



**M.Sc. INORGANIC CHEMISTRY**  
**(For students admitted from the academic year 2015-2016)**

**CURRICULUM AND SYLLABUS**

**UNDER CHOICE BASED CREDIT SYSTEM**

**FACULTY OF SCIENCE AND HUMANITIES**  
**SRM UNIVERSITY**  
**SRM NAGAR, KATTANKULATHUR – 603 203**

**M.Sc. INORGANIC CHEMISTRY**  
(For students admitted from the academic year 2015-2016)

**CURRICULUM**

SUBJECT CODE	TITLE OF THE SUBJECT	L	T	P	Total of L+T+P	C
<b>SEMESTER I</b>						
PCY15101	Inorganic Chemistry-I	3	3	-	6	4
PCY15102	Organic Chemistry-I	3	3	-	6	4
PCY15103	Physical Chemistry-I	3	3	-	6	4
PCY15E01/ PCY15E02	Major Elective-1 (Nanochemistry / Chemistry of Nanoscience and Technology)	3	3	-	6	3
PCY15104	Inorganic Chemistry Practical	-	-	6	6	3
<b>Total</b>		12	12	6	30	18
<b>SEMESTER II</b>						
PCY15201	Inorganic Chemistry-II	4	1	-	5	4
PCY15202	Organic Chemistry-II	4	1	-	5	4
PCY15203	Physical Chemistry-II	4	-	-	4	4
PCY15E51/ PCY15E52	Skill Based Elective-1 (Analytical Chemistry/Advanced Analytical Methods)	2	2	-	4	4
	Open Elective-1	2	-	-	2	2
PCY15204	Organic Chemistry Practical	-	1	4	5	3
PCY15205	Physical Chemistry Practical	-	1	4	5	3

<b>Total</b>		16	6	8	30	<b>24</b>
<b>SEMESTER III</b>						
PCY15311	Organometallic Chemistry	4	2	-	6	4
PCY15312	Photo Inorganic Chemistry	4	2	-	6	4
PCY15313	Bioinorganic Chemistry	4	2	-	6	4
PCY15E53	Skill based Elective-2 (Applications of Computer in Chemistry)	2	2	-	4	4
	Open Elective-2	2	-	-	2	2
PCY15314	Advanced Inorganic Chemistry Practical	-	-	6	6	2
<b>Total</b>		16	8	6	30	<b>20</b>
<b>SEMESTER IV</b>						
Xxxxxxxx	Major Elective- 2	3	-	-	3	3
PCY15401	Seminar*	-	-	1	1	1
PCY15402	Project Work	-	-	28	28	14
<b>Total</b>		3	-	29	32	<b>18</b>
<b>Total number of credits to be earned for the award of degree</b>		<b>80</b>				

Mode for opting specialization: The number of seats in each specialization course would be upto a maximum of 30% of the total eligible candidates

**Note:**

\* - Continuous Assessment (Full Internals)

L – Lecture Hours, T – Tutorial Hours, P – Practical Hours & C – Credits

### MAJOR ELECTIVES

SEMESTER	SUBJECT CODE	TITLE OF THE SUBJECT	L	T	P	Total of L+T+P	C
I	PCY15E01	Nanochemistry	3	3	-	6	3
	PCY15E02	Chemistry of Nanoscience and Technology)	3	3	-	6	3
IV	PCY15E03	Solid State Chemistry	3	-	-	3	3
	PCY15E08	Medicinal Inorganic Chemistry	3	-	-	3	3

## SYLLABUS

### SEMESTER I

Subject Code	Title of the Subject	L	T	P	Total of L+T+P	C
PCY15101	Inorganic Chemistry-I	3	3	-	6	4
<b>INSTRUCTIONAL OBJECTIVES</b>						
(i)	To study in depth about atomic structure , periodic table , bonding and structure					
(ii)	To gain knowledge about the main group chemistry					
(iii)	To acquire knowledge about coordination chemistry					
(iv)	To study in detail about the reaction mechanism of complexes					

#### **UNIT I Atomic Structure and Periodic Table**

Atom as nucleus with orbital electrons, concept of wave-functions, quantum numbers and spin, shape of s, p and d orbitals and their radial distribution functions, electronic configuration of atoms, Aufbau principle, Pauli Exclusion Principle and Hund's rule. Slater's rules for the determination of screening constants; arrangement of elements in Groups in the Periodic Table- s-block, p-block, d-block and f-block elements; periodic properties, ionic radii, ionization potential, electron affinity, electronegativity (Pauling, Mulliken and Alfred-Rochnow scales) atomic states and terms symbols.

#### **UNIT II Bonding and Structure**

Types of bonds, ionic, covalent, coordinate, double and triple bonds, orbital symmetry and overlaps. Concept of MO and VB theory, concept of hybridization, the extent of orbital participation in molecular bonding, bond energy and covalent radii. Concept of resonance, bond moment and molecular dipole moment, polarizing power and polarizability and Fajan's rules.

#### **UNIT III Main Group Chemistry**

**Main Group Chemistry:** Chemistry of boron – borane, higher boranes, carboranes, borazines and boron nitrides. Chemistry of silicon – silanes, higher silanes, multiple bonded systems, disilanes, silicon nitrides, siloxanes and silicates. P-N compounds, cyclophosphazenes and cyclophosphazanes. S-

N compounds –  $S_4N_4$ , (SN)<sub>x</sub>.

**Ionic Model** – Lattice energy – Born-Landeequation – Kapustinskiequation – High Tc superconductors – Solid state reactions – Types and examples.

### UNIT IV Coordination Chemistry

**Theories of Metal-Ligand bond:** VB theory and its limitations – Crystal field theory – splitting of d-orbitals under various geometries – Factors affecting splitting – CFSE and evidences for CFSE (Structural and thermodynamic effects) – Spectrochemical series – Jahn Teller distortion – Spectral and magnetic properties of complexes – Site preferences – Limitations of CFT – Ligand field theory – MO theory – sigma – and pi-bonding in complexes – Nephelauxetic effect – The angular overlap model.

### UNIT V Reaction Mechanism of complexes

#### Coordination Chemistry –

**Reaction Mechanism:** Kinetics and mechanism of reactions in solution – labile and inert complexes – Ligand displacement reactions in octahedral and square planar complexes – acid hydrolysis, base hydrolysis and anation reactions – trans effect – theory and applications. Electron transfer reactions – electron exchange reactions – complementary and non-complementary types – inner sphere and outer sphere processes – Application of Electron transfer reactions in inorganic complexes – isomerization and racemization reactions of complexes – Molecular rearrangement – reactions of four and six-coordinate complexes – Interconversion between stereoisomers. Reactions of coordinated ligands – Template effect and its application for the synthesis of Macrocyclic ligands – Unique properties.

#### Text Books

1. Day, M.C and Selbin, J (1985): Theoretical Inorganic Chemistry, 2<sup>nd</sup> Edition, Affiliated East West Press Pvt. Ltd.
2. Cotton, F. A and Wilkinson, G (2009): Advanced Inorganic Chemistry, 4<sup>th</sup> Edition, A Wiley- Interscience Publication, John-Wiley & Sons, USA.
3. Huheey, J.E (1983): Inorganic Chemistry, 3<sup>rd</sup> Edition, Harper & Row publisher, Singapore.

#### References

1. Kettle, S.F.A. (1996): Physical Inorganic Chemistry – A Coordination Chemistry Approach, Spectrum, Academic Publishers, Oxford University Press.
2. Adamson, A.W (1975): Inorganic Photochemistry, John Wiley & Sons, New York.
3. Basolo, F. and Pearson, R.G (1967): Mechanism of Inorganic Reactions, John Wiley, New York.



## SEMESTER I

Subject Code	Title of the Subject	L	T	P	Total of L+T+P	C
PCY15102	Organic Chemistry-I	3	3	-	6	4
<b>INSTRUCTIONAL OBJECTIVES</b>						
(i)	To gain knowledge on the importance of basic organic chemistry					
(ii)	To acquire knowledge about aromaticity					
(iii)	To understand the substitution reaction mechanisms					
(iv)	To acquire knowledge in stereochemical aspects of organic molecules					
(v)	To gain knowledge about the reagents and their application to organic chemistry					

### UNIT I Structure, Bonding and Reactive Intermediates

**Structure and Bonding** Localized Chemical Bonding: Electronic Structure of molecules; VB and MO - Inductive and Field Effects, Bond distances, Bond angles and Bond energies. Delocalized Chemical Bonding: Bond energies and Bond distances in compounds containing delocalized bonds - Cross conjugation-Resonance - Hyperconjugation and Keto – Enol tautomerism.

**Reactive Intermediates:** Generation, Structure, Stability and Reactivity of Carbocations and Carbanions, Free radicals, Carbenes, Nitrenes and Benzyne.

### UNIT II Aromaticity

Huckel's theory of aromaticity, Concept of homoaromaticity and antiaromaticity. Electron occupancy in MO's. Systems with 2, 4, 8 and 10 electrons, systems of more than 10 electrons, alternant and non-alternant hydrocarbons (azulene type). Bonding properties of systems with  $(4n + 2)\pi$  electrons and  $4n\pi$  electrons, Aromaticity of benzenoid, heterocyclic and non-benzenoid compounds. Annulenes, Sydnones and Fullerenes. NMR concept of Aromaticity

### UNIT III Substitution Reactions

**Aliphatic Nucleophilic substitutions:** The  $S_N2$ ,  $S_N1$ , mixed  $S_N1$  and  $S_N2$  and SET mechanisms. The neighbouring group mechanism, neighbouring group participation by  $\sigma$  and  $\pi$ - bonds, anchimeric assistance. Classical and nonclassical carbocations, phenonium ions and norbornyl system. The  $S_N1$  mechanism. Nucleophilic substitution at an allylic, aliphatic trigonal and a vinylic carbon. Reactivity effects of substrate, attacking nucleophile, leaving group and reaction medium.

**Aromatic Nucleophilic Substitution:** The  $S_NAr$ ,  $S_N1$ , benzyne and  $S_{RN}1$  mechanisms. Reactivity - effect of substrate, structure, leaving group and attacking nucleophile.

#### **UNIT IV Stereochemistry**

Fundamentals of Organic Stereochemistry: Principles of symmetry-Stereoisomerism-Optical isomerism-Definitions-Conventions used in Stereochemistry: Newmann, Sawhorse and Fischer notations and interconversions and representations. Nomenclature, correlation of configuration, Cahn-Ingold-Prelog rules for simple molecules, Optical activity and chirality-Types of molecules exhibiting optical activity-Fischer projection-absolute configuration. Molecules with more than one chiral center-molecular chirality-Atropisomerism-Biphenyl, allenes and spiranes.Methods of determining configuration.Prochiral centers-Asymmetric synthesis-racemisation and resolution.

Geometrical Isomerism: E&Z Nomenclature, Determination of configuration of geometrical isomers. Stereochemistry of addition and elimination reactions.Stereoselective and stereospecific synthesis(Elementary examples)Conformational Analysis. Basic concepts of conformation analysis-conformation of ethane, substituted ethane, n-butane and cyclohexane

#### **UNIT V Reagents**

Use of the following reagents in organic synthesis:, Diazomethane, Dicyclohexylcarbodiimide, DIBAL, Grignard, Lead tetraacetate, Lithium aluminium hydride, Lindlar's catalyst, N-Bromosuccinimide, Osmium tetroxide, PCC, Raney Nickel, Selenium dioxide, Wittig reagent.

#### **Text Books**

1. March, J (2000): Advanced Organic Chemistry: Reactions, Mechanisms and Structure, 5<sup>th</sup> edition, Wiley.
2. Morrison, R.T and Boyd, R.N (1992): Organic Chemistry, 6<sup>th</sup> edition, Pearson.

#### **References**

1. Nasipuri, D (2002): Stereochemistry of organic compounds-Principles and applications., 2<sup>nd</sup> edition, New Age International.
2. Bansal, R.K (1975): Organic Reaction Mechanisms, Tata McGraw Hill.

## SEMESTER I

Subject Code	Title of the Subject	L	T	P	Total of L+T+P	C
PCY15103	Physical Chemistry-I	3	3	-	6	4
<b>INSTRUCTIONAL OBJECTIVES</b>						
(i)	To understand the theories and concepts of electrochemistry.					
(ii)	To suggest the applications of electrochemistry.					
(iii)	To understand the thermodynamic properties and its determination.					
(iv)	To make the students understand and appreciate the concepts of chemical kinetics.					

### UNIT I Ions in Solutions

Conductivity of solutions and their measurement - the Arrhenius ionisation theory - transport numbers and mobilities of ions - measurement of transport numbers - Hittorff method and moving boundary method - ionic activities and activity coefficients and their determination by various methods - Debye-Huckel-Onsager theory - ionic atmosphere - Debye-Huckel limiting law - dissociation constant of acids and bases.

### UNIT II Electrochemical Cells

Electromotive force - measurement of EMF – the cell EMF and the cell reaction - reversible cells - types of half cells - classification of cells - the standard EMF of a cell - electrochemical potential - standard electrode potentials - calculation of the EMF of a cell - Nernst equation and its limitations - calculation of solubility products - standard free energies and entropies of aqueous ions - electrode concentration cells - electrolyte concentration cells - cells with liquid junctions - oxidation - reduction reactions, measurement of PH, concentration cells - decomposition voltages - concentration polarisation and over voltage - polarography.

### UNIT III Chemical Kinetics - I

Simple collision theory, absolute reaction rate theory (ARRT), thermodynamic treatment, potential energy surfaces, application of ARRT to simple bimolecular process; chain reactions – general characteristics, study of kinetics of chain reaction like  $H_2-Br_2$  reaction, decomposition of acetaldehyde and  $N_2O_5$ , study of  $H_2-O_2$  explosive reactions. Theory of unimolecular reactions-Lindemann, Hinshelwood, RRKM and Slater treatment- steady state approximation, principle of microscopic reversibility and detailed balancing - kinetic isotope effect.

#### **UNIT IV Chemical Thermodynamics**

Second law of thermodynamics-concept of entropy-Gibbs function- Gibbs –Helmholtz equation- Maxwell relations- Thermodynamic equation of state- thermodynamics of systems of variable composition- partial molar quantities, partial molar volume-chemical potential, Gibbs-Duhemequation – Experimental determinations of fugacity of real gases. Third law of thermodynamics – absolute entropies-determination-exception to third law – Unattainability of absolute zero

#### **UNIT V Surface Phenomenon and Catalysis**

Introduction-adsorption of gases on solids- physisorption and chemisorptions, adsorption isotherms- Freundlich – Langmuir-BET-Temkin adsorption isotherm-Adsorption on liquid surface-surface tension-Gibbs's adsorption isotherm-surface area determination.

Specific and general acid-base catalysis.Bronsted catalysis law. Acidity functions. Enzyme catalysis (single substrate reactions only).Michaelis-Menton kinetics. Influence of pH and temperature on enzyme catalysis. Kinetics of heterogeneous catalysis (Langmuir Hinshelwood mechanism and Eley-Rideal mechanism)

#### **Text Books**

1. Gurudeep Raj (2006): Advanced Physical chemistry, 32<sup>nd</sup> edition, Goel Publishing House, Krishna Prakashan Media (P) Ltd.
2. Bockris J.O.M and Reddy,A.K.N (2008): Electrochemistry, volumes 1 and 2, Springer.
3. Laidler,J (1987): Chemical Kinetics, 3<sup>rd</sup> edition, Harper & Row.

#### **References**

1. Glasstone,S (2004) : An Introduction to Electrochemistry, Affiliated East West press, New Delhi.
2. Arthur W. Adamson, Alice P. Gast (1997): Physical chemistry of surfaces, 6<sup>th</sup>Edition,Wiley Eastern Ltd.
3. Glasstone, S (2012): Thermodynamics for chemists, East West press.

## SEMESTER I

Subject Code	Title of the Subject	L	T	P	Total of L+T+P	C
PCY15E01	Major Elective-1a (Nanochemistry)	3	3	-	6	3
<b>INSTRUCTIONAL OBJECTIVES</b>						
(i)	To educate students on the basics of nanochemistry					
(ii)	To make students understand the various techniques involved in the characterisation of nanomaterials					
(iii)	To acquire knowledge on the synthesis of nanomaterials					
(iv)	To envision the importance of nanomaterials					

### UNIT I Nanochemistry – An Introduction

Definition of nanodimensional materials - Some historical milestones in the saga of nano forms - Size effects - Importance of nanomaterials - Classification of nanomaterials - Simple examples of unique properties of nanosized materials - Elementary aspects of bionanotechnology - Some important recent discoveries in nanoscience and technology.

### UNIT II Techniques in Nanochemistry

Techniques for characterisation of nanoscale materials (Basic aspects): Atomic force microscopy (AFM)-Transmission electron microscopy (TEM)-Resolution and scanning transmission electron microscopy (STEM) Scanning Tunneling Microscopy (STM) Scanning nearfield optical microscopy (SNOM) and surface plasmon spectroscopy.

### UNIT III Synthesis of Nanomaterials

Chemical methods in preparation of nanomaterials: Sol – gel technique – co-precipitation hydrolysis – sonochemical method – combustion technique – colloidal precipitation – template process.

**Inorganic Nanoparticles and Nanoporous Materials:** Oxide nano particles – Oxomolybdates – Nano catalysis – Porous silicon – Transition and Non transition metal phosphates.

## **UNIT IV Carbon Clusters and Nanostructures**

Nature of carbon bond – New carbon structures – Carbon clusters: Discovery of C<sub>60</sub> – Alkali doped C<sub>60</sub> – Superconductivity in C<sub>60</sub> – Larger and smaller fullerenes. Carbon nanotubes: Synthesis – Single walled carbon nanotubes – Structure and characterization – Mechanism of formation – Chemically modified carbon nanotubes – Doping – Functionalizing nanotubes – Application of carbon nanotubes. Nanowires – Synthetic strategies – Gas phase and solution phase growth – Growth control – Properties.

## **UNIT V Organic Films and Supramolecular Assembly**

Organic films - insulating and passivating layers – electron transfer – Organic nanostructures – Optical properties – Organic semiconductors – Active organic devices. Polymerization – Sizes of polymers – Nanocrystals – Conductive polymers – Block co-polymers. Supramolecular structures – Transition-metal mediated types - Dendritic molecules – Supramolecular dendrimers – Micelles – Biological nanostructures – Examples of proteins

**Applications of nanomaterials:** Applications of Nanoparticle in various fundamental research, industries, medical field and environmental issue; toxicity, biosafety and ethical issue in application of Nanoparticles.

### **Text Books**

1. Rao, C. N. R, Muller, A and Cheetam, A.K. (Eds) (2004): The Chemistry of Nanomaterials, Vol.1, and 2, Wiley – VCH, Weinheim.
2. Poole, C. P and Owens, Jr: F. J (2003): Introduction to Nanotechnology Wiley Interscience, New Jersey.
3. Kenneth J. Klabunde (Ed) (2001), Nanoscale materials in Chemistry, Wiley-Interscience, New York.

### **References**

1. Pradeep, T (2007): Nano: The Essentials in understanding nanoscience and nanotechnology, Tata McGraw Hill, New Delhi.
2. Gleiter, H (2000): Nanostructured Materials: Basic Concepts, Microstructure and Properties.
3. Tang, T and Sheng, P. (2004): Nano Science and Technology – Novel Structures and Phenomena, Taylor & Francis, New York, 2004.

## SEMESTER I

Subject Code	Title of the Subject	L	T	P	Total of L+T+P	C
PCY15E02	Major Elective -1b (Chemistry of Nanoscience and Technology)	3	3	-	6	3
<b>INSTRUCTIONAL OBJECTIVES</b>						
(i)	To understand the basic concept of nano science and technology.					
(ii)	To acquire knowledge about synthesis, preparation and characterization of nanomaterials					
(iii)	To gain knowledge on application of nanomaterials.					

### UNIT I Basic Aspects of Nanotechnology

Introduction and classification - What is nanotechnology - Classification of nanostructures - Nanoscale architecture - How nanoscale dimensions affect properties - Carbon and inorganic nanostructure - self assembled materials - Making thin organic films –nanopatterning surfaces by self-assembly - Templated nanostructures.

### UNITII Characterization Methods

X-ray diffraction - XPS Working Principle, Instrumentation and Applications. Impedance Analysis - Micro hardness –nanoindentation– Nuclear Magnetic Resonance (NMR). Differential scanning calorimeter (DSC)- Thermogravimetric/Differential Thermal Analyzer (TG/DTA)-UV-Visible Spectrophotometer - FTIR – Principle and Applications – Photoluminescence (PL) Spectroscopy.

### UNITIII Lithographic Methods

Introduction – Lithography – Photolithography - Phase-shifting photolithography - Electron beam lithography - X-ray lithography - Focused ion beam (FIB) lithography - Neutral atomic beam lithography - Nanomanipulation and Nanolithography - Soft Lithography - Assembly of Nanoparticles and Nanowires Other Methods for Microfabrication.

#### **UNIT IV Sensors**

Static and Dynamic Characteristics - Inorganic Nanotechnology Enabled Sensors - Gas Sensing with Nanostructured Thin Films - Nanotechnology Enabled Mechanical Sensors - Nanotechnology Enabled Optical Sensors - Magnetically Engineered Spintronic Sensors - Organic Nanotechnology Enabled Sensors - Surface Materials and Surface Modification.

#### **UNIT V Energy Devices**

Nanoscale Electronic and Ionic Transport – Energy Conversion and Storage in Electrochemistry - Overview of the Principles of Operation of Energy Conversion and Storage Devices - Solar Cells - Nanomaterials and Nanostructured Films as Electro active Electrodes - Nanomaterials as Electrolytes - Lithium Ion Batteries - Fuel Cells. Quantum Dot Sensitizers.

#### **Text Books**

1. Robert W. Kelsall, Ian W. Hamley and Mark Geoghegan (2005): Nanoscale Science and Technology John Wiley & Sons, Ltd., UK.
2. Pradeep, T (2008): Nano: The Essentials: Understanding Nanoscience and Nanotechnology, Tata McGraw-Hill Publishing Company Limited, New Delhi.

#### **References**

1. Rao, C. N. R, Thomas, P. J. and Kulkarni, G. U (2007): Nanocrystals: Synthesis, Properties and Applications, Springer .
2. Kourosh Kalantar-zadeh and Benjamin Fry (2008): Nanotechnology - Enabled Sensors, Springer.
3. Guozhong Gao (2004): Nanostructures & Nanomaterials: Synthesis, Properties & Applications, Imperial College Press .

## SEMESTER I

Subject Code	Title of the Subject	L	T	P	Total of L+T+P	C
PCY15104	Inorganic Chemistry Practical	-	-	6	6	3
<b>INSTRUCTIONAL OBJECTIVES</b>						
(i)	To enable the students, to apply the principle in the semi-micro analysis of an inorganic salt mixture.					

### Semi – micro qualitative analysis:

Analysis of mixtures containing two familiar and two less familiar cations from the following W, Pb, Se, Te, Mo, Cu, Cd, As, Sb, Ce, Be, Th, Zr, Ti, V, Cr, Mn, U, Ni, Co, Zn, Ca, Ba, Sr, Li, Mr (insoluble and interfering anion may be avoided).

### Any eight combinations of different salts.

### General scheme for distribution of marks in practical examination

Time: 6 h (One day Examination) Marks: 50 (External) + 50 (Internal)

Identification of ions: 20 Marks

Procedure : 10 Marks

Record : 10 Marks

Viva-Voce : 10 Marks

Internal : 50 Marks

**Total : 100**

### Text Books

1. Vogel's (1987): Qualitative Inorganic Analysis, Revised by G Svehla, 6<sup>th</sup> Edition, Longman.
2. Ramanujam, V.V (1974): "Inorganic Semi-micro Qualitative Analysis", The National Publishing Co, Chennai.

## SEMESTER II

Subject Code	Title of the Subject	L	T	P	Total of L+T+P	C
PCY15201	Inorganic Chemistry-II	4	1	-	5	4
<b>INSTRUCTIONAL OBJECTIVES</b>						
(i)	To understand the various concepts of acids and bases					
(ii)	To understand the basic principles of ionic bond					
(iii)	To gain knowledge in nuclear chemistry					
(iv)	To educate students on the various spectroscopic techniques and its applications to some selected molecules					

### UNIT I Acids and Bases

Acids and Bases: Bronsted and Lewis acids and bases, pH, pK<sub>a</sub>, acid-base concept in non-aqueous media, buffer solution, Protonic acids-Proton Affinities-Differentiation and leveling solvents-Hammett scale-Acidic behavior of the binary hydrides-Cosolvating agents - Oxyacids-Organic acids-Acetic acid and the Inductive Effect, Aromatic Acids and Resonance Effects - Hydrolysis and Aquoacids- Basic precipitations-Amphoteric oxides-Nonprotonic concept of Acid-Base reactions-Lux Concept-Solvent Ion theory of Acids and Bases-Liquid Ammonia, Acetic acid as a solvent, Bromine trifluoride, Dinitrogen tetroxide, Liquid hydrogen chloride-Hard and Soft Acids and Bases - Classification - Acid - Base strength and Hardness and Softness - Symbiosis-Theoretical basis of Hardness and Softness-Electronegativity and Hardness and Softness.

### UNIT II Ionic Bond and Crystal Structure

Radius Ratio rules-Calculation of some limiting radius ratio values for C.N. 3 (planar triangle), C.N. 4 (tetrahedral), C.N. 6 (octahedral). Classification of ionic structures - AX (ZnS, NaCl, CsCl), AX<sub>2</sub> (fluorite, rutile, beta-cristobalite) and AX<sub>3</sub> types (Structures only), Layer structure - CdI<sub>2</sub>, Nickel arsenide structures-Lattice energy-Born-Landee equation derivation-Important points arising from Born-Landee equation-Schottky defect and Frenkel defect-explanation and calculation of number of defects formed per cm<sup>3</sup>-Metal excess defect-F centers and interstitials-Metal deficiency defect-positive ions absent-extra interstitial negative ions-Semiconductors and transistors-Rectifiers-Photovoltaic cell-Transistors-steps in the manufacture of memory chips for computers.

### UNIT III Nuclear Chemistry

Radioactive decay – Theories of decay processes – Laws of radioactivity – Detection and measurement of radiations – Nuclear structure – Composition of nuclei – properties of nuclei – nuclear radii, nuclear spin etc – nuclear forces – its characteristics – Meson field theory – nuclear stability – characteristics – nuclear models – liquid drop, shell and collective models. Artificial radioactivity – Nuclear reactions transmutations, stripping and pickup, fission, fusion, spallation and fragmentation reactions – scattering reactions – nuclear cross section. Nuclear reactors – charged particle accelerators – neutron sources – gamma ray and X-ray sources. Applications of nuclear science in agriculture and biology – neutron activation and isotopic dilution analysis.

### UNIT IV Spectroscopic Techniques

**Infrared and Raman Spectroscopy:** Structural elucidation of coordination compounds containing the following molecules/ions as ligands –  $\text{NH}_3$ ,  $\text{H}_2\text{O}$ ,  $\text{CO}$ ,  $\text{NO}$ ,  $\text{OH}^-$ ,  $\text{SO}_4^{2-}$ ,  $\text{CN}^-$ ,  $\text{SCN}^-$ ,  $\text{NO}_2^-$  and  $\text{X}^-$  (X = halogen).

**Electron Paramagnetic Resonance Spectroscopy:**

EPR of  $d^1$  and  $d^9$  transition metal ions in cubic and tetragonal ligand fields, evaluation of g values and metal hyperfine coupling constants.

### UNIT V Studies and Applications of Lanthanides and Actinides

Spectral and magnetic properties, use of lanthanide compounds as shift reagents, Modern methods of separation of lanthanides and actinides, Organometallic chemistry applications of lanthanide and actinide compounds in Industries

#### Text books

1. Bodie, E. Douglas and Darl H. McDaniel (1970): Concepts and Models in Inorganic Chemistry, Indian Edition, Oxford & IBH Publishing Co, New Delhi.
2. Friedlander, J.W, Kennady and Miller, J.M (1981): Nuclear and Radiochemistry, 3<sup>rd</sup> Edition.
3. Cotton and Wilkinson (1988): Advanced Inorganic Chemistry, 5<sup>th</sup> ed., John Wiley & Sons, New York.

#### References

1. Kaim, W and Schwederski, B (1994): Bioinorganic Chemistry, Inorganic elements in the Chemistry of Life, John Wiley & Sons, New York.
2. James E. Huheey, Ellen A Keiter and Richard L. Keiter (2006): Inorganic Chemistry, Principles of Structures and Reactivity, 4<sup>th</sup> ed, Addison-Wesley, New York.

## SEMESTER II

Subject Code	Title of the Subject	L	T	P	Total of L+T+P	C
PCY15202	Organic Chemistry– II	4	1	-	5	4
<b>INSTRUCTIONAL OBJECTIVES</b>						
(i)	To gain knowledge in the addition reactions and its applications					
(ii)	To acquire knowledge about Elimination reactions					
(iii)	To understand the rearrangements and its mechanisms					
(iv)	To acquire knowledge in photochemistry of organic molecules					
(v)	To gain knowledge in pericyclic concerted reactions					

### UNIT I Addition Reactions

**Addition to Carbon - Carbon Multiple Bonds:** Mechanistic and stereochemical aspects of addition reactions involving electrophiles, nucleophiles and free radicals - regio and chemoselectivity, orientation and reactivity. Addition to cyclopropane ring. Hydrogenation of double and triple bonds - Hydrogenation of aromatic rings and Hydroboration. Sharpless asymmetric epoxidation.

**Addition to Carbon - Hetero Multiple Bonds:** Steric course of addition reactions to C=O and C=N, Cram's rule, Aldol condensation, Cannizzaro, Perkin, Knoevenagel condensations, Claisen - Schmidt, Claisen, Dieckman, Benzoin and Stobbe condensations, Wittig, Grignard, Mannich, Michael reaction. Hydrolysis of Carbon-Nitrogen bond, Isocyanates and isothiocyanates.

### UNIT II Elimination Reactions, Esterification and Hydrolysis

**Elimination Reactions:** Types of elimination reactions, Mechanisms, Stereochemistry and Orientation. Hofmann and Saytzeffrules. Syn elimination versus anti- elimination, competition between elimination and substitution, factors influencing elimination and substitution reaction, dehydration, dehydrogenation, dehalogenations, decarboxylative eliminations, pyrolytic eliminations, molecular rearrangement during elimination and Fragmentation reactions.

**Esterification and hydrolysis:** Mechanism of hydrolysis of Esters, amides and acyl halides, Esterification of acids and trans esterification.

### **UNIT III Rearrangements**

#### **Rearrangement involving migration to electron-deficient carbon**

Wagner-Meerwein, Pinacol-Pinacalone, Benzil-Benzilic, Wolf rearrangements.

#### **Rearrangement involving migration to electron-deficient nitrogen**

Beckmann, Hofmann, Curtius, Lossen, Schmidt rearrangements

#### **Rearrangement involving migration to electron-deficient oxygen**

Baeyer-Villiger oxidation, Hydroperoxide rearrangement.

#### **Rearrangement involving migration to electron-rich carbon**

Favorskii, Stevens, Neber rearrangements

### **UNIT IV Photochemistry**

Organic Photochemistry – Fundamental concepts – Jablonski diagram – Energy transfer, characteristics of photoreactions, photoreduction and photooxidation, photoreactions of ketones and enones, Norrish Type I and II reactions. Photochemistry of alkenes, dienes and aromatic compounds, reactions of unactivated centres – Photolytic cycloadditions and photolytic rearrangements – Photosensitisation – Photoadditions – Barton reaction – PaternoBuchi reaction.

### **UNIT V Pericyclic Reactions**

Concerted reactions – stereochemistry-orbital symmetry and concerted symmetry and correlation diagram – Frontier molecular orbital approach – Woodward and Hoffmann rules – Electrocyclic reactions – cycloaddition reactions – sigmatropic rearrangements – selection rules and examples with simple molecules – 1,3 and 1,5 hydrogen shifts – Cope and Claisen rearrangements.

### **Text Books**

1. March, J (2000): Advanced Organic Chemistry: Reactions, Mechanisms and Structure, 5<sup>th</sup> edition, Wiley.
2. Morrison, R.T. and Boyd, R.N (1992): Organic Chemistry, 6<sup>th</sup> edition, Pearson.

### **References**

1. Finar, I.L (1975): Organic Chemistry, Vol.II, 5<sup>th</sup> edition, ELBS.
2. Bansal, R.K (1975): Organic Reaction Mechanisms, Tata McGraw Hill.
3. Carey F. A and Sundberg, R.J (2002): Advanced Organic Chemistry, Parts A & B, Plenum, 2002

## SEMESTER II

Subject Code	Title of the Subject	L	T	P	Total of L+T+P	C
PCY15203	Physical Chemistry - II	4	-	-	4	4
<b>INSTRUCTIONAL OBJECTIVES</b>						
(i)	To have a good foundation in understanding the physical and mathematical aspects of quantum mechanics.					
(ii)	To become familiar with the aspects of group theory.					
(iii)	To understand and appreciate the concepts of statistical thermodynamics.					
(iv)	To know about electrochemical phenomena.					

### UNIT I Electrochemical Phenomena

Evidences for electrical double layer. Electrocapillary phenomena-Electro capillary curves, Electro-osmosis, electrophoreses. Streaming and Sedimentation potentials. Zeta potentials and its determination by electrophoresis, influence of ions on Zeta potential. Helmholtz-Perrin, Guoy-Chapmann and Stern models of electrical double layer-Applications and limitations. Kinetics of electrode process. Energy barrier at electrode surface- electrolyte interface, overpotential, Butler – Volmer equation, Tafel equation

### UNIT II Chemical Kinetics II

Comparison between gas phase and solution reactions, Cage effect. The influence of the solvent on the reactions between ions and reaction between ions and neutral molecules. Influence of ionic strength on rates of reactions in solution. Arrhenius equation to reaction in solution, Significance of volume and entropy of activation. Primary and secondary salt effect.

### UNIT III Statistical Thermodynamics

Aims of statistical thermodynamics, definition of state of a system, ensembles (microcanonical and canonical) Boltzmann distribution law and its derivation. Boltzmann-Planck equation: partition functions, thermodynamic properties from partition functions, partition function and equilibrium constant; Quantum statistics- Fermi Dirac and Bose-Einstein statistics, photon gas, electron gas according to such statistics: population inversion, negative Kelvin temperature, Einstein's and Debye's theories of heat capacities of solids. Nuclear spin statistics-statistical basis of entropy of H<sub>2</sub> gas- ortho and para nuclear states- Calculation of entropy in terms of ortho-para ratio – residual entropy of H<sub>2</sub> at 0 K.

### **UNIT IV Basics of Group Theory**

Symmetry elements and symmetry operations, group and its properties, Multiplication table, point symmetry groups. Schoenflies symbol, representations of groups by matrices, Irreducible representation of groups, the Great Orthogonality theorem, construction of character table ( $C_{2v}$ ,  $C_{3v}$  only). Applications of group theory to normal modes analysis, Selection rules for fundamental vibrational transition – IR and Raman activity of fundamentals in  $H_2O$ ,  $BF_3$ , – The rule of mutual exclusion.

### **UNIT V Basics of Quantum Mechanics**

de-Broglie's concept, experimental verification- Compton effect - Heisenberg's uncertainty principle – derivation of Schrodinger wave equation - requirements of the acceptable wave function. Operators, linear operators, method of getting the following quantum mechanical operators: Position, Momentum, kinetic energy, potential energy, total energy, angular momentum. Hermiticity and proving the quantum mechanical operators are Hermitian operation- commutator algebra-evaluation of commutators - eigen functions and eigen values - postulates of quantum mechanics.

### **Text Books**

1. Prasad, R. K (2010): Quantum chemistry, 4<sup>th</sup> edition, New Age International.
2. Cotton F. A (2004): Chemical applications of group theory, 3<sup>rd</sup> edition, John Wiley & Sons.
3. Rajaram J (2013): Chemical Thermodynamics: Classical, Statistical and Irreversible, Dorling Kindersley (India) Pvt Ltd.

### **References**

1. Bockris J.O.M and Reddy, A.K.N (2008): Electrochemistry, volumes 1 and 2, Springer.
2. Banwell, C.N (2013): Fundamentals of molecular Spectroscopy, 5<sup>th</sup> edition., TMH, New Delhi.
3. Gilbert W. Castellan (2004): Physical Chemistry, 4<sup>th</sup> edition, Narosa Publishing House.

## SEMESTER II

Subject Code	Title of the Subject	L	T	P	Total of L+T+P	C
PCY15E51	Skill Based Elective-1a ( Analytical Chemistry)	2	2	-	4	4
<b>INSTRUCTIONAL OBJECTIVES</b>						
(i)	To learn the fundamental principles of analytical chemistry.					
(ii)	To understand the difference between accuracy and precision, significance of figures, and be able to apply statistical analysis to rely on or reject results.					
(iii)	To understand the different types of titrations and their applications.					
(iv)	To understand the different chromatographic methods and their applications.					

### UNIT I Errors and Evaluations

Systematic and random errors, Effects of errors on analytical results, Accuracy, precision, Absolute and Relative errors, Significant figures, mean, mean deviation and median, standard deviation, variance, confidence limits, application of statistics, Reliability and rejection of results, Q test, Analysis of variance.

### UNIT II Types of Titrations

Redox titration: Redox potentials, theory and feasibility of redox titration, calculation of potentials at different stages of titrations, redox indicators, their choice and applications.

Precipitation titrations: Theory and types, Mohr, Volhard and Fajan's methods.

Adsorption indicators: theory, choice and applications.

Complexometric titrations: Theory, Stepwise and overall formation constants, Titrations involving chelates (EDTA). Metallochromic indicators: Theory and Choice, Masking and demasking methods and applications.

### UNIT III Chromatography

Solvent extraction, principles, types and applications of paper, column, thin layer, gas and ion exchange Chromatographic techniques. Adsorbents, columns, detection methods, estimations, preparative column, GC, MS techniques: methods, principles and uses.

#### **UNIT IV Thermal Methods of Analysis**

**Thermogravimetric analysis:** Principle, Thermal analysis of silver nitrate, methods of obtaining thermograms, TGA, factors influencing the thermogram, Instrumentation, precautions in the use of thermo balance and applications.

**Differential Thermo Analysis:** Theory, principle, instrumentation and applications, DTA of calcium oxalate monohydrate, thermal analysis of calcium monohydrate.

**Thermometric titrations:** Theory, instrumentation, technique of thermometric titrations applications of thermometric titrations in complexometric and redox titrations.

#### **UNIT V Electro analytical Techniques**

**Polarography:** Introduction, Instrumentation, Ilkovic equation and its verification. Derivation of wave equation, Determination of half wave potential, qualitative and quantitative applications.

**Amperometry:** Basic principles, instrumentation, nature of titration curves and analytical applications.

**Theory of Electrogravimetric analysis,** electrode reactions, overpotential, completeness of deposition, electrolytic separation of metals with controlled cathode potential.

#### **Textbooks**

1. Skoog, D.A, West,D.M and Holler,F.J and Crouch,S.R (2007): Fundamentals of Analytical Chemistry, 8<sup>th</sup>Edn., Saunders College Pub.
2. Miller, J.C and Miller,J.N (1988): Statistics for Analytical Chemistry – Ellis Horwood.Chichester..
3. Skoog, Willard and Dean (1988): Instrumental methods of analysis. 8<sup>th</sup> Edition, East West Press, New Delhi. 1988.

#### **References**

1. Christian, G.D and J.E. O'Reilly (1986): Instrumental Analysis, Allyn & Bacon.
2. Sivasankar,B (2012): Instrumental methods of analysis, Oxford University Press
3. Kaur,H (2001): Instrumental methods of Chemical analysis, PragatiPrakashan, 1<sup>st</sup> Edition, Meerut

## SEMESTER II

Subject Code	Title of the Subject	L	T	P	Total of L+T+P	C
PCY15E52	Skill Based Elective-1b (Advanced Analytical Methods)	2	2	-	4	4
<b>INSTRUCTIONAL OBJECTIVES</b>						
(i)	To know the principle and applications of electrochemical techniques.					
(ii)	To elucidate the molecular structure by applications of chemical spectroscopy.					
(iii)	To understand the basic concepts in surface imaging					
(iv)	To know about biochemical analysis and the applications of sensors.					

### UNIT I Advanced Electrochemical Techniques

Principles, Instrumentation-Electrochemical scanning tunneling microscopy and Electrochemical Atomic force microscopy. Spectro-electrochemistry - Principle, applications. Impedance measurements, Chronomethods - Principles, Chrono-potentiometric – amperometric and coulometric measurements - Instrumentation and Applications.

### UNIT II Applications of Chemical Spectroscopy

Infrared Spectroscopy: Fourier Transform infrared spectroscopy - Applications. Combined Applications - UV, IR, NMR and Mass in the elucidation of molecular structure. Chemical Analysis- Non-destructive techniques- Wavelength and energy dispersive X-ray fluorescence spectroscopy (WDS and EDS)-X-ray absorption spectroscopy (XANES and EXAFS)-Destructive technique- inductively coupled plasma-atomic emission spectroscopy (ICP-AES).

### UNIT III Surface Analytical Techniques

Basic concepts in surface imaging - Electron Spectroscopy for Chemical Analysis (ESCA): Principles, Instrumentation, and Analytical Applications. Auger electron spectroscopy: Principles, Instrumentation, Applications. Surface enhanced Raman Spectroscopy (SERS): Principles, Instrumentation, Nanoparticulate SERS substrates, Surface enhanced resonance Raman scattering (SERRS), SERRS of Ag and Au metal colloids, Thin solid films, Langmuir-Blodgett Monolayers, SERRS mapping and imaging, Applications.

#### **UNIT IV Chemiluminescence**

Introduction, principle, types. Measurement of chemiluminescence, Instrumentation quantitative chemiluminescences. Gas phase chemiluminescence'sanalysis. Electro-chemiluminescence.

#### **UNIT V Bioanalytical Chemistry**

Relevance of Bioassaying and Biochemical Analysis-Spectroscopic methods and fluorimetric methods-Quantitation of Enzymes and Optical Methods of Detection of Enzymes, Immobilization Methods, Mass Spectrometry of Biomolecules, Matrix-assisted laser desorption/ionization (MALDI); Electrochemical Sensors and Biosensors in Bioanalysis-Immunoassaying.

#### **Text Books**

1. Sharma, Y. R. (2007): Elementary Organic Spectroscopy-Principles and Applications, 5<sup>th</sup> Edition S. Chand Publishers.
2. Kamalesh Bansal, (2009): Analytical spectroscopy ,Campus Book International,

#### **References**

1. Fritz Scholz, (2010): Electroanalytical Methods: Guide to Experiments and Applications, 2<sup>nd</sup> Edition, Springer,.
2. D J O'Connor, Brett A Sexton, Roger S C Smart (Eds), (2010): Surface Analysis Methods in Materials Science, 2<sup>nd</sup> Edition, Springer,.
3. John F Watts, John Wolstenholme, (2011): An Introduction to Surface Analysis by XPS and AES, 2<sup>nd</sup> Edition, Wiley VCH,.
4. Susan R. Mikkelsen and Eduardo Cortón, (2004) :Bio Analytical Chemistry, John Wiley & Sons Inc.

## SEMESTER II

Subject Code	Title of the Subject	L	T	P	Total of L+T+P	C
PCY15204	Organic Chemistry Practical	-	1	4	5	3
<b>INSTRUCTIONAL OBJECTIVES</b>						
(i)	To understand the separation methods of organic mixtures.					
(ii)	To impart knowledge in the synthesis of organic compounds.					

### Qualitative Analysis of an organic mixture containing two components.

Pilot separation, bulk separation, analysis, derivatization.

- Detection of elements (N, Cl, S) by Lassaigne's test
- Detection of the following functional groups by systematic chemical analysis: Aromatic amino (-NH<sub>2</sub>), aromatic nitro (-NO<sub>2</sub>), Amido (-CONH<sub>2</sub>, including imide), Phenolic -OH, Carboxylic acid (-COOH), Carbonyl (>C=O); only one test for each functional group is to be reported.

### Preparation of Organic compounds (Single stage).

- 2,4,6-trinitrophenol(picric acid)from phenol (nitration)
- Benzophenoneoxime from Benzophenone (addition reaction)
- Benzophenoneoxime to Benzanilide(rearrangement)
- 4-nitrobenzoic acid to 4-nitrobenzanilide (Substitution)
- o-chlorobenzoic acid from anthranillic acid (Sandmeyer reaction)
- p-benzoquinone from hydroquinone (oxidation)
- 2,4,6-tribromophenol from phenol (bromination)

### General scheme for distribution of marks in practical examination

Time: 6 h (One day Examination) Marks: 50 (External) + 50 (Internal)

Qualitative analysis: 10 Marks

Preparation : 10 Marks

Procedure : 10 Marks

Record : 10 Marks

Viva-Voce : 10 Marks

Internal : 50 Marks

**Total : 100**

**Text Books**

1. Vogel (1996): A Textbook of Practical Organic Chemistry, 5<sup>th</sup> edition, Prentice Hall,
2. Fieser and Fieser (2006): Reagents in Organic Synthesis, Wiley, 2006

**References**

1. Mann & Saunders (1960): Practical Organic Chemistry, 4<sup>th</sup> edition, Longmans.
2. Clarke.H. T (1975): A Handbook of Quantitative & Qualitative Analysis, Arnold Heinemann.
3. March,J (2000): Advanced Organic Chemistry: Reactions, Mechanisms and Structure, 5<sup>th</sup> edition, Wiley.

## SEMESTER II

Subject Code	Title of the Subject	L	T	P	Total of L+T+P	C
PCY15205	Physical Chemistry Practical	-	1	4	5	3
<b>INSTRUCTIONAL OBJECTIVES</b>						
(i)	To motivate the students to understand the principles of chemical kinetics, potentiometric and conductometric titrations.					
(ii)	To impart knowledge with respect to the phase transformation of different systems.					

### LIST OF EXPERIMENTS

1. Determination of rate constant of Acid hydrolysis of an ester.
2. Determination of molecular weight of substances by Rast method.
3. Determination of Critical Solution Temperature (CST) of phenol- water system and effect of impurity on CST.
4. Study of phase diagram of two components forming a simple eutectic.
5. Distribution of benzoic acid between water and benzene.
6. Adsorption of oxalic acid/acetic acid on charcoal.
7. Determination of  $E_a$  of saponification of Ester by conductometry method.
8. Determination of equivalent conductance, degree of dissociation and dissociation constant of weak acid by conductometry.
9. Determination of relative strength of two acids by conductance measurements.
10. Titration of  $\text{AgNO}_3$  vs Halide mixture by potentiometry.
11. Redox titrations ( $\text{MnO}_4^-$  vs  $\text{I}^- / \text{Cr}_2\text{O}_7^{2-}$  vs  $\text{Fe}^{2+}$ ) by potentiometry.
12. Determination of dissociation constant of weak acids by potentiometry.

### General scheme for distribution of marks in practical examination

Time: 6 h (One day Examination) Marks: 50 (External) + 50 (Internal)

Observations including tables and figures: 20 Marks

Procedure : 10 Marks

Record : 10 Marks

Viva-Voce : 10 Marks

Internal : 50 Marks

**Total : 100**

### **Text Books**

1. Yadav, J. B (2005): Advanced Practical Physical Chemistry, 22<sup>nd</sup> edition, Goel publishing House, Krishna Prakashan Media Ltd.
2. Venkatesan, V, Veeraswamy, R and Kulandaivelu, A.R (1997): Basic Principles of Practical Chemistry", 2<sup>nd</sup> edition, Sultan Chand and Sons Publication, New Delhi.

### **References**

1. Findlay's (1985): Practical Physical Chemistry, Revised and edited by B.P. Levitt 9<sup>th</sup> edition, Longman, London.
2. Chatwal, G.R. and Anand, S.K (2000): Instrumental Methods of Chemical Analysis, Himalaya Publishing House, Delhi.

### SEMESTER III

Subject Code	Title of the Subject	L	T	P	Total of L+T+P	C
PCY15311	Organometallic Chemistry	4	2	-	6	4
<b>INSTRUCTIONAL OBJECTIVES</b>						
(i)	To study in depth the properties of organometallic compounds					
(ii)	To gain knowledge in various catalytic processes of organometallic compounds					
(iii)	To understand the various reactions of organometallic compounds					
(iv)	To identify the applications of organometallic compounds					

#### UNIT I Introduction

Compounds with transition metal to carbon bonds: classification of ligands, nomenclature, eighteen electron rule; transition metal carbonyls: range of compounds and structure, bonding, vibrational spectra, preparation, reactions; transition metal organometallics: square planar complexes, metal alkyls, metal alkylidenes, metal alkylidynes and metal arenes.

#### UNIT II $\pi$ Complexes of Unsaturated Molecules

Synthesis, structure, bonding and reactivity of transitional metal complexes with alkenes, cyclopentadienyl (Metallocenes), Benzenoid,  $\pi$ -allyl, and enyl systems. Complexes with cyclic  $\pi$  donors: Cyclopentadiene, benzene, cycloheptatriene and cyclooctatetraene complexes.

#### UNIT III Catalytic Processes

Hydrosilation reaction, hydride elimination, abstraction, cyclooligomerisation, olefin isomerisation, ethylene dimerization using  $\text{RhCl}_3$  catalyst. Fischer Tropsch process, water gas shift reaction. Oxidation of Aldehydes, Cyclohexanol, Cyclohexanone, p-Xylene.

#### UNIT IV Properties and Reactions of Organometallic Compounds

Complex formation, reactions with active oxygen compounds, reactions with halogen, reactions with alkyl halides, acid halides, reactions with oxygen, carbonyls and others.

Metal carbonyls, isocyanides and acetylides: Preparation, structure, reactions of metal carbonyls with alkyl halides, reactions of metal carbonyls with metal alkyls, cyanides and isocyanides complexes, acetalynide complex adduct formation. Complexes: 2, 3, 4, 5, 6 and 7 electron donor carbametallic compounds, aromaticity of cyclopentadienyls.

## **UNIT V Applications of Organometallic Compounds**

Introduction, organometallics in medicine, organometallic compounds in agriculture and horticulture, organometallics in Industry and environmental aspects of organometallic compounds.

### **Text Books**

1. Mehrotra, R. C and Singh, A (2000): Organometallic Chemistry: A Unified Approach, Wiley Eastern.
2. Rochow, E. G (1964): Organometallic Chemistry, Reinhold, New York.
3. Zeiss, H (1960): Organometallic chemistry, Reinhold, New York.

### **References**

1. Stone, F. G. A. and West, R (1988): Advances in Organometallic Chemistry, volume 42, Academic Press, London.
2. Powell, P (1991): Principles of Organometallic Chemistry, 2<sup>nd</sup> Edition., ELBS.
3. Lippard, S. J (1983): Progress in Inorganic Chemistry, Vol. 30, John Wiley.

## SEMESTER III

Subject Code	Title of the Subject	L	T	P	Total of L+T+P	C
PCY15312	Photo Inorganic Chemistry	4	2	-	6	4
<b>INSTRUCTIONAL OBJECTIVES</b>						
(i)	To educate students on the principles of photochemistry					
(ii)	To understand the various photochemical properties of transition metal complexes					
(iii)	To acquire knowledge in charge transfer photochemistry					
(iv)	To know the various photochemical reactions taking place on solid surfaces					

### UNIT I Principles of Photochemistry

Absorption, excitation, photochemical laws, quantum yield. Absorption and emission for complexes with different ground state /excited state for  $ML_6$  complexes. Potential energy function and energy levels for  $ML_6$  complexes. Flash photolysis, stopped flow techniques. Energy dissipation by radiative and non-radiative processes, absorption spectra. Frank-Condon principle, photochemical stages – primary and secondary processes. Jablonski diagram for photochemical process

### UNIT II Photochemical Properties of Transition Metal Complexes

Photo physical process, Photochemical process, Photo substitution reactions, photoredox reactions, Photorearrangement reaction, Prompt and Delayed Photochemical reactions, Photolysis rules and ligand field theory

### UNIT III Charge Transfer Photochemistry

Introduction, charge transfer absorption spectra, types of charge transfer excitations and their energy level scheme for charge transfer excitations, Types of reactions observed by charge transfer metal complexes.

### UNIT IV Ligand Field Photo chemistry of Transition Metal Complexes

Photochemistry  $Cr(III)$  of complexes : Photo-substitutions, properties of ligand field excited states, Photo aquation reactions, photolysis rule , photoisomerization , photo racimization, photoanation reactions, sensitizer, energy transfer process, Mechanism of photosensitization, photo reactive excited state. The Doublet hypothesis, Role of quartet excited states, Photochemistry of  $Co(III)$  complexes : Introduction, energy level diagram, Photo aquations in  $Co(III)$  amine,  $Co(III)$  cyanide complexes,  $Fe(II)$  low spin complexes,  $Ru(II)$  ammine derivative complexes, Photo redox properties of  $Ce(III)$  and  $Ce(IV)$  complexes, photochemistry of  $Cu(II)$  (1,3 diketone) complexes

### **UNITV Photochemical Reactions on Solid Surface**

Introduction, photo electron transfer mechanism, energy level diagram of solid acceptor and donor levels, Examples of photo catalytic metal/mixed metal oxides and their applications, semiconductor supported metal oxides for photolysis of water, Decomposition of organic pollutants, experimental setup, end product of organic products, carbon dioxide reduction, nitrogen fixations, solar energy conversion and its storage. Chemiluminescence's in coordination complexes, Triplet state and Franck-Condon state.

### **Text Books**

1. Adamson, A.W and Fleischauer, P.D (1975): Concepts of Inorganic Photochemistry, Wiley, New York.
2. Ferraudi, G.J (1988): Elements of Inorganic Photochemistry, Wiley, New York.

### **References**

1. Lever, A. B. P (1984): Inorganic Electronic Spectroscopy, Elsevier Science.
2. VeeraReddy, K (1998): Symmetry and Spectroscopy of Molecules, New Age International.
3. Huheey, J. E (1983): Inorganic Chemistry, 3<sup>rd</sup> Edition, Harper and Row Publisher, Singapore.

### SEMESTER III

Subject Code	Title of the Subject	L	T	P	Total of L+T+P	C
PCY15313	Bioinorganic Chemistry	4	2	-	6	4
<b>INSTRUCTIONAL OBJECTIVES</b>						
(i)	To study in depth about the essential elements of life					
(ii)	To gain knowledge about oxygen carriers					
(iii)	To understand the basic concepts of enzymes and acquire knowledge about metalloenzymes					
(iv)	To study in detail about the characterization techniques					

#### UNIT I Introduction

Essential elements in biology, distribution of elements in biosphere, bio-availability, biostability, building blocks of the biosphere; sugars (carbohydrates), fatty acids (lipids), nucleotides (nucleic acids) and amino acids (proteins), Biological importance of water, and the chemistry of biopolymers.

#### UNIT II Oxygen Storage and Transport

O<sub>2</sub> binding properties of heme (haemoglobin and myoglobin) and non-heme proteins hemocyanin & hemerythrin), their coordination geometry and electronic structure, cooperativity effect, Hill coefficient and Bohr Effect; characterization of O<sub>2</sub> bound species by Raman and infrared spectroscopic methods; representative synthetic models of heme and non-heme systems.

#### UNIT III Electron Transfer Proteins and Nitrogen Fixation

Electron transfer proteins - active site structure and functions of ferredoxin, rubredoxin and cytochromes and their comparisons. Cytochrome P<sub>450</sub> and its mechanism of action.

Enzymatic reduction of Nitrogen to Ammonia - Nitrogenase Structure and mechanism. Transition-metal-dinitrogen complexes and insights into N<sub>2</sub> binding, reduction to ammonia. Molybdenum Nitrogenase - Spectroscopic and other studies. Model Systems for Nitrogenase.

#### UNIT IV Enzymes and Metalloenzymes

Enzymes- Nomenclature and classification, chemical kinetics, the free energy of activation and the effects of catalysts, kinetics of enzyme catalyzed reactions-

Michaelis-Menten constant equation- effect of pH, temperature on enzyme reactions, factors contributing to the catalytic efficiency of enzymes.

Metalloenzymes: Zinc enzymes - Carboxypeptidase and Carbonic anhydrase. Iron enzyme - Catalase, Peroxidase and Cytochrome P-450. Copper enzymes – Superoxide dismutase. Molybdenum enzymes - Oxatransferase enzymes, Xanthine oxidase. Vitamin B12 Coenzyme (Adenosyl Coenzyme).

### **UNIT V Characterisation Techniques**

Physical techniques in bioinorganic chemistry: Brief description of the techniques – UV-Vis, Raman, X-Ray crystallography, paramagnetic NMR and EPR spectroscopy, EXAFS, magnetic susceptibility and electrochemistry

#### **Text Books**

1. Lippard and Berg (1994): Principles of Bioinorganic Chemistry, Univ. Science Books.
2. Kaim, W. and Schwederski (1994): Bioinorganic Chemistry: Inorganic perspective in the chemistry of Life, An Introduction and Guide, Wiley, Chichester.

#### **References**

1. David.E.Fenton (1995): Biocoordination Chemistry, Oxford Chemistry Primer.
2. Bertini, Gray, Lippard and Valentine (1988): Bioinorganic Chemistry, Viva books Pvt. Ltd.

## SEMESTER III

Subject Code	Title of the Subject	L	T	P	Total of L+T+P	C
PCY15E53	Skill based Elective-2 (Applications of Computer in Chemistry)	2	2	-	4	4
<b>INSTRUCTIONAL OBJECTIVES</b>						
(i)	To introduce the basics of computers.					
(ii)	To learn C language and its applications in solving problems in Chemistry					

### UNIT I Recapitulation of Computer Basics

PC hardware, operating systems, data storage and backup, networks, information technology. Basic operations using windows.

### UNIT II Computer Programming

Constants, variables, bits, bytes, binary and ASCII formats, arithmetic expressions, hierarchy of operations, inbuilt functions. Elements of the BASIC language. BASIC keywords and commands. Logical and relative operators. Strings and graphics. Compiled versus interpreted languages.

### UNIT III Word Processing- I

Handling numeric data: spreadsheet software (Excel), simple calculations, statistical analysis, plotting graphs using a spreadsheet (radial distribution curves for hydrogenic orbitals, gas kinetic theory, spectral data, pressure-volume curves of van der Waals gas, data from phase equilibria studies), graphical solution of equations, solving equations numerically (e.g. pH of a weak acid ignoring/ not ignoring the ionization of water, volume of a van der Waals gas, equilibrium constant expressions).

### Word Processing- II

Numeric modelling, numerical curve fitting, linear regression (rate constants from concentration- time data, molar extinction coefficients from absorbance data), numerical differentiation (e.g. handling data from potentiometric titrations), integration (e.g. entropy/enthalpy change from heat capacity data). Numerical solution of differential equations (e.g. kinetics).

#### **UNIT IV Molecular Modelling**

Visualization of 3D structures, calculation of molecular structures and properties (e.g., conformational energies of butane, rotation of 1,3-butadiene, distribution of isomers, energies of orbitals and total energy as a function of bond angle for H<sub>2</sub>O, simulation of Diels-Alder reaction, S<sub>N</sub>2 reactions).

#### **UNIT V Chemical Information on the Web**

Chemical abstracts. Structures and properties.

Software: Microsoft Office, ChemOffice, MicrocalOrigin, Scifinder, scopus, literature search (ACS, RSC, Wileyinterscience (Free alternatives: Open Office ([www.openoffice.org](http://www.openoffice.org)), ISIS Draw (<http://www.mdli.com>; registration required), ArgusLab ([www.planaria-software.com](http://www.planaria-software.com))).

#### **Text Books**

1. Noggle, J. H (1985):Physical chemistry on a Microcomputer. Little Brown & Co.
2. Venit, S.M (1996):Programming in Basic: Problem solving with structure and style.Jaico Publishing House,Delhi.

#### **References**

1. Engel, T. & Reid, P (2010): Physical Chemistry, 2<sup>nd</sup> Ed. Pearson.

### SEMESTER III

Subject Code	Title of the Subject	L	T	P	Total of L+T+P	C
PCY15314	Advanced Inorganic Chemistry Practical	-	-	6	6	2
<b>INSTRUCTIONAL OBJECTIVES</b>						
(i)	To motivate the students to understand separation and gravimetric techniques.					
(ii)	To impart knowledge of synthesis and characterization of the inorganic complexes.					
(iii)	To practice the estimation of metal ions by spectrophotometric methods.					

**A. Quantitative analysis:**

Separation and estimation of mixtures by volumetric and gravimetric methods: some typical recommended mixtures are:

(i) Cu-Ni (ii) Cu- Fe (iii) Cu-Zn (iv) Ba-Ca(v) Ni-Zn.

**B. Inorganic complex preparation and characterization:**

1. tris-triphenylphosphine copper(I) nitrate
2. tris-acetylacetonato iron (III)
3. cisandtrans-dichlorobis (ethylenediamine) cobalt (III) chloride
4. bispyridine iodide nitrate
5. trans-bisglycinato copper(II)
6. Prussian blue
7. Tetrammine copper(II)
8. Hexamine cobalt(II) chloride
9. Hexamine nickel(II) chloride

**C. Spectrophotometric estimation:(any three)**

Cu, Mn, Ni, Fe, V, Cr, Co.

### **General scheme for distribution of marks in practical examination**

Time: 6 h (One day Examination) Marks: 50 (External) + 50 (Internal)

Quantitative analysis (A) : 20 Marks

Preparation (B) : 10 Marks

Record : 10 Marks

Viva-Voce : 10 Marks

Internal : 50 Marks

**Total : 100 Marks**

### **References**

1. Bassett et al, J (1989): Text Book of Quantitative Chemical Analysis, 5<sup>th</sup> Edition, ELBS, Longman, U.K.
2. Vogels (2002): Textbook of Quantitative Chemical Analysis, 6<sup>th</sup> Edition.
3. Gurdeepraj (2001): Advanced Practical Inorganic Chemistry, Goel Publishing House.

## SEMESTER IV

Subject Code	Title of the Subject	L	T	P	Total of L+T+P	C
PCY15E03	Solid State Chemistry	3	-	-	3	3
<b>INSTRUCTIONAL OBJECTIVES</b>						
(i)	To study in depth about amorphous solids					
(ii)	To gain knowledge about ceramic and composite materials					
(iii)	To understand the mechanical properties of materials					
(iv)	To study the magnetic behavior of compounds					

### UNIT I Introduction

Crystalline and amorphous solids-crystal systems, point groups, types of close packing - hcp and ccp, packing efficiency, radius ratios; polyhedral description of solids; structure types -NaCl, ZnS, Na<sub>2</sub>O, CdCl<sub>2</sub>, wurtzite, nickel arsenide, CsCl, CdI<sub>2</sub>, rutile and Cs<sub>2</sub>O, perovskite ABO<sub>3</sub>, K<sub>2</sub>NiF<sub>4</sub>, spinels.

### UNIT II Amorphous Solids and Semiconductor Devices

Amorphous solid, oxide glasses, chalcogenide glasses, amorphous carbon, graphite, diamond, alkaline graphite compounds.

Diodes, p-n junction, transistor, interstitial and cheverel compound, superconductivity compound, properties of super conductivite compounds.

### UNITIII Ceramic and Composite Materials

Ceramic materials- Definition, types, polarization, polarizibility, electric properties, dielectric properties, piezoelectric, pyroelectric and ferroelectric effect.

Composite- Definition, fiber, concrete, asphalt, wood, several other types of composite material.

### UNIT IV Electrical and Optical Conductivity of Solids

Electrical conductivity, origin of valence and conduction band in solids, classification of material, time dependent of conductivity, mobility of charge carriers, metal-metal junction, metal- semiconductor junction, optical properties of material, refractive index, inorganic colored solid, LASER and photoluminescence.

### UNIT V Mechanical Properties and Magnetic Behavior of Materials

Mechanical behaviour, mechanical properties, fractures of metal, ductile fracture, brittle fracture, toughness and impact testing.

Introduction to magnetism, behavior of substance in a magnetic field, magnetic moments, Diamagnetism, Paramagnetism, Experimental determinations of susceptibility, Ferromagnetism, Antiferromagnetism, Ferrimagnetions, Magnetizations of a ferromagnetic substance.

### **Text Books**

1. Wells, A. F (1984) :Structural Inorganic Chemistry, 5<sup>th</sup>Edition .
2. Huheey, J. E (1983): Inorganic Chemistry, 3<sup>rd</sup> Edition, Harper and Row Publisher, Singapore.
3. West, A. R (1999): Basic Solid State Chemistry, 2<sup>nd</sup>Edition, John Wiley and Sons Ltd.

### **References**

1. Haney, N. B (1967): Solid State Physics, Prentice-Hall.
2. Keer, H. V (1993): Principles of Solid State, New Age International Publishers.
3. Pillai, S. O (2005): Solid State Physics, New Age International Publishers.

## SEMESTER IV

Subject Code	Title of the Subject	L	T	P	Total of L+T+P	C
PCY15E08	Medicinal Inorganic Chemistry	3	-	-	3	3
<b>INSTRUCTIONAL OBJECTIVES</b>						
(i)	To gain knowledge on various toxic metals					
(ii)	To acquire knowledge on the interactions of metal ions and its complexes					
(iii)	To identify the various metal complexes as drugs					
(iv)	To acquire knowledge on the mode of action of various therapeutic drugs					

### **UNIT I Introduction to Metal Ion Toxicity**

Metal ion toxicity in humans and animals. General aspects of Pb(II), Cd(II), and Hg(II) toxicity, biochemical and physiological effects due to Pb(II), Cd(II), and Hg(II) ion toxicity. Detoxifications using chelating agents.

### **UNIT II Interactions of Metal Ions and Metal Complexes**

Structure and functions of amino acids, proteins, peptides, enzymes, nucleosides, nucleotides and comparative study of structures and functions of these biomolecules. Metal ion binding sites present in amino acids, peptides, proteins, enzymes, nucleoside and nucleotide. Interactions of metal ion and metal complexes with these biomolecules.

### **UNIT III Metal Complexes as Drugs**

Introduction to Pt(II) chemistry – Thermodynamic and kinetic principles – Cis and Trans influences.

Discovery applications and structure-effect relationships. CisPt(NH<sub>3</sub>)<sub>2</sub>Cl<sub>2</sub> and its mode of action. Drug resistance and DNA repair mechanism.

**UNIT IV Bio-energetics and ATP cycle:** Metal complexes in transmission of energy, chlorophylls, photosystem I and photosystem II in cleavage of water, Model systems.

**Metallo enzymes:** Apoenzymes, Holoenzyme & Coenzyme. The principle involved and role of various metals in i) Zn-enzyme- Carboxyl peptidase & Carbonic anhydrase. ii) Fe-enzyme-Catalase Peroxidase & Cytochrome P-450 iii) Molybdenum-Oxotransferase enzymes, Xanthine oxidase.

## **UNIT V Metal Complexes in Clinical Chemistry**

Theory and mode of action of therapeutic chelating agents, Single ligand Chelation Therapy –Aminopolycarboxylic acids, Desferrioxamine, pencillamine, triethylenetetramine Mixed ligand chelation therapy - Metallothionens in detoxification. Role of metal ions in the action of antibiotics-Bleomycin, adriamycin and tetracyclines. Gold-Containing drugs used in therapy of Rheumatoid arthritis, Atherapeutic agent for Menkes disease: Copper-histidine - Anti viral chemotherapy and metal peptide interaction.

### **Text Books**

1. Helmut Sigel (1973): Metal ions in biological system, Vol.9, Marcel Dekker INC, New York and Basel.
2. Helmut Sigel (1973): Metal ions in biological system (Concepts on metal ion toxicity), Vol.7 Marcel Dekker INC, New York and Basel.
3. Kaim, Wand Schewederski, B (1994): Bioinorganic Chemistry: Inorganic Elements in the Chemistry of Life, John Wiley & Sons, New York, USA.

### **References**

1. Guy Berthon (1995): Handbook of Metal-Ligand interactions in Biological fluid, Bioinorganic medicine, Vol.2, Marcel Dekker INC, New York and Basel.
2. Rosette M. Roat- Malone (2007): Bioinorganic Chemistry: A Short Course, Wiley.
3. Ivano Bertini (1994): Bioinorganic Chemistry, Mill Valley, CA: University Science Books.

## SEMESTER IV

Subject Code	Title of the Subject	L	T	P	Total of L+T+P	C
PCY15401	Seminar*	-	-	1	1	1
INSTRUCTIONAL OBJECTIVES						
(i)	To make the student understand and present the topic of interest related to chemistry in a class room					

### Purpose

To train the students in preparing and presenting technical topics.

### Mode of Assessment

The students are expected to give at least two presentations on their topics of interest which will be assessed by a committee constituted for this purpose. The students will be tested both in subject matter and mode of presentation.

The components in the subject matter include :

Knowledge in the subject and plan of work, originality, logical development, answer to the questions, summary and references.

Component in the mode of presentation include:

1. Communication skill
2. Usage of audio visual aids
3. Language and diction

This course is mandatory and a student has to pass the course to become eligible for the award of degree.

The Committee constituted by the Head of the Department will evaluate the presentation and will award the marks based on

Economy of time

Voice as a tool of communication

Blackboard use and teaching aids

Comprehensible arguments and organization.

Accessible delivery

Accessible visuals in support of arguments.

Relating to the audience

### Mark Distribution

Abstract submission :05 Marks

Presentation :10 Marks

Question session :05 Marks

**Total 20Marks**

## SEMESTER IV

Subject Code	Title of the Subject	L	T	P	Total of L+T+P	C
PCY15402	Project Work	-	-	28	28	14

### PURPOSE

To undertake research in an area related to the program of study.

### INSTRUCTIONAL OBJECTIVE

M.Sc. projects should be socially relevant and research oriented ones.

Each student is expected to do an individual project. The project work is carried out in two phases – Phase I in III semester and Phase II in IV semester.

The project internally will be evaluated by the concerned guide.

The student shall be capable of identifying a problem related to the program of study and carry out wholesome research on it leading to findings which will facilitate development of a new/improved product, process for the benefit of the society.

Phase II of the project work shall be in continuation of Phase I only. At the completion of a project the student will submit a project report, which will be evaluated (end semester assessment) by duly appointed examiner(s). This evaluation will be based on the project report and a viva voce examination on the project.

The method of assessment for both Phase I and Phase II is shown in the following table:

### Assessment Tool Weightage

Review I: 40 Marks

Review II : 40 Marks

### Review I & II Mark Distribution

Attendance : 5 Marks

Novelty : 5 Marks

Submission of hard copy : 15 Marks

Presentation : 10 Marks

Question session : 5 Marks

**Total 40Marks**

### Seminar- 20 Marks

Report evaluation : 70 Marks

Viva : 30 Marks

**Total 200 Marks**

Student will be allowed to appear in the final viva voce examination only if he / she has submitted his / her project work in the form of paper for presentation / publication in a conference / journal and produced the proof of acknowledgement of receipt of paper from the organizers / publishers.

