
4. Environmental Pollution Analysis, S. M. Khopkar, New Age International publication(2011).
5. Water And Water Pollution (hand book) Ed., Seonard'l Ciacere, Vol I to IV, MarcelDekker inc.N.York(1972)
6. Water pollution, Arvind kumar, APH publishing (2004)
7. Introduction to Potable Water Treatment Processes Simon Parsons, Bruce Jefferson, Paper back publication.
8. Guidelines for drinking-water quality, Third edition, (incorporating first and second addenda). WHO report.
9. Soil pollution, S.G. Misra and Dinesh Mani, APH Publishing Corporation, (2009).
10. Soil Pollution: origin, monitoring and remediation, Abrahim Mirsal, Springer (2010).
11. Noise Pollution, Donald F Anthrop, Lexington Books, (1973)
12. Noise Effects Handbook: A Desk Reference to Health and Welfare Effects of Noise (1981) Available at NCL laboratories e- Library.
13. Chemistry, Emission Control, Radioactive Pollution and Indoor Air Quality Edited by Nicolas Mazzeo, InTech Publications (2011).
14. Environmental Protection Against Radioactive Pollution: N. Birsen, Kairat K. Kadyrzhanov, Springer publication , (2003).
15. Environmental law in India, Mohammad Naseem, Wolters Kluwer.
16. Environmental Protection, Law And Policy In *India* Kailash Thakur google books (1997).

17. Green chemistry An Introductory text, Mzike Lancaster, Royal Society of Chemistry (2002)
18. Pesticide Analysis Ed K. G. Das, Dekker (1981)
19. Analytical, Agricultural Chemistry S. L Chpra J.S Kanwar Kalyani publication
20. Soil and plant Analysis C.S Piper, Hans Publication

SEMESTER – III

RJSPGCHEA304

Pharmaceutical and Organic Analysis

UNIT I Pharmaceutical Analysis **15**

1.1 General idea regarding the Pharmaceutical Industry, definition and classification of drugs, introduction to pharmaceutical formulations, classification of dosage forms.Role of FDA in pharmaceutical industries. (7L)

1.2 Sources of impurities in pharmaceutical products and raw materials. (4L)

1.3 Standardization of finished products and their characteristics, officialmethods of quality control. (4L)

UNIT II Drugs **15**

2.1 Analysis of compounds based on functional groups, instrumental methods for analysis of drugs, assays involving chromatographic separations, proximate assays, assays of enzyme containing substances, biological and microbiological assays and tests. (8L)

2.2 Limit tests, solubility tests, disintegration tests, stability studies, impurity profile of drugs, bioequivalence and bioavailability studies.Polymers in pharmaceuticals and novel drug delivery systems. (7L)

UNIT III Forensic Science **15**

3.1 Analytical Chemistry in Forensic Science: General idea. (2L)

3.2 Forensic Analysis: Blood, DNA profiling, Hair analysis, Alcohol in body fluids, systematic drug identification. (5L)

3.3 Analytical Toxicology: Isolation, identification and determination of:

3.3.1 Narcotics: Heroin, morphine and cocaine.

3.3.2 Stimulants: Amphetamines and caffeine.

3.3.3 Depressants: Benzodiazepines, Barbiturates and Mandrax.

3.3.4 Hallucinogens: LSD and Cannabis.

3.3.5 Metabolites of drugs in blood and urine of addicts.

3.3.6 Viscera, stomach wash, vomit and postmortem blood for poisons like– cyanide, arsenic, mercury, insecticides and pesticides. (8L)

UNIT IV Cosmetic Analysis **15**

4.1 Cosmetics: Introduction. Evaluation of cosmetic materials, raw materials and additives. Formulation, standards and methods of analysis. (2L)

4.2 Deodorants and antiperspirants: Al, Zn, Boric acid, chlorides, sulphates, hexachlorophene, methanamine, phenolsulphonates and urea. (3L)

4.3 Face powder: Fats, fatty acids, boric acid, barium sulphate, Ca, Mg, Ti, Fe, oxides of Ti, Fe and Al (total). (3L)

4.4 Hair tonic: 2,5-diaminotoluene, potassium borates, sodium perborate, pyrogallol, resorcinol, salicylic acid, dithioglycollic acid (in permanent wavers) (3L)

4.5 Creams and Lotions: Types of emulsions, chloroform soluble materials, glycerol, pH emulsion, ash

analysis, nonvolatile matter (IR spectroscopy) (2L)

4.6 Lipsticks: General analysis, determination of - nonvolatile matter, lakes and fillers, trichloroethylene-acetone soluble contents. (2L)

References

1) Analytical Biochemistry, David J Holmes and Hazel Peck, Longman, 1983.
2) Bioanalytical Chemistry, Susan R Mikkelesen and Eduardo Cotton, John Wiley and Sons, 2004.
3) Analysis of food and beverages, George Charalanbous, Academic press, 1978.
4) Harry's Cosmetology, 7th Ed, Longman Scientific Co.
5) Formulation and Function of Cosmetics, Joseph Stefan Jellinek, Wiley Interscience, 1971.
6) Cosmetic Technology, Edward Sagarin, Interscience Publishers, 1957.
7) Modern Cosmetics, Edgar George Thommsen, Francis Chilson, Drug and Cosmetic Industry, 1947.
8) Encyclopedia of Industrial Chemical Analysis, Foster Dee Snell et al, Interscience Publishers, 1967.
9) Government of India Publications of Food, Drug and Cosmetic Act and Rules.
10) The Handbook of Drug Laws, M L Mehra, University Book Agency, Ahmedabad, 1997.
11) Chemical Analysis of Drugs, Takeru Higuchi, Interscience Publishers, 1995.
12) Text book of Pharmaceutical Analysis, Kenneth Antonio Connors, Wiley, 2001.
13) Food Processing and Preservation, B Sivasankar, Prentice - Hall of India Private Limited, 2007.
14) Food Additives, R M Pandey and S K Upadhyay, INTECH, Open Science/Open Minds.
15) Food Science, B Srilakshmi, New Age International (P) Ltd. Publishers, 2003.
16) Food Contaminants: Sources and Surveillance, Edited by C Creaser, R Purchase, Elseiver, 1991.
17) The Chemical Analysis of Food and Food Products, Morris B Jacobs.
18) FSSAI (Food Safety and Standards Authority of India) Manuals of Methods of Analysis of Foods (Oils and Fats, Milk and Milk Products, Food Additives), Ministry of Health and Family Welfare, Government of India.
19) Fundamentals of Urine and Body Fluid Analysis, Nancy A Brunzel, Elsevier health Sciences, 2013.
20) Lab Manual on Blood analysis and Medical Diagnostics, Dr Gayatri Prakash, S Chand and Company Ltd, New Delhi.
21) Manual of Medical Laboratory Techniques, S Ramakrishnan and K N Sulochana,Jaypee brothers Medical Publishers (P) Ltd, 2012.
22) Indian Pharmacopeia, Volume I and II.
23) Forensic Chemistry, Suzanne Bell, Pearson Prentice Hall Publication, 2006.
24) Forensic Chemistry, David E Newton, Infobase Publishing, 2007.
25) Encyclopedia of Analytical Chemistry, Volume 3, Academic Press, 1995.
26) AOAC Volume I and II.

SEMESTER-III
PRACTICALS
RJSPGCHEAPR301

Group – A:

1. Determination of the pK value of an indicator.
2. Determination of copper and bismuth in mixture by photometric titration.
3. Estimation of strong acid, weak acid and salt in the given mixture conductometrically.
4. Analysis of mixture of carbonate and bicarbonate (present in ppm range) using pHmetry.
5. Determination of copper by extractive photometry using diethyldithiocarbamate.

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Group – B:

1. Estimation of drugs by non aqueous titration: Pyridoxine hydrochloride, Sulphamethoxazole.
2. Determination of percentage purity of methylene blue indicator.
3. Estimation of cholesterol and Uric acid in the given sample of blood serum
4. Estimation of fluoride in a tooth paste.
5. Determination of silica by molybdenum blue method.

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Group–C:

1. Total reducing sugars before and after inversion in honey using: (a) Cole's Ferricyanide (b) Lane - Eynon method.
2. Analysis of lactose in milk
3. Estimation of Caffeine in tea
4. Estimation of Vitamin C in lemon Juice/squash by Dichlorophenol-indophenol method
5. Iodine value of oil / fat
6. Analysis of alcoholic beverages (Beer) for alcohol content by distillation followed by specific gravity method, acidity by titration, total residue by evaporation.

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Group – D:

1. To analyze Pyrolusite for: Fe by colorimetry and / or Mn by volumetry.
2. To analyze Magnelium for Mg by complexometry.
3. Analysis of Bauxite for Ti by colorimetry / Al by gravimetry / Fe (volumetry)
4. Analysis of water sample: Total hardness and salinity.
5. Analysis of water sample: Acidity and sulphate(Benzidine method).

NOTE:

1. The candidate is expected to submit a journal 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. Use of non-programmable calculator is allowed both at the theory and the practical examination.

SEMSTER-IV

RJSPGCHEA401

Quality in Analytical Chemistry

UNIT I Separation Science **15**

1.1 Membrane separation processes: operating principles and applications of microfiltration, ultra-filtration, reverse osmosis, dialysis and electro-dialysis. (8L)

1.2 Applications of Solvent extraction in Analytical Chemistryrecapitulation 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 (7L)

UNIT II Separation, Analysis and Standardization of Herbal based products. 15

2.1 Herbs as a raw material: Defination 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 materials,drying and processing of herbal raw material. (6L)

2.2 Extraction of herbal materials: Choice of solvent for extraction, methods used for extraction and principles involved in extraction. (3L)

2.3Standardization of herbal formulation and herbal extracts: Standardization of herbal extract as per WHO cGMP guidelines, Physical, Chemical,Spectral and toxilogical standardization,qualitative and quantitative esimations. (6L)

UNIT III Green Chemistry 15

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 (4L)

3.2 Organic solvents: environmentally benign solutions, solvent free systems, supercritical fluids (only introduction) Ionic liquids as catalysts and solvents (4L)

3.3 Emerging Green Technologies: photochemical reactions (advantages and challenges), examples. Chemistry using microwaves, sonochemistry and electrochemical synthesis. (4L)

3.4 Designing Greener Processes: Inherently Safer Designs (ISD), Process intensification (PI) in-process monitoring. (3L)

UNIT IV Advanced Techniques 15

4.1 Electrophoresis: introduction, factors affecting migration rate, supporting media (gel, paper, cellulose, acetate, starch, polyacrylamide, agarose, sephedax and thin layers) (2L)

4.2 Techniques of Electrophoresis: low and high voltage, sds-page, continuous electrophoresis, capillary electrophoresis, zone, gel, isoelectric focusing, isotaechophoresis and miceller electro kinetic capillary chromatography, instrumentation, detection and applications. (8L)

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). (5L)

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.

SEMESTER-IV

RJSPGCHEA402

Advanced Instrumental Techniques

UNIT I Spectral Methods III **15**

NMR Spectroscopy

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) (9L)

1.2 Radio waves in imaging- principle instrumentation and applications of MRI (3L)

1.3 Application of NMR to other nuclei C^{13}, P^{31} and F^{19} spectroscopy (3L)

UNIT-II Spectral Methods IV **15**

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 (9L)

2.2 Raman spectroscopy: Principle Theory Instrumentation , techniques(SERS and Resonance Raman) and Applications of Raman spectroscopy (6L)

UNIT III Radiochemical And Thermal Methods **15**

3.1 Activation analysis- NAA ,radiometric titrations and radio-release methods (7L)

3.2 Thermal analysis- Principle, Interfacing , instrumentation and Applications of (a) Simultaneous Thermal Analysis- TG-DTA and TG-DSC (b) Evolved gas analysis- TG-MS and TG-FTIR (8L)

UNIT IV Hyphenated Techniques **15**

4.1 concept of hyphenation, need for hyphenation, possible hyphenations. (2L)

4.2 Interfacing devices and applications of GC – MS, ICP -MS, GC - IR, Tandem Mass Spectrometry, LC – MS: HPLC-MS, CE-MS. (13L)

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

SEMESTER – IV

RJSPGCHEA403

Selected Topics in Analytical Chemistry

UNIT I Effluent Treatment **15**

1.1 Effluent treatment plant general construction and process flow charts (3L)
1.2 Treatment and disposal of Sewage. (3L)
1.3. Effluent parameters for metallurgical industry. (2L)
1.4 Permissible limits for metal (example Cr, As, Pb, Cd etc) traces in the effluent. (2L)
1.5 Recovery of metals from effluent, modern methods – Electrodialysis, Electrodeposition and Ion Exchange etc. (3L)
1.6 Recycle and reuse of process and treated (effluent) water (2L)

UNIT – II Solid Waste Management **15**

2.1 Solid waste management: objectives, concept of recycle, reuse and recovery (3L)
2.2 Methods of solid waste disposal. (2L)
2.3 Treatment and disposal of sludge / dry cake (3L)
2.4 Managing non-decomposable solid wastes (2L)
2.5 Bio- medical waste : Introduction , Classification and methods of disposal (5L)

UNIT – III Plastics and Polymers **15**

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. (5L)
3.2 Metallic impurities in plastic and their determination, (2L)
3.3 Impact of plastic on environment as pollutant. (2L)
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. (3L)
3.5 Role of Organo silicones in paints and their impact on environment. (3L)

UNIT – IV: Metallurgy **15**

4.1 Ores and minerals: Dressing of ores, pollution due to metallurgical processes (ore dressing, calcination, smelting) (3L)
4.2 Chemical analysis of ores for principal constituents : Galena, Pyrolusite, Bauxite, Hematite, Monazite

(4L)

4.3 Alloys: definition, analysis of Cupronickel, Magnelium, Steel And Stainless Steel, Bronze, Gun metal. (4L)

4.4 Techniques of purification: Zone refining, analysis of high purity materials like s i l i c o n , vacuum fusion and extraction techniques. (4L)

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).**

SEMESTER – IV

RJSPGCHEA404

(INTELLECTUAL PROPERTY RIGHTS & CHEMINFORMATICS)

Unit 1: **[15L]**

Introduction to Intellectual Property: **[2L]**

Historical Perspective, Different types of IP, Importance of protecting IP.

Patents: **[5L]**

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.

Industrial Designs: **[2L]**

Definition, How to obtain, features, International design registration.

Copyrights: **[2L]**

Introduction, How to obtain, Differences from Patents.

Trade Marks: **[2L]**

Introduction, How to obtain, Different types of marks – Collective marks, certification marks, service marks, trade names etc.

Geographical Indications: **[2L]**

Definition, rules for registration, prevention of illegal exploitation, importance to India.

Unit 2: **[15L]**

Trade Secrets: **[2L]**

Introduction and Historical Perspectives, Scope of Protection, Risks involved and legal aspects of Trade Secret Protection.

IP Infringement issue and enforcement: **[2L]**

Role of Judiciary, Role of law enforcement agencies – Police, Customs etc.

Economic Value of Intellectual Property: **[5L]**

Intangible assests and their valuation, Intellectual Property in the Indian context – Various Laws in India Licensing and Technology transfer.

Different International agreements: **[6L]**

(a) World Trade Organization (WTO): [5L]

(i) General Agreement on Tariffs and Trade (GATT), Trade Related Intellectual Property Rights (TRIPS) agreement

(ii) General Agreement on Trade Related Services (GATS) Madrid Protocol.

(iii) Berne Convention

(iv) Budapest Treaty

(b) Paris Convention [6L]

WIPO and **TRIPS, IPR** and Plant Breeders Rights, IPR and Biodiversity.

Unit III: **[15L]**

Introduction to Cheminformatics: **[5L]**

History and evolution of cheminformatics, Use of Cheminformatics, Prospects of cheminformatics, Molecular modeling and structure elucidation.

Representation of molecules and chemical reactions: **[5L]**

Nomenclature, Different types of notations, SMILES coding, Matrix representations, Structure of Molfiles and Sdfiles, Libraries and toolkits, Different electronic effects, Reaction classification.

Searching Chemical Structures: **[5L]**

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: **[15L]**

Applications:

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, Ligandbased and Structure based Drug design, Application of Cheminformatics in Drug Design.

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.

SEMESTER – IV

RJSPGCHEA404

RESEARCH METHODOLOGY

Unit 1: **[15L]**

Print: **[5L]**

Primary, Secondary and Tertiary sources.

Journals:

Journal abbreviations, abstracts, current titles, reviews, monographs, dictionaries, text-books, current contents, Introduction to Chemical Abstracts and Beilstein, Subject Index, Substance Index, Author Index, Formula Index, and other Indices with examples.

Digital: **[5L]**

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.

Information Technology and Library Resources: **[5L]**

The Internet and World wide web, Internet resources for Chemistry, finding and citing published information.

Unit II: DATA ANALYSIS **[15L]**

The Investigative Approach:

Making and recording Measurements, SI units and their use, Scientific methods and design of experiments.

Analysis and Presentation of Data:

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.

Unit III: METHODS OF SCIENTIFIC RESEARCH AND WRITING SCIENTIFIC PAPERS [15L]

Reporting practical and project work, Writing literature surveys and reviews, organizing a poster display, giving an oral presentation.

Writing Scientific Papers:

Justification for scientific contributions, bibliography, description of methods, conclusions, the need for illustration, style, publications of scientific work, writing ethics, avoiding plagiarism.

Unit IV: CHEMICAL SAFETY & ETHICAL HANDLING OF CHEMICALS **[15L]**

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.

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

Practical course

RJSPGCHEAPR401

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

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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

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Group – C:

1. Analysis of Calcium, Iron and phosphorous in milk.
2. Determination of SAP value of oil.
3. Estimation of Aldehyde in lemon grass oil / Cinnamon oil
4. Estimation of Glucose by Folin-Wu method
5. Analysis of water sample : Mn^{2+} by colorimetric method

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Group – D: Project Evaluation

NOTE:

3. The candidate is expected to submit a journal certified by the Head of the Department / institution at the time of the practical examination.
4. 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. Use of non-programmable calculator is allowed both at the theory and the practical examination.

M.Sc. (Analytical Chemistry) Semester – III & IV

Paper Pattern

Internal Exam

1. Class Test : 20 marks
2. Presentation : 20 marks

Paper Pattern for Semester End Examination

Maximum Mark: 60 Duration : 2Hrs

There will be 5 questions each of 12 marks.

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

The pattern for above questions is as follows:

- Each question will have five sub questions of 4 marks each.
- Learners have to attempt any 3 questions out of 5.

Q. 5 will have 8 sub questions of 3 marks each (2 questions will be from each unit).

Learners have to attempt any 4 questions out of 8.

Practical Exam

Practical exam will be of 50 marks.

- Experiment : 40 marks
- Journal : 5 marks
- Viva : 5 marks