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# S. P. MANDALI'S RAMNARAIN RUIA AUTONOMOUS COLLEGE



# Syllabus for SEMESTER III and IV Program: M.Sc. (RPSCHEI) Course: Inorganic Chemistry

Credit based semester and grading system with effect from the academic year 2022-2023

	Μ	I.SC. SEMESTER III INORGANIC CHEMISTRY		
<b>Course Code</b>	Unit	Торіс	Credits	Lectures
	Ι	Descriptive Crystal Chemistry		15
RPSCHEI301	II	Imperfection in crystals and Non Stoichiometry	4	15
KFSCHEI501	III	Methods of Preparations	4	15
	IV	Behavior of Inorganic Solids		15
	Ι	Spectral Methods		15
	II	Hyphenated Techniques	_	15
RPSCHEI302	III	Radiochemical and Thermal Methods	4	15
	IV	Electroanalytical Methods		15
	Ι	Bioinorganic Chemistry		15
	II	Reactivity of Chemical Species –I		15
RPSCHEI303	III	Reactivity of Chemical Species –II	4	15
	IV	Synthesis, Structure, Bonding and Stereochemistry		15
	I	Manufacture and Applications of Inorganic Compounds		15
	I	Manufacture and Applications of morganic compounds Metallurgy		15
<b>RPSCHEIEC-I 304</b>	III	Inorganic Pharmaceuticals	4	15
			_	_
	IV	Environmental Monitoring and Assessment		15
	Ι	Advances in Nanomaterials		15
	II	Inorganic Materials		15
RPSCHEIEC-II 304	III	Nuclear Chemistry and Some Selected Topics	4	15
	IV	Safety in Chemistry Laboratories		15
RPSCHEI3P1				
RPSCHEI3P2	-	- · · ·		
RPSCHEI3P3	-	Practical	8	16
RPSCHEI3P4	-			

M.Sc. Semester IV Inorganic Chemistry				
Course Code	Unit	Торіс	Credits	Lectures
	Ι	Inorganic Materials Properties – I (Electrical and Thermal Properties)		15
RPSCHEI401	II	Inorganic Materials Properties – II (Magnetic and Optical Properties)	4	15
	III	Diffraction Methods		15
	IV	Molecular Spectroscopy		15
	Ι	Clusters and The Isolobal Analogy		15
RPSCHEI402	II	Applications of Organometallic Chemistry to Organic Synthesis	4	15
	III	Inorganic Cluster and Cage compounds		15
	IV	Inorganic – Rings – Chains –Polymer		15
	Ι	Symmetry in Chemistry		15
	II	N.M.R. Spectroscopy	. 4	15
RPSCHEI403	III	ESR and Mossbauer Spectroscopy		15
	IV	Catalysis		15
	Ι	Intellectual Property - I		15
	II	Intellectual Property - II		15
RPSCHEIOC-I 404	III	Cheminformatics – I	4	15
	IV	Cheminformatics – II		15
	Ŧ			1.7
	I	Review of Literature		15
	II	Data Analysis		15
RPSCHEIOC-II 404	III	Methods of Scientific Research And Writing Scientific Papers	4	15
	IV	Chemical Safety & Ethical Handling Of Chemicals		15
RPSCHEI4P1				
RPSCHEI4P2				
RPSCHEI4P2 RPSCHEI4P3		Practical		16
RPSCHEI4P4				

#### SEMESTER – III

#### **RPSCHEI301**

#### Credits 4

#### PAPER – I SOLID STATE CHEMISTRY

#### **Course Objectives:**

- Initially, the learner is introduced to structures of some compounds of the type AB, AB<sub>2</sub>, AB<sub>3</sub> along with oxides ABO<sub>3</sub> and AB<sub>2</sub>O<sub>4</sub> and how these polyhedra are linked through corner, edge or face is discussed.
- Hereafter, the difference between the perfect and imperfect crystals and the Classification of proposed schemes for defects and importance of thermodynamics in the formation of defects is brought to the notice of the learner.
- Along with the above concepts, the learner understands the methods of synthesis of inorganic materials with special emphasis of growing of single crystals from different phases of matters, thin film preparation and solid solutions.
- Last but not the least, the most important feature of this paper is to study the diffusion by measuring the concentration of the atoms at different distances from the release point after a given time has elapsed. In this unit, attention is confined to diffusion when the concentration of the diffusing species is very small, so that concentration effects are not important, or where the diffusion coefficient does not depend on concentration or position. This is equivalent to stipulating that the diffusion coefficient is a constant.

## **Course Outcomes:**

- Predict the structures of some known type of compounds based on their stoichiometry like AB, AB<sub>2</sub> etc.
- Classify the oxides based on structure whether inverse, normal or random and how the polyhedra forms by sharing its corner, edge or face.
- Have a clear distinction between Perfect and imperfect crystals and how these defects lead to change the properties of solids.
- Be well versed with the methods available to synthesize the inorganic solids based on the compositions.
- Identify the importance of Single Crystal and its method of preparation.
- Understand the behavior studies of solids using diffusion as property. Applications of Liquid Crystals.

	PAPER – I SOLID STATE CHEMISTRY					
Unit	Topics Description Constal Chamister	Lecture				
Ι	Descriptive Crystal Chemistry 1.1 Simple structures:	(15)				
	Structures of <b>AB</b> type compounds (PbO and CuO), <b>AB</b> <sub>2</sub> type ( $\beta$ cristobalite, CaC <sub>2</sub> and Cs <sub>2</sub> O),					
	A <sub>2</sub> B <sub>3</sub> type (Cr <sub>2</sub> O <sub>3</sub> and Bi <sub>2</sub> O <sub>3</sub> ), AB <sub>3</sub> (ReO <sub>3</sub> , Li <sub>3</sub> N), ABO <sub>3</sub> type, relation between ReO <sub>3</sub> and					
	perovskite $BaTiO_3$ and its polymorphmic forms, Oxide bronzes, Ilmenite structure,					
	AB <sub>2</sub> O <sub>4</sub> type, normal, inverse, and random spinel Structures.					
	1.2 Linked Polyhedra:					
	1.2.1 Corner sharing: tetrahedral structure (Silicates) and octahedral structure (ReO <sub>3</sub> ) and					
	rotation of $ReO_3$ resulting in VF <sub>3</sub> , $RhF_3$ and calcite type structures.					
	1.2.2 Edge sharing: tetrahedral structures (SiS <sub>2</sub> ) and octahedral structures (BiI <sub>3</sub> and AlCl <sub>3</sub> ).					
	pyrochlores, octahedral tunnel structures and lamellar structures.					
II	Imperfection in crystals and Non- Stoichiometry	(15)				
	<b>2.1 Point defects</b> : 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, colourcentres.					
	2.2 Line defects: Edge and Screw Dislocations. Mechanical Properties and Reactivity of Solids.					
	2.3 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.					
III	Methods of Preparations	(15)				
	3.1 Methods of Synthesis: Chemical Method, High Pressure Method, Arc Technique and					
	Skull Method (with examples).					
	3.2 Different methods for single crystal growth:					
	3.2.1 Crystal Growth from Melt: Bridgman and Stockbargar, Czochralski and					
	Vernuilmethods.					
	3.2.2 Crystal growth from liquid solution: Flux growth and temperature gradient methods					
	3.2.3 Crystal growth from vapor phase: Epitaxial growth methods.					
	<b>3.3 Thin film preparation</b> : Physical and Chemical methods.					
	<b>3.4 Solid Solutions:</b> Formation of Substitutional, Interstitial and Complex Solid Solutions;					
	Mechanistic Approach; Study of Solid solutions by X-ray Powder Diffraction and Density					
	Meenansite Approach, Study of Solid Solutions by A-ray Fowder Diffraction and Delisity					

	Measurement.			
IV	Behavior of Inorganic Solids	(15)		
	4.1 Diffusion in Solids: Fick's Laws of Diffusion; Kirkendal Effect; Wagner mechanism,			
	Diffusion and Ionic Conductivity; Applications of Diffusion in Carburizing and non-			
	Carburizing Processes in Steel Making.			
	4.2 Solid state reactions: General principles and factors influencing reactions of solids,			
	Reactivity of solids.			
	4.3 Liquid Crystals: Introduction and classification of thermotropic liquid crystals,			
	Polymorphism in liquid crystal, Properties and applications of liquid crystals.			

- A.F. Wells, Structural Inorganic Chemistry, 4<sup>th</sup> Edition, Clarendon Press-Oxford University Press, 1975.
- Ulrich Muller, Inorganic Structural Chemistry, 2<sup>nd</sup> Edition, John Wiley & Sons Ltd, 2006.
- Anthony R. West, Solid State Chemistry and its Applications, Student Edition, 2<sup>nd</sup> Edition, John Wiley & Sons Ltd, 2014.
- Lesley E. Smart, Elaine A. Moore, Solid State Chemistry Introduction, 3<sup>rd</sup> Edition, Taylor & Francis Group, LLC, 2005.
- Richard J. D. Tilley, Understanding Solids: the Science of Materials, John Wiley & Sons Ltd, 2004.
- 6. Richard J. D. Tilley, Crystals and CrystalStructures, John Wiley & Sons Ltd, 2006.
- William D. Callister, David G. Rethwisch, Materials Science and Engineering An Introduction, John Wiley & Sons Ltd, 2014.

#### SEMESTER – III

#### **RPSCHEI302**

#### Credits 4

#### PAPER – II ADVANCED INSTRUMENTAL TECHNIQUES

#### **Course Objectives:**

- The learner should know the recent developments in this fields which will enable them to attain industrial readiness.
- The learner is introduced to the surface analytical techniques, electron spectroscopy and NQR is introduced in the first unit.
- The second unit aims at introducing the learner to the hyphenated techniques which will basically bridge the gap between the academic and industry.
- The third unit focuses on thermal methods and radiochemical methods.
- The fourth unit deals with electroanalytical methods with special reference tovoltammetry. Voltammetry includes various types. As a whole this unit four encompasses the methods, instrumentation, various types of microelectrodes and their working.
- Apart from the general coverage, importance is given to the study of organic systems by electrochemical methods. Modern techniques used for chemical analysis and mechanistic studies are introduced so that real world analysis problems can be investigated.
- Focus will be on analytical applications of these techniques and utilizing the correct technique for solving specific analysis problems.

# **Course Outcome:**

After studying this course the students will be able to-

- Understand the basic working principles and applications of surface analytical techniques (such as SIMS,PIXE),electron spectroscopy and Nuclear quadrupole resonance.
- Understand the advantages of development of hyphenated techniques and the different types of interfaces that are used to achieve this hyphenation.
- Know the essential principles underlying the applications of thermal methods and radiochemical methods.
- Develop a working knowledge of various methods used in Voltammetry.
- Explain anodic, cathodic and adsorptive stripping methods in voltammetry.
- Select a suitable method of voltammetry for the analysis of a particular sample.

# PAPER - II ADVANCED INSTRUMENTAL TECHNIQUES

Unit	Topics	Lecture			
Ι	Spectral Methods	(15)			
	1.1. Surface Analytical Techniques: Preparation of the surface, difficulties involved in the				
	surface analysis.				
	<b>1.2.</b> Principle, instrumentation and applications of the following:				
	i) Secondary Ion mass spectroscopy ii) Particle-Induced X-Ray Emission.				
	<b>1.3.</b> Electron Spectroscopy: principles, instrumentation and applications of the following				
	ESCA (XPS), AUGER, UPS				
	1.4. Nuclear Quadrupole Resonance (NQR), ENDOR, ELDOR.				
II	Hyphenated Techniques	(15)			
	<b>2.1</b> Introduction, need for hyphenation, possible hyphenations.				
	2.2 Interfacing devices and applications of the following- GC-MS, GC-IR, MS-MS, Tandem				
	Mass Spectrometry, LC-MS HPLC-MS, ICP-MS, Spectro-electrochemistry and radio				
	chromatography.				
III	Radiochemical And Thermal Methods	(15)			
	<b>3.1</b> Enthalpimetric methods and thermometric titrations.				
	<b>3.2</b> Thermal analysis- Principle, Interfacing, instrumentation and Applications of Simultaneous				
	Thermal Analysis- TG-DTA and TG-DSC, Evolved gas analysis- TG-MS and TG-FTIR				
	3.3 Activation analysis- NAA, radiometric titrations and radio-release methods Radiometric				
	titrations and Applications				
	3.4 Auto, X-ray and Gamma Radiography				
IV	Electroanalytical Methods	(15)			
	<b>4.1</b> Current Sampled (TAST) Polarography, Normal and Differential Pulse Polarography,				
	Differential double Pulse Polarography				
	<b>4.2</b> Potential Sweep methods- Linear Sweep Voltammetry and Cyclic voltammetry.				
	4.2.1 Potential Step method- Chronoamperometry				
	4.2.2 Stripping Voltammetry- anodic, cathodic, and adsorption				
	4.2.3 Chemically and electrolytically modified electrodes and ultra- microelectrodes in				
	voltammetry				
	<b>4.3</b> Applications of electrochemical methods in Organic synthesis				

- D. A. Skoog, F. J. Holler and J.A. Niemann, Principles of Instrumental Analysis, 5<sup>th</sup> Edition, 2004.
- H. H. Willard, L. L. Merritt Jr., J. A. Dean and F. A. Settle Jr., Instrumental Methods of Analysis, 7<sup>th</sup>Edition, CBS 1986.
- 3. R. D. Braun, Introduction to Instrumental Analysis, McGraw Hill, 1987.
- 4. G. D. Christian, Analytical Chemistry, 4<sup>th</sup>Edition, John Wiley, New York, 1986.
- D. A. Skoog, D. M. West and F. J. Holler Holt- Saunders, Fundamentals of Analytical Chemistry, 6<sup>th</sup>Edition, 1992.
- 6. A. J. Bard and Marcel Dekker, Electroanalytical Chemistry, New York, (A series of volumes).
- 7. J.J. Lingane, Electroanalytical Chemistry, 2<sup>nd</sup> Edition, Interscience, New York, 1958.
- A. M. Bond, Marcel Dekker, Modern Polarographic Methods in Analytical Chemistry, New York, 1980.
- 9. KamlaZutski, Introduction to polarography and allied techniques, 2006.
- John C. Vickerman and Ian S. Gilmore, Surface Analysis The Principal Techniques, 2<sup>nd</sup> Edition, John Wiley & Sons, Ltd., 2009.

#### SEMESTER – III

#### **RPSCHEI303**

#### Credits 4

#### PAPER – III BIOINORGANIC AND COORDINATION CHEMISTRY

#### **Course Objectives:**

- The first objective of this paper is to teach the underlying principles of bioinorganic chemistry, introductory material followed by detailed discussions of specific bioinorganic chemistry topics.
- The second objective is to study the reactivity of Lewis acids and bases, classification based on the Frontier Molecular Orbital (FMO) method and determination of the strengthof oxoacids based on Pauling's rule.
- The third objective is to study the relative stabilities of different oxidation states in aqueous solution for individual elements. Parameters governing the potential and pHunder which species are stable in water are also studied.
- The fourth objective of is to enhance the learner's knowledge of thermodynamic and kinetic stabilities of complexes as an aid in devising methods for the synthesis of coordination compounds and/or understanding synthetic reactions.
- It further includes the bonding and stereochemistry of coordination compounds.

# **Course Outcome:**

- Know the importance of Iron, Zinc, Manganese and Nickel in different biological processes.
- Illustrate the reactivity of Lewis acids and bases and Classification based on Frontier Molecular Orbital concept.
- Know the different features of groups from 13-17 with respect to the acidity.
- Predict the strength, hardness and softness of acids and bases.
- Be well versed with the Latimer, Pourbaix and Frost diagrams.
- Know the different routes of synthesizing coordination complexes.
- Differentiating between sigma and pi bonding of coordination complexes and geometries of tetrahedral and octahedral.
- Rationalize the chiral and fluxional behavior of coordination complexes.

# PAPER – III BIOINORGANIC AND COORDINATION CHEMISTRY

Unit	Topics	Lecture		
Ι	Bioinorganic Chemistry	(15)		
	<b>1.1</b> Coordination geometry of the metal ion and functions.			
	1.2 Zn in biological systems: Carbonic anhydrase, protolytic enzymes, e.g. carboxy peptidase,			
	Zinc finger			
	<b>1.3</b> Role of metal ions in biological electron transfer processes: iron sulphur proteins,			
	1.4 Less common ions in biology e.g. Mn (arginase; structure and reactivity), Ni (urease;			
	structure and reactivity)			
	1.5 Biomineralization			
II	Reactivity of Chemical Species –I	(15)		
	2.1 Recapitulation of the definition of Lewis acids and bases,			
	2.2 Classification of Lewis acids and bases based on frontier Molecular orbital topology,			
	Reactivity matrix of Lewis acids and bases.			
	2.3 Group Characteristic of Lewis acids (Group -1, 13- 17).			
	<b>2.4</b> Pauling rules to determine the strength of oxoacids; classification and Structural anomalies.			
III	Reactivity of Chemical Species –II	(15)		
	<b>3.1</b> Pourbaix Diagrams.			
	3.1.1 Amphoteric behavior, Periodic trends in amphoteric properties of p-block and d-block			
	elements			
	3.1.2 Measures of hardness and Softness of Acids and Bases			
	3.1.3 Applications of acid-base Chemistry: Super acids and Super bases, heterogeneous			
	acid-base reactions.			
	3.1.4 Pauling and Drago-Wayland Equation			
	3.2 Latimer Diagrams			
	3.3 Frost diagrams			
IV	Synthesis, Structure, Bonding and Stereochemistry	(15)		
	4.1 Synthesis of Coordination Compounds			
	Addition Reactions, Substitution Reactions, Redox Reactions, Thermal Dissociation of Solid			
	Complexes, Reactions in Absence of Oxygen, Reactions of Coordination Compounds, Trans			
	Effect.			
	4.2 Structure and Bonding.			
	4.2.1 Molecular Orbital Theory for Complexes with Coordination Number 4 and 5 for the			
	central ion (sigma as well as Pi bonding)			

4.2.2 Angular Overlap Model for octahedral and tetrahedral complexes for sigma and pi bond.

#### 4.3 Stereochemistry of Coordination Compounds.

- 4.3.1 Chirality and Fluxionality of Coordination Compounds with Higher Coordination Numbers.
- 4.3.2 Geometries of Coordination compounds from Coordination number 6 to 9.

- Wolfgang Kaim, Brigitte Schwederski and Axel Klein, Bioinorganic Chemistry: Inorganic Elements in the Chemistry of Life, 2<sup>nd</sup> Edition, John Wiley & Sons Ltd, 2013.
- 2. Robert R. Crichton, Biological Inorganic Chemistry An Introduction, Elsevier, 2008.
- 3. Gary Wulfsberg, Inorganic Chemistry, Viva Books PA Ltd., New Delhi, 2002.
- 4. James E. House, Inorganic Chemistry, 2<sup>nd</sup> Edition, Elsevier, 2013.
- 5. W.W.Porterfield, Inorganic Chemistry-An Unified Approach, Academic press, 1993.
- D.F.Shriver, P.W.Atkins and C.H. Langford, Inorganic Chemistry, 3<sup>rd</sup>edition Oxford University Press, 1999.
- Asim K.Das, Fundamental Concepts of Inorganic Chemistry, (Volumes-I, II and III) CBS Publication, 2000.
- 8. F. Basolo and R. G. Pearson, Mechanisms of Inorganic Reactions, Wiley, New York, 1967.
- 9. J.D.Lee, Concise Inorganic Chemistry, 5<sup>th</sup>Edition, Blackwell Science Ltd., 2005.
- F. A. Cotton, G. Wilkinson, C. Murillo and M. Bochmann, Advanced Inorganic Chemistry, 6th ed., John Wiley, New York, 1999.
- Catherine E. Housecroft and Alan G. Sharpe, Inorganic Chemistry, 2<sup>nd</sup> Edition, Pearson Education Limited, 2005.

# S. P. MANDALI'S RAMNARAIN RUIA AUTONOMOUS COLLEGE M.SC. INORGANIC CHEMISTRY SEMESTER – III RPSCHEIEC - I 304 Credits 4

# PAPER – IV APPLIED CHEMISTRY I

#### **Course Objectives:**

- This paper highlights the manufacturing processes, economic relevance and applications of inorganic materials and or products withemphasis on the extraction, processing, recovery and recycling of some industrially important metals.
- Further, this course discusses the relevance of Inorganic chemistry in the arena of pharmaceuticals and also includes the supramolecular chemistry which is an interdisciplinary field of science covering the chemical, physical and biological features of molecular assemblies that are organized and held together by intermolecular interactions.
- Also, the course underlinesthe significance of Environmental Monitoring and Assessment, how data on each component are collected, what standards and regulations apply, how impacts are predicted, what mitigation measures can be used to minimize or eliminate impacts, what some of the limitations of these methods are, and where further information can be obtained. It also included the different acts comes under Environmental Agencies.

#### **Course Outcome:**

- Have a clear idea of the some important inorganic chemicals and materials and their application in day to day life.
- Understand how metals are extracted, recovered and recycled.
- Be well versed with the inorganic chemicals or materials used in pharmaceuticals.
- Understand the importance of environment monitoring and assessment.
- Have an idea about the different aspects of environmental legislation pertaining to ewaste, Forest Act and plastic manufacture.

# **PAPER – IV APPLIED CHEMISTRY I**

Unit	Topics	Lecture
I	Manufacture and Applications of Inorganic Compounds	(15)
	1.1 Ceramics and refractory materials	
	<b>1.2</b> Cement	
	<b>1.3</b> Fertilizers and micronutrients	
	1.4 Inorganic pesticides	
	1.5 Inorganic Pigments	
II	Metallurgy	(15)
	2.1 Occurrence, extraction and metallurgy of Zirconium, Hafnium, Niobium, Tantalum	
	Platinum and Palladium metals. Physical and chemical properties and applications of	
	these metals, compounds of these metals, alloys and their uses.	
	2.2 Recycling& recovery of metals with reference to Silver, Lead, Nickel and Chromium	
III	Inorganic Pharmaceuticals	(15)
	3.1 Radiopharmaceuticals containing Tc and Bi, contrast agents for X-ray and NMR	
	imaging. Gastrointestinal agent's viz. (i) antacids (aluminium hydroxide, milk of	
	magnesia, sodium bicarbonate and (ii) Cathartics(magnesium sulphate and sodium	
	phosphate). Topical agent's viz. (i) protective and adsorbents (talc, calamine), (ii)	
	antimicrobial agents(potassium permanganate, tincture iodine, boric acid) and	
	astringents (potash alum).	
	<b>3.2</b> Supramolecular chemistry	
IV	Environmental Monitoring and Assessment	(15)
	4.1 Environmental Monitoring:	
	Advantages of Environmental Monitoring, Deterioration of environmental quality with	
	reference to anthropogenic impact; Methods of assessment of environmental quality-	
	Short term studies/surveys, Rapid assessment, Continuous short and long term	
	monitoring.	
	4.2 Environmental Impact Assessment (EIA):	
	Need of EIA; Scope and objectives; Environmental Impact Assessment techniques-Ad-	
	hoc method, checklist method, overlay mapping method, simulation and modeling	
	technique, and system diagram technique; Merits and Demerits of EIA studies.	
	4.3 Objectives and Provisions of Acts and Rules:	
	Indian Forest Act 1927, Forest Conservation Act 1980, Environment (Protection) Act	
	1986, National Green Tribunal Act 2010, E-waste Management and Handling Rules	
	,	

- 1. Fathi Habashi, Handbook of Extractive Metallurgy, Volume I-IV, WILEY-VCH, 1997.
- Thomas W. Swaddle, Inorganic Chemistry- An Industrial and Environmental Perspective, Elsevier Science & Technology Books, 1997.
- 3. Karl Heinz Buchel, Hans-Heinrich Moretto and Peter Woditsch, Industrial Inorganic Chemistry, WILEY-VCH, 2000.
- Kent and Riegel, Handbook of Industrial Chemistry and Biotechnology, Volume I, Springer, 2007.
- Peter Morris and Riki Therivel, Methods of Environmental Impact Assessment, Routledge, Taylor & Francis Group,2009.
- Philippe Sands, Principles of International Environmental Law, Cambridge University Press, 2<sup>nd</sup> Edition, 2003.
- Gilbert M. Masters, Wandell P. Ela, Introduction to Environmental Engineering and Science, 3<sup>rd</sup> Edition, Pearson Education Limited, 2014.
- 8. Thomas F. P. Sullivan, Environmental Law Handbook, 22<sup>nd</sup> Edition, Bernan Press, 2014.
- 9. Indian Forest Act 1927, NGT Act 2010, Sales and Usage Rules 2011.

# S. P. MANDALI'S RAMNARAIN RUIA AUTONOMOUS COLLEGE M.SC. INORGANIC CHEMISTRY SEMESTER – III RPSCHEIEC - II 304 Credits 4 PAPER – IV APPLIED CHEMISTRY II

# **Course Objectives:**

- The primary objective of this paper is to highlight the different types of nano materials, preparation methods and applications of nano materials in various fields.
- The courseemphasizes on the classification, preparation and applications of fillers and fibers and it also includes the some industrially important chemicals, its application and manufacturing.
- It further envisages the discussion on nuclear chemistry with emphasis on separation of fission product from nuclear fuels. This also includes the introduction to Super Heavy elements, their discovery and preparation.
- The essentials such as laboratory safety, handling of hazardous chemicals and legislations associated with it have also been included in this course.

#### **CourseOutcome:**

- Know the nano materials and how they are synthesized.
- Have a clear idea of the some important inorganic chemicals and materials and their application in day to day life.
- Understand purification of nuclear waste from nuclear reactions.
- Be well versed with the super heavy elements and its importance in Chemistry
- Understand the importance of Safety in Chemical Lab
- Have an idea about the Environment Protection act.

# **PAPER – IV APPLIED CHEMISTRY II**

Unit	Topics	Lecture				
Ι	Advances in Nanomaterials	(15)				
	1.1 Types of nanomaterials, e.g. nanotubes, nanorods, solid spheres, core-shell					
	nanoparticles, mesoporous materials; General preparative methods for various					
	nanomaterials.					
	1.2 Some important properties of nanomaterials: optical properties of metal and					
	semiconductor nanoparticles, magnetic properties.					
	1.3 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.					
	1.4 Applications of nanomaterials in electronics, energy, automobiles, sports and toys,					
	textile, cosmetics, medicine, space and defense. Environmental effects of					
	nanotechnology					
II	Inorganic Materials	(15)				
	2.1 Classification, manufacture and applications;	~ ~ ~				
	2.1.1 Inorganic fibers					
	2.1.2 Inorganic fillers					
	2.1.3 Study of (i) Condensed phosphates, and (ii) Coordination polymers.					
	<b>2.2 Preparation, properties and uses of industrially important chemicals</b> – potassium					
	permanganate, sodium thiosulphate, bleaching powder, hydrogen peroxide, potassium					
	dichromate, Lime, Chlorine and Caustic soda.					
III	Nuclear Chemistry and Some Selected Topics	(15)				
	3.1 Nuclear Chemistry:	(10)				
	3.1.1 Introduction toof nuclear fuels and separation of fission products from spent fuel					
	rods by PUREX process.					
	3.1.2 Super heavy element:, discovery, preparation, position in the periodic table.					
	3.2 Some Selected Topics					
	3.2.1 Isopoly and Hetropoly acids,					
	3.2.2 Intercalation compounds					
	3.2.3 Inorganic explosives (mercury fulminate, Lead azide)					
	8					

IV		Safety in Chemistry Laboratories	(15)	
	<b>4.1</b> Goo	4.1 Good Laboratory Practices: Elements of Good Laboratory Practices; Standard		
	Ope	rating Procedures; Quality Assurance		
	<b>4.2</b> Han	dling of Hazardous Materials		
	4.2.1	Toxic Materials (Various types of toxins and their effects on humans)		
	4.2.2	Explosives and Inflammable Materials		
	4.2.3	Types of fire extinguishers		
	4.2.4	Bioactive materials.		
	4.3 Lega	al provisions regarding Chemical Laboratories.		
	<b>4.4</b> Envi	ironment Protection Act, 1986.		

- 1. Sulabha K. Kulkarni, Nanotechnology-Principles and Practices, Capital Publishing Co., 2007.
- 2. ThomasW. Swaddle, Inorganic Chemistry- An Industrial and Environmental Perspective, Elsevier Science & Technology Books, 1997.
- 3. Karl Heinz Buchel, Hans-Heinrich Moretto and Peter Woditsch, Industrial Inorganic Chemistry, WILEY-VCH, 2000.
- 4. Kent and Riegel, Handbook of Industrial Chemistry and Biotechnology, Volume I, Springer, 2007.
- Philippe Sands, Principles of International Environmental Law, Cambridge University Press, 2<sup>nd</sup> Edition, 2003.
- Gilbert M. Masters, Wandell P. Ela, Introduction to Environmental Engineering and Science, 3<sup>rd</sup> Edition, Pearson Education Limited, 2014.

#### **SEMESTER – III**

#### PRACTICAL

#### **RPSCHEI3P1:** Analysis of Alloys

- 1. Analysis of Brass alloy:
  - i) Cu content by iodometric method,
  - ii) Zn content by complexometric method.
- 2. Analysis of Magnelium alloy:
  - i) Al content by gravimetric method as basic succinate,
  - ii) Mg content by complexometric method.
- 3. Analysis of Bronze alloy:
  - i) Cu content by complexometric method,
  - ii) Sn content by gravimetric method.
- 4. Analysis of steel nickel alloy:Ni content by homogeneous precipitation method.

#### **RPSCHEI3P2:** Solvent Extraction

- 1. Separation of Co and Ni using n-butyl alcohol and estimation of Co
- 2. Separation of Mn and Fe using isoamyl alcohol and estimation of Mn
- 3. Separation of Cu and Fe using n-butyl acetate and estimation of Cu
- 4. Separation of Fe and Mo using isoamyl alcohol and estimation of Mo

#### **RPSCHEI3P3: Inorganic Preparations**

- 1. Preparation of V(oxinate)<sub>3</sub>
- 2. Preparation of  $Co(\alpha$ -nitroso- $\beta$ -naphthol)<sub>3</sub>
- 3. Preparation of Ni(salicylaldoxime)<sub>2</sub>
- 4. Hexaamine cobalt (III) chloride
- 5. Preparation of Trans-bis (glycinato) Cu(II)

#### **RPSCHEI3P4:** Analysis of the following Commercial 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 colorimetry by 1, 10-phenonthroline method.
- 4. Nycil powder for its Zn content complexometrically.

#### **References for Practical:**

- 1. G H Jeffery, J Bassett, J Mendhem, R C Denney, Vogel's Textbook Of Quantitative Chemical Analysis, 3<sup>rd</sup> Edition, Longman Scientific & Technical,1989.
- 2. R Gopalan, V Ramalingam, Concise Coordination Chemistry, Vikas Publishing House Pvt. Ltd. 200.
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#### SEMESTER – IV

#### **RPSCHEI401**

#### Credits 4

#### PAPER – I SOLID STATE CHEMISTRY AND MOLECULAR SPECTROSCOPY

#### **Course Objectives:**

- The primary objective of this paper is to study the electrical properties of inorganic solids with emphasis on Thomson and Seebeck effect which throw light on development ofelectric potential across a temperature gradient.
- The second objective is to study magnetic behavior of inorganic materials in presence and absence of applied magnetic fields.
- This also includes the structural and magnetic behavior of alloys, hardness and softness of magnets of different inorganic materials. The study of transition metal oxides and their applications in different electronic fields such as Bubble memory for data storage devices has been explored.
- The essential aspect of solid state chemistry is included for the learner to understand applications of XRD and gives a clear idea about instrumental methods like XRD and its different types.
- A thorough discussion on the basic principles and applications of Molecular spectroscopy at the advanced level supplements the objectives.

### **Course Outcome:**

- Understand the electrical properties of inorganic solids and how these materials can be used as superconductors.
- Learn the importance of inorganic materials in making batteries and sensors.
- Know how hopping model is used to describe carrier transport in a disordered semiconductor or in amorphous solid.
- Know transition metal oxides such as spinels, garnets and the strength of magnets
- Understand the thermal properties and optical behavior of inorganic solids.
- Know the different models available to understand optical properties of inorganic solids
- Elucidate the structure by powder diffraction and single crystal X-ray diffraction patterns.
- Understand different instrumental methods of structure determination by X-ray diffraction method and its different types like electron and neutron diffraction.
- Comprehend the general principles and theory of spectroscopy
- Grasp the specialties and applications of various types of spectroscopic methods.

# PAPER – I SOLID STATE CHEMISTRY AND SPECTROSCOPY

Unit	PAPER – I SOLID STATE CHEMISTRY AND SPECTROSCOPY Topics	Lecture		
Ι	Inorganic MaterialsProperties – I(Electrical and Thermal Properties)	(15)		
	1.1 Electrical properties of solids:Conductivity: Solid Electrolytes; Fast IonConductors;			
	Mechanism of Conductivity; Hopping Conduction.			
	1.2 Other Electrical Properties: Thomson and Seebeck Effects; Thermocouples and their			
	Applications; Hall Effect; Dielectric, Ferroelectric, Piezoelectric and PyrroelectricMaterials			
	and their Inter-relationships and Applications.			
	1.3 Thermal Properties: Introduction, Heat Capacity and its Temperature Dependence;			
	Thermal Expansion of Metals; Ceramics and Polymers and Thermal Stresses.			
II	Inorganic Materials Properties – II (Magnetic and Optical Properties)	(15)		
	2.1 Magnetic properties: Behaviour of substances in magnetic field, mechanism of			
	ferromagnetic and antiferromagnetic ordering, super exchange, Hysteresis, Hard and soft			
	magnets, structures and magnetic Properties of Metals and Alloys.			
	2.2 Transition metal Oxides: Spinels, garnets, Ilmenites, Perovskite and Magneto plumbites,			
	Application in transformer cores, information storage, magnetic bubble memory devices and			
	as permanent magnets.			
	2.3 Optical properties: Color Centers and Birefringence; Luminescent and Phosphor			
	Materials, Coordinate Model, Phosphor Model, Anti Stokes Phosphor; Ruby Laser and			
	Neodymium Laser			
III	Diffraction Methods	(15)		
	<b>3.1 X-Ray Diffraction:</b> Bragg Condition, Miller Indices, Laue Method, Bragg Method, Debye			
	Scherrer Method of X-Ray Structural Analysis of Crystals			
	<b>3.2 Electron Diffraction:</b> Scattering of electrons, Scattering Intensity versus Scattering Angle,			
	Weirl Measurement Technique and Elucidation of Structures of Simple gas Phase			
	Molecules.			
	3.3 Neutron Diffraction: Scattering of Neutrons: Scattering of neutrons by Solids and			
	Liquids, Magnetic Scattering, Measurement Technique.			
IV	Molecular Spectroscopy	(15)		
	4.1 Rotational spectroscopy: Einstein coefficients, classification of poly atomicMolecules			
	spherical top, symmetric top and asymmetric top molecules, rotationalSpectra of			
	polyatomic molecules Stark modulated microwave Spectrometer.			
	4.2 Infrared spectroscopy: Fundamental modes of vibrations, selection rules, IR absorption			
	bands of metal - donor atom, effect of complexation on the IR spectrum of ligands			
	1	l		

formations on the IR of ligands like NH<sub>3</sub>, CN-, CO, olefins (C=C) and C<sub>2</sub>O<sub>4</sub><sup>2-</sup>

- **4.3 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.
- 4.4 Ligand Field Theory: Electronic structures of free atoms and ions; Splitting of levels and terms in a chemical environment; Construction of energy level diagrams; Direct product ; Correlation diagrams for d<sup>2</sup> ions in octahedral and tetrahedral ligand field; Methods of Ascending and Descending Symmetry; Hole formalism.

- Anthony R. West, Solid State Chemistry and its Applications, Student Edition, 2<sup>nd</sup> Edition, John Wiley & Sons Ltd, 2014.
- Lesley E. Smart, Elaine A. Moore, Solid State Chemistry Introduction, 3<sup>rd</sup> Edition, Taylor & Francis Group, LLC, 2005.
- Richard J. D. Tilley, Understanding Solids: the Science of Materials, John Wiley & Sons Ltd, 2004.
- 4. Richard J. D. Tilley, Crystals and Crystal Structures, John Wiley & Sons Ltd, 2006.
- William D. Callister, Jr. and David G. Rethwisch, Materials Science and Engineering -An Introduction, John Wiley & Sons Ltd, 2014.
- Colin N. Banwell and Elaine M. McCash, Fundamentals of molecular spectroscopy, 4<sup>th</sup> Edition.
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- 8. H.S. Randhawa, Modern Molecular Spectroscopy, McMillan India Ltd., 2003
- R.S. Drago, Physical Methods for Chemists, 2<sup>nd</sup> Edition, Saunders College Publishing 1992.
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#### SEMESTER - IV

#### **RPSCHEI402**

#### Credits 4

#### PAPER – II ORGANOMETALLIC AND MAIN GROUP CHEMISTRY

#### **Course Objectives:**

- The basic objective of the course of organometallic chemistry will be explained in this course.
- This course aimsto study large clusters which have been researched upon with the objective of developing catalysts that may duplicate or improve upon the properties of previously known heterogeneous catalysts; the surface of a large cluster may in these cases mimic in some degree the behavior of the surface of a solid catalyst. This also includes the concept of isolability which shows similarities between organometallic chemistry and organic chemistry. Such similarities can be envisioned on a broader scale by considering frontier orbital of the isolobal molecular fragments of which organometallic compounds are composed.
- Further, the study of various industrial applications of organometallic compounds using as catalyst is brought about in this course. This course also throws light on appropriate pairing of palladium with suitable ligands and their applications in certain industrially important coupling reactions.
- The structure, bonding and classification of inorganic clusters and cage compounds is also discussed in detail in this course. Before considering organometallic clusters, we willfind it useful to examine the capacity of boron to form clusters. The types of orbital interactions involved in boron-based clusters will provide useful background to understand the types of interactions that occur in organometallic clusters containingtransition metals.
- Finally, fine aspects of some important main group elements compounds and polymers which find an application in day to day life are introduced to the learner.

# **Course Outcome:**

- Understand the Bonding, electron count of metal clusters
- Be well versed with the Synthesis of various palladium Coupling complexes and its properties along with applications.
- Know the Homogenous and heterogeneous catalytic applications of organometallic compounds in various industrial fields.
- Understand the Chemistry of cage and cluster compounds
- Explain the preparation methods and properties of silicates, inorganic polymers.

# PAPER – II ORGANOMETALLIC AND MAIN GROUP CHEMISTRY

Unit	Topics	Lecture
Ι	Clusters and The Isolobal Analogy	(15)
	1.1 Metal Cluster	
	1.1.1 Carbonyl Cluster	
	1.1.1.1 Low Nuclearity Carbonyl Cluster (LNCC)	
	1.1.1.2 High Nuclearity Carbonyl Cluster (HNCC)	
	1.1.1.3 Electron Counting for LNCC and HNCC	
	1.1.1.4 Capping Rules: Limitation and Exceptions	
	1.1.1.5 Synthesis and reactions of Metal Carbonyl clusters	
	1.1.1.6 Wade's Rule	
	1.2 Halide type Clusters	
	1.3 Total Valence Electron Counts in d-block organometallic clusters	
	1.4 Chevrel Phases	
	1.5 Zintl Ions	
	1.6 Concept of Isolobality and Isolobal Analogies	
II	Applications of Organometallic Chemistry to Organic Synthesis	(15)
	2.1 Alkene Metathesis	
	2.1.1 Synthesis of Grub's and Schrock Catalysts	
	2.1.2 Mechanism of Metathesis: Ring Opening Metathesis, Ring Closing Metathesis, Cross	
	Metathesis	
	2.2 Palladium Catalyzed C-C and C-N Cross Coupling Reactions	
	2.2.1 Discovery and Industrial application of Cross Coupling Reactions	
	2.2.2 The Heck Reaction	
	2.2.3 Suzuki-Miyaura Coupling	
	2.2.4 Sonogashira Coupling	
	2.2.5 Stille Coupling	
	2.2.6 Negishi Coupling	
	2.2.7 Buchwald-Hartwig C-N Cross Coupling	
	2.3 Methanol Carbonylation and Alkenes Oxidation: The Monsanto Process and The Wacker	
	Process	
	2.4 Fischer- Tropsch Synthesis, Hydrosilylation of Alkenes, Hydroformylation using Cobalt	
	Catalyst, Water gas Shifts Reaction, Carbonylation of Alcohol	
	, , , , , , , , , , , , , , , , , , ,	

III		Inorganic Cluster and Cage compounds	(15)		
	<b>3.1</b> Bora	anes			
	3.1.1	Introduction			
	3.1.2	Method for Classifying Structures			
	3.1.3	Wade's rules and its Origin			
	3.1.4	Structural correlations and Bonding			
	3.1.5	Synthesis of higher boranes			
	3.1.6	Characteristic reactions of boranes			
	<b>3.2</b> Cart	poranes			
	3.2.1	Introduction			
	3.2.2	Method for Classifying Structures			
	3.2.3	Wade's rules			
	3.2.4	Synthesis of Carboranes			
	<b>3.3</b> Hete	proboranes			
	3.3.1	Introduction			
	3.3.2	Method for Classifying Structures			
	<b>3.4</b> Met	allaboranes and Metallacarboranes			
	3.4.1	Introduction			
	3.4.2	Method for Classifying Structures			
	<b>3.5</b> Poly	hedral Skeletal Electron Pair approach or Mingo's Rules			
	<b>3.6</b> Elec	tron precise compounds and their relation to clusters			
IV		Inorganic – Rings – Chains –Polymer	(15)		
	<b>4.1</b> Silic	ates: Types of Silicates			
	<b>4.2</b> Zeol	ites			
	<b>4.3</b> Silic	cones			
	4.4 Phospho Nitrilic Compounds: Phosphazenes and Phosphazines Polymers				
	<b>4.5</b> Sulp	hur Nitrogen Compounds: S <sub>4</sub> N <sub>4</sub> and S <sub>3</sub> N <sub>3</sub>			
	<b>4.6</b> Flur	ocarbons			

- **1.** B D Gupta and A J Elias, Basic Organometallic Chemistry- Concept, Synthesis and Applications, 2<sup>nd</sup> Edition, University Press, 2013.
- Gary O. Spessard and Gary L. Miessler, Organometallic Chemistry, Oxford University Press, 2<sup>nd</sup> Edition, 2010.
- Catherine E. Housecroft and Alan G. Sharpe, Inorganic Chemistry, 2<sup>nd</sup> Edition, Pearson Education Limited, 2005.
- 4. F. A. Cotton, G. Wilkinson, C. Murillo and M. Bochmann, Advanced Inorganic Chemistry, 6th ed., John Wiley, New York, 1999.
- 5. D. F. Shriver, P. W. Atkins and C.H. Langford, Inorganic Chemistry, 3<sup>rd</sup> edition Oxford University Press, 1999.
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- 7. James E. House, Inorganic Chemistry, 2<sup>nd</sup> Edition, Elsevier, 2013.
- Robert H. Crabtree, The Organometallic Chemistry Of The Transition Metals, 4<sup>th</sup>Edition, John Wiley & Sons Ltd, 2005.

#### SEMESTER – IV

#### **RPSCHEI403**

#### Credits 4

#### PAPER - III SYMMETRY, SPECTROSCOPY TECHNIQUES AND CATALYSIS

#### **Course Objectives:**

- The primary aim of this paper is to learn about the point groups, character table and basic application of symmetry in spectroscopy and chemical bonding. This also aims to learn the selection rule for Infrared and Raman-active transitions.
- Secondly, the learner explores how nuclear spins are affected by a magnetic field, and is able to explain what happens when radiofrequency radiation is absorbed. The learner will be able to predict the number of proton and carbon NMR signals expected from a compound given its structure and predict the splitting pattern in the proton NMR spectrum of a compound given its structure.
- The third unit makes the learnerunderstand the hyperfine parameters, recoil energy, quadruple splitting and chemical shift / isomer shift by using Mossbauer spectroscopy.

#### **Course Outcome:**

- Describe the selection rule for infrared-active transitions.
- Determine whether the molecular vibrations of a triatomic molecule are Raman active.
- Analyze the hybridization of given compounds.
- Understand the concepts of equivalent and non-equivalent hydrogen.
- Know the effect of structure on chemical shift and coupling constants.
- Elucidate the electronic structure of free radicals and paramagnetic transition metal complexes.
- Illustrate the magnetic properties of the materials and its order of orientation.

<b>r</b>	PAPER – III SYMMETRY, SPECTROSCOPY TECHNIQUES AND CATALYSIS					
Unit I	Topics Symmetry in Chemistry	Lecture				
I	<b>1.1</b> Recapitulation of Points groups and Character tables.	(15)				
	<b>1.2</b> Applications of Group theory in Infrared and Raman spectroscopy. Molecular Vibrations,					
	determining the Symmetry Types of the Normal Modes; symmetry-based Selection Rules of					
	IR and Raman, application in Infrared and Raman spectroscopy for molecules belongs to point					
	group $C_{2v}$ , $C_{3v}$ , $C_{4v}$ , $D_{2h}$ , $D_{3h}$ , $D_{\infty h}$ and $T_d$ .					
	<b>1.3</b> Group theory and quantum mechanics. Wave function as bases for irreducible representation.					
	<b>1.4</b> Symmetry Adapted Linear Combinations - (SALC) - projection operators and their use to construct SALC.					
	1.5 Molecular Orbital Theory. Transformation properties of atomic orbitals, MO's for Sigma and					
	pi - molecular orbitals in ABn molecules, AB4 (tetrahedral) and AB6 (octahedral) molecules,					
	Hybrid orbitals.					
II	N.M.R. Spectroscopy	(15)				
	1.1 Nuclear Magnetic Resonance (NMR) Spectroscopy: Nuclear spin and its interaction with					
	applied field, population of energy state, relaxation time, <sup>1</sup> H NMR Spectroscopy: Chemical					
	Shift; Multiplet Splitting of NMR peaks arises through Spin-Spin Coupling, Multiplet					
	Splitting when more than two spins interact.					
	<b>1.2</b> Pulse technique in NMR: The magnetization vector, spin-spin relaxation, spin-lattice relaxation.					
	1.3 <sup>13</sup> C NMR Spectroscopy: Fourier Transform NMR; Off-Resonance and Spin-Decoupled,					
	DEPT, Applications, 2-D NMR Spectroscopy (COSY). Nuclear Overhauser Effect					
	Spectroscopy (NOESY).					
	1.4 Solid-state NMR					
	1.5 Magnetic Resonance Imaging (MRI);					
	<b>1.6</b> NMR Spectroscopy of <sup>19</sup> F, <sup>15</sup> N and <sup>31</sup> P nuclides.					
III	ESR and Mossbauer Spectroscopy	(15)				
	3.1 Electron spin Resonance Spectroscopy-					
	3.1.1 Basic principle, hyperfine splitting (isotropic systems)					
	3.1.2 g-value and the factors affecting thereof; interactions affecting electron energies in					
	paramagnetic complexes (Zero-field splitting and Kramer's degeneracy);					

3.1.3	An isotropic effect (the g-value and the hyperfine couplings); The EPR of triplet states;					
	Structural applications to transition metal complexes.					
3.2 Mos	sbauer Spectroscopy:					
3.2.1	Basic principles of Mössbauer spectroscopy, instrumentation, spectral parameters					
	Mössbauer Parameters- Isomer Shifts, quadrupole splitting, Magnetic hyperfine					
	interaction.					
3.2.2	Application of Mössbauer spectroscopy with respect to Oxidation states of metal ion in					
	compounds, Structural elucidation, Covalent and ionic compounds and High spin low					
	spin behavior					
	Catalysis	(15)				
<b>4.1</b> Intro	oduction, history and importance of catalysis, concept of activity, selectivity, poisoning,					
pron	notion, turnover number and deactivation,					
<b>4.2</b> Type	es of catalysis: homogeneous catalysis: examples of homogeneous catalysis in gasphase,					
and	in solution phase, acid-base catalysis.					
4.3 Hete	progeneous catalysis: heterogeneous catalysis with gaseous reactants, liquid reactants, and					
gase	ous reactants, biocatalysis, autocatalysis, negative catalysis, characteristics of catalytic					
reac	tions, activation energy and catalysis, theories of catalysis: the intermediate compound					
form	nation theory, the adsorption theory.					
<b>4.4</b> Mec	hanism of heterogeneous catalysis, kinetics of heterogeneous catalytic reactions,					
Langmuir-Hinshelwood model, Catalysis by semiconductors, Boundary Layer theory,						
Wolkenstein's theory.						
<b>4.5</b> Preparation and Characterization of Catalysts: General methods of preparation of catalysts:						
prec	ipitation, sol-gel, hydrothermal, impregnation, hydrolysis, vapour deposition. Activation					
of c	atalysts: calcinations, reduction. Catalyst characterization: surface area, pore size					
distr	ibution, particle size determination, XPS, AES, UV-Vis, FTIR and thermal methods.					
	3.2 Mos 3.2.1 3.2.2 4.1 Intro prom 4.2 Type and 4.3 Hete gase reac form 4.4 Mec Lang Wol 4.5 Prep prec of ca	<ul> <li>Structural applications to transition metal complexes.</li> <li>3.2 Mossbauer Spectroscopy:</li> <li>3.2.1 Basic principles of Mössbauer spectroscopy, instrumentation, spectral parameters Mössbauer Parameters- Isomer Shifts, quadrupole splitting, Magnetic hyperfine interaction.</li> <li>3.2.2 Application of Mössbauer spectroscopy with respect to Oxidation states of metal ion in compounds, Structural elucidation, Covalent and ionic compounds and High spin low spin behavior</li> <li>Catalysis</li> <li>4.1 Introduction, history and importance of catalysis, concept of activity, selectivity, poisoning, promotion, turnover number and deactivation,</li> <li>4.2 Types of catalysis: homogeneous catalysis: examples of homogeneous catalysis in gasphase, and in solution phase, acid-base catalysis.</li> <li>4.3 Heterogeneous catalysis: heterogeneous catalysis with gaseous reactants, liquid reactants, and gaseous reactants, biocatalysis, autocatalysis, negative catalysis; characteristics of catalytic reactions, activation energy and catalysis, theories of catalysis: the intermediate compound formation theory, the adsorption theory.</li> <li>4.4 Mechanism of heterogeneous catalysis, kinetics of heterogeneous catalytic reactions, Langmuir-Hinshelwood model, Catalysis by semiconductors, Boundary Layer theory, Wolkenstein's theory.</li> </ul>				

- K. Veera Reddy, Symmetry and Spectroscopy of molecules, 2<sup>nd</sup> Edition, New Age International publishers.
- F. A. Cotton, Chemical applications of Group Theory, John Wiley and Sons, Pvt. Ltd., 2006.
- R. L. Carter, Molecular symmetry and Group theory, John Wiley and Sons, Pvt. Ltd., 1996.
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- Heterogeneous Catalysis, D. K. Chakrabarty and B. Viswanathan, Hardcover Oct 2008 New Age International Publishers.
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- G H Jeffery, J Bassett, J Mendhem, R C Denney, Vogel's Textbook Of Quantitative Chemical Analysis, 3<sup>rd</sup> Edition, Longman Scientific & Technical, 1989.
- R Gopalan, V Ramalingam, Concise Coordination Chemistry, Vikas Publishing House Pvt. Ltd., 2000.
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#### **SEMESTER – IV**

#### **RPSCHEIOC - I 404**

#### Credits 4

#### PAPER – IV INTELLECTUAL PROPERTY RIGHTS & CHEMINFORMATICS

#### **Course Objectives:**

- This course aims to introduce the basic tenets of intellectual property rights and patent law.
- The learner, being in the final stage of their Master's course will be familiarized with the procedure of obtaining copyrights, trademarks, etc.
- The legal aspects of trade secrets, various legislation and role of the judiciary in the protection of intellectual property rights will also be explored.
- The course will further cover the use of computers in the application of chemical concepts via Cheminformatics such as in drug design, modelling structures, etc.
- The aim of this paper is to introduce the students to technical aids and software models imperative to research- both academic and industrial.

#### **Course outcome:**

- Be well versed with the concept of intellectual property and the terms involved with respect to Indian Patent Law.
- Have a clear distinction between patents and copyrights.
- Understand the economical impact and legislature involved in Intellectual property rights.
- Have a brief idea about software tools pertaining to Cheminformatics and Molecular Modeling.
- Be able to conduct structure and sub-structure search online, determine SMILES codes for various molecules.
- To gain knowledge about the application of the research based tools.

# PAPER – IV INTELLECTUAL PROPERTY RIGHTS & CHEMINFORMATICS

I       Intellectual Property - I         1.1 Introduction: Historical Perspective, Different types of IP, Importance of protecti IP.       1.2 Patents: Historical Perspective, Basic and associated right, WIPO, PCT syste Traditional Knowledge, Patents and Health care-balancing promoting innovation w public health, Software patents and their importance for India.         1.3 Industrial Designs: Definition, How to obtain, features, International desi registration.       1.4 Copyrights: Introduction, How to obtain, Differences from Patents.         1.5 Trade Marks: Introduction, How to obtain, Different types of marks – Collect marks, certification marks, service marks, trade names etc.       1.6 Geographical Indications: Definition, rules for registration, prevention of illege exploitation, importance to India.         II       Intellectual Property - II         2.1 Trade Secrets: Introduction and Historical Perspectives, Scope of Protection, Ritinvolved and legal aspects of Trade Secret Protection.         2.2 IP Infringement issue and enforcement: Role of Judiciary, Role of law enforcement agencies – Police, Customs etc.         2.3 Economic Value of Intellectual Property: Intangible assests and their valuated Intellectual Property in the Indian context – Various Laws in India Licensing a Technology transfer.         2.4.1 World Trade Organization (WTO): General Agreement on Tariffs and Tra (GATT), Trade Related Intellectual Property Rights (TRIPS) agreement, Gene Agreement on Trade Related Services (GATS) Madrid Protocol, Bene Convention, Budapest Treaty         2.4.2 Paris Convention: WIPO and TRIPS, IPR and Plant Breeders Rights, IPR a Biodiversity.		Lecture
<ul> <li>IP.</li> <li>1.2 Patents: Historical Perspective, Basic and associated right, WIPO, PCT syste Traditional Knowledge, Patents and Health care-balancing promoting innovation w public health, Software patents and their importance for India.</li> <li>1.3 Industrial Designs: Definition, How to obtain, features, International desi registration.</li> <li>1.4 Copyrights: Introduction, How to obtain, Differences from Patents.</li> <li>1.5 Trade Marks: Introduction, How to obtain, Different types of marks – Collect marks, certification marks, service marks, trade names etc.</li> <li>1.6 Geographical Indications: Definition, rules for registration, prevention of illegexploitation, importance to India.</li> <li>11 Intellectual Property - II</li> <li>2.1 Trade Secrets: Introduction and Historical Perspectives, Scope of Protection, Risinvolved and legal aspects of Trade Secret Protection.</li> <li>2.2 IP Infringement issue and enforcement: Role of Judiciary, Role of law enforcemagencies – Police, Customs etc.</li> <li>2.3 Economic Value of Intellectual Property: Intangible assests and their valuatie Intellectual Property in the Indian context – Various Laws in India Licensing a Technology transfer.</li> <li>2.4.1 World Trade Organization (WTO): General Agreement on Tariffs and Tra (GATT), Trade Related Intellectual Property Rights (TRIPS) agreement, Gene Agreement on Trade Related Services (GATS) Madrid Protocol, Ber Convention, Budapest Treaty</li> <li>2.4.2 Paris Convention: WIPO and TRIPS, IPR and Plant Breeders Rights, IPR a Biodiversity.</li> <li>11 Cheminformatics – I</li> </ul>		(15)
<ul> <li>1.2 Patents: Historical Perspective, Basic and associated right, WIPO, PCT syste Traditional Knowledge, Patents and Health care-balancing promoting innovation w public health, Software patents and their importance for India.</li> <li>1.3 Industrial Designs: Definition, How to obtain, features, International desi registration.</li> <li>1.4 Copyrights: Introduction, How to obtain, Differences from Patents.</li> <li>1.5 Trade Marks: Introduction, How to obtain, Different types of marks – Collect marks, certification marks, service marks, trade names etc.</li> <li>1.6 Geographical Indications: Definition, rules for registration, prevention of illege exploitation, importance to India.</li> <li>11 Intellectual Property - II</li> <li>2.1 Trade Secrets: Introduction and Historical Perspectives, Scope of Protection, Ris- involved and legal aspects of Trade Secret Protection.</li> <li>2.2 IP Infringement issue and enforcement: Role of Judiciary, Role of law enforcemen- agencies – Police, Customs etc.</li> <li>2.3 Economic Value of Intellectual Property: Intangible assests and their valuatie Intellectual Property in the Indian context – Various Laws in India Licensing a Technology transfer.</li> <li>2.4.1 World Trade Organization (WTO): General Agreement on Tariffs and Tra (GATT), Trade Related Intellectual Property Rights (TRIPS) agreement, Gene Agreement on Trade Related Services (GATS) Madrid Protocol, Ben Convention, Budapest Treaty</li> <li>2.4.2 Paris Convention: WIPO and TRIPS, IPR and Plant Breeders Rights, IPR a Biodiversity.</li> <li>11 Cheminformatics – I</li> </ul>	ıg	
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3.1 History and evolution of cheminformatics, Use of Cheminformatics, Prospects	_	(15)
	of	
cheminformatics, Molecular modeling and structure elucidation.		

	3.2 Representation of molecules and chemical reactions: Nomenclature, Different types					
	of notations, SMILES coding, Matrix representations, Structure of Molfiles and Sdfiles,					
	Libraries and toolkits, Different electronic effects, Reaction classification.					
	3.3 Searching Chemical Structures: 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.					
IV	Cheminformatics – II	(15)				
	4.1 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,					
	4.2 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.					
	<b>4.3</b> Application of Cheminformatics in Drug Design.					

- Vivien Irish, Intellectual Property Rights for Engineers, 2<sup>nd</sup> Edition, British Library, 2008.
- 2. David I. Bainbridge, Intellectual Property, 8th Edition, Pearson, 2010.
- Stephen Elias and Richard S tim, Patent Copyright & Trade Mark, 8<sup>th</sup> Edition, Nolo and Richard, 2013.
- 4. Johann Gasteiger and Thomas Engel, Chemoinformatics, Wiley-VCH, 2003.
- 5. Andrew R. Leach, Valerie J. Gillet, An Introduction to Chemoinformatics, Springer, 2007.
- 6. Barry A. Bunin, Jurgen Bajorath, Brian Siesel and Guillermo Morales, Chemoinformatics- Theory, Practice and Products, Springer, 2007.

#### SEMESTER - IV

#### **RPSCHEIOC - II 404**

#### Credits 4

#### **PAPER – IV RESEARCH METHODOLOGY**

#### **Course Objectives:**

- This course aims to introduce the basic principles of scientific research. The student who
  will soon obtain a Master's degree in Science will be introduced to the systematic
  methodology of conducting fundamental research, right from literature surveys to
  developing a problem.
- They will be taught methods in statistical analysis of data pertaining to research, writing of research papers in the various formats available.
- Finally they will be guided about laboratory safety protocols which are absolutely essential for the new research student.

#### **Course Outcomes:**

- Understand basics of research methodology
- Get the technical know-how of research from developing a problem.
- Be able to write a research paper, study formats of existing research papers and review papers.
- Be aware about importance of lab-safety and the safety protocols in R&D laboratories.

Unit	Topics	Lecture					
Ι	Review of Literature	(15)					
	<b>1.1 Print:</b> Primary, Secondary and Tertiary sources.						
	1.2 Journals: Journal abbreviations, abstracts, current titles, reviews, monographs,						
	dictionaries, textbooks, current contents, Introduction to Chemical Abstracts and						
	Beilstein, Subject Index, Substance Index, Author Index, Formula Index, and other						
	Indices with examples.						
	1.3 Digital: Web sources, E-journals, Journal access, TOC alerts, Hot articles, Citation						
	Index,Impact factor, H-index, E-consortium, UGC infonet, E-books, Internet						
	discussiongroups and communities, Blogs, preprint servers, Search engines, Scirus,						
	Google Scholar, ChemIndustry, Wiki-databases, ChemSpider, Science Direct,						
	SciFinder, Scopus.						
	1.4 Information Technology and Library Resources: The Internet and World Wide						
	Web, Internet resources for Chemistry, finding and citing published information.						
II	Data Analysis	(15)					
	2.1 The Investigative Approach: Making and recording Measurements, SI units and their						
	use, Scientific methods and design of experiments.						
	2.2 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.						
III	Methods Of Scientific Research And Writing Scientific Papers	(15)					
	3.1 Reporting practical and project work, Writing literature surveys and reviews, organizing						
	a poster display, giving an oral presentation.						
	3.2 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.						

# **PAPER – IV RESEARCH METHODOLOGY**

IV	Chemical Safety & Ethical Handling Of Chemicals	(15)
	4.1 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	
	pressure.	
	4.2 Safe storage and disposal of waste chemicals, recovery, recycling and reuse of laboratory	
	chemicals, procedure for laboratory disposal of explosives, identification, verification	
	and segregation of laboratory waste, disposal of chemicals in the sanitary	
	sewer system, incineration and transportation of hazardous chemicals.	

- C. R. Kothari, ResearchMethodology- Methods and techniques, New Age International (P) Limited Publisher, 2004.
- 2. YogeshKumar Singh, Fundamental of ResearchMethodology and Statistics, New Age International (P) Limited Publisher, 2006.
- 3. Carol Ellison, Concise Guide to WritingResearchPpaers, McGraw-Hill, 2016.
- IntroductoryStatistics, Prem S. Mann, C. Jay Lacke, 7<sup>th</sup> Edition, John Wiley and Sons, 2010.
- 5. Statistics From A to Z Confusing Concepts Clarified, Andrew A. Jawlik, John Wiley and Sons, 2016.

#### **SEMESTER – IV**

### PRACTICAL

#### **RPSCHEI4P1:** Analysis of ores/alloys

- 1. Analysis of galena ore:
  - i) Pb content as PbCrO4 by gravimetric method using 5% potassium chromate
  - ii) Fe content by colorimetrically using 1, 10- phenonthroline
- 2. Analysis of Zinc blend ore:
  - i) Zn content by complexometric method
  - ii) Fe content by colorimetric method (Azide method)
- 3. Analysis of Pyrolusite ore:
  - i) Mn content by complexometric method
  - ii) Acid insoluble residue by gravimetric method

# **RPSCHEI4P2:** Coordination Chemistry

- 1. Determination of Stability constant of  $[Zn(NH_3)_4]^{2+}$  by potentiometry.
- 2. Determination of Stability constant of [Ag(en)]<sup>+</sup> 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 complex  $[Ni(H_2O)_6]^{2+}$  and  $[Ni(en)_3]^{2+}$

#### **RPSCHEI4P3:** Commercial sample Analysis

- 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. Soil for mixed oxide content by gravimetric method.
- 5. Fertilizer for potassium content by flame photometry.

#### **RPSCHEI4P4:** Project Evaluation

#### **References for Practical:**

- 1. G H Jeffery, J Bassett, J Mendhem, R C Denney, Vogel's Textbook Of Quantitative Chemical Analysis, 3<sup>rd</sup> Edition, Longman Scientific & Technical,1989.
- 2. R Gopalan, V Ramalingam, Concise Coordination Chemistry, Vikas Publishing House Pvt. Ltd. 200.
- 3. H N Patel, S P Turakhia, S SKelkar, S R Puniyani, Post Graduate Practical Chemistry Part I, Himalaya Publishing House, 5<sup>th</sup> Edition, 2008.

#### **MODALITY OF ASSESSMENT**

### **Theory Examination Pattern:**

A) Internal Assessment - 40%

**Presentation: 20 Marks** 

**Continuous Internal Assessment (CIA): 20 Marks** 

For each paper, students are evaluated from their presentation based on the topic selected from syllabus. The assessment of presentation is as follows:

Sr. No	Evaluation type	Marks
1	Presentation content	10
2	Presentation skills	05
3	Viva	05
4	Continuous Internal Assessment (CIA) e.g. Test, Group discussion, assignment, open-book tests etc.	20
	Total	40

#### B) External examination - 60 %

#### Semester End Theory Assessment - 60 marks

- i. Duration These examinations shall be of **2.5 hours** duration.
- ii. Paper Pattern:
- 1. There shall be 04 questions each of 15 marks. On each unit, there will be one question.
- 2. All questions shall be compulsory with internal choice within the questions.

Questions	Options	Marks	Questions on	
Q.1) A)	Any 3 out of 5	12	Unit I	
Q.1) B)	Any 1 out of 2	3		
Q.2) A)	Any 3 out of 5	12	Unit II	
Q.2) B)	Any 1 out of 2	3		
Q.3) A)	Any 3 out of 5	12	Unit III	
Q.3) B)	Any 1 out of 2	3		
Q.4) A)	Any 3 out of 5	12	Unit IV	
Q.4) B)	Any 1 out of 2	3		

#### **Practical Examination Pattern:**

#### **Semester End Practical Examination: 50 marks**

Experimental Work	40
Viva	05
Journal	05

#### PRACTICAL BOOK/JOURNAL

The students are required to present a duly certified journal for appearing at the practical examination, failing which they will not be allowed to appear for the examination.

In case of loss of Journal, a Lost Certificate should be obtained from Head/ Coordinator / In- charge of the department; failing which the student will not be allowed to appear for the practical examination.

# Overall Examination and Marks Distribution Pattern Semester: III

Course	3	01		302			Grand
							Total
	Internal	External	Total	Internal	External	Total	
Theory	40	60	100	40	60	100	200
Practical	cal 50		50	100			
Course	303			3	04		Grand
							Total
	Internal	External	Total	Internal	External	Total	
Theory	40 60		100	40	60	100	200
Practical		50		I	50	100	

Total: 600 marks

Semester: IV

Course	4	01		402			Grand
							Total
	Internal	External	Total	Internal	External	Total	
Theory	40	60	100	40	60	100	200
Practical			50			50	100
Course	403			404			Grand
							Total
	Internal	External	Total	Internal	External	Total	
Theory	40	60	100	40	60	100	200
Practical	ractical		50			50	100

Total: 600 marks