

# **M.Sc. CHEMISTRY SYLLABUS 2023-24**

Course Structure						
Course Code	Subject	L	T	P	Credit	Contact Hours
<b>SEMESTER-I</b>						
20MSC501T	Organic Chemistry-I	3	0	0	3	3
20MSC501P	Organic Chemistry-I Practical	0	0	3	1.5	3
20MSC502T	Inorganic Chemistry-I	3	0	0	3	3
20MSC502P	Inorganic Chemistry-I Practical	0	0	3	1.5	3
20MSC503T	Physical Chemistry-I	3	0	0	3	3
20MSC503P	Physical Chemistry-I Practical	0	0	3	1.5	3
20MSC504T	Analytical Chemistry-I	2	0	0	2	2
20MSC504P	Analytical Chemistry-I Practical	0	0	3	1.5	3
20MSC505T	Environmental and Green Chemistry	2	0	0	2	2
<b>Total</b>		<b>13</b>	<b>0</b>	<b>12</b>	<b>19</b>	<b>25</b>
<b>SEMESTER-II</b>						
20MSC506T	Organic Chemistry-II	3	0	0	3	3
20MSC506P	Organic Chemistry- II Practical	0	0	3	1.5	3
20MSC507T	Inorganic Chemistry-II	3	0	0	3	3
20MSC507P	Inorganic Chemistry- II Practical	0	0	3	1.5	3
20MSC508T	Physical Chemistry-II	3	0	0	3	3
20MSC508P	Physical Chemistry- II Practical	0	0	3	1.5	3
20MSC509T	Analytical Chemistry-II	2	0	0	2	2
20MSC509P	Analytical Chemistry- II Practical	0	0	3	1.5	3
20MSC510T	Theoretical & Computational Chemistry	2	1	0	3	5
20MSC510P	Theoretical & Computational Chemistry Practical	0	0	2	1	2
<b>Total</b>		<b>13</b>	<b>1</b>	<b>14</b>	<b>21</b>	<b>30</b>
<b>SEMESTER-III</b>						
	Stream Elective-I	3	0	0	3	3
	Stream Elective-II	3	0	0	3	3
	Stream Elective-III	3	0	0	3	3
	Stream Elective-IV	3	0	0	3	3
	Stream Elective-V	3	0	0	3	3
	Stream Elective Lab*	0	0	3	1.5	3
20RM601	Research Methodology	1	0	0	1	1
20MSC635P	Research Project Phase I*	0	0	16	8	16
<b>Total</b>		<b>11</b>		<b>19</b>	<b>20.5</b>	<b>35</b>
<b>SEMESTER-IV</b>						
20MSC636P	Research Project (Experiment, Dissertation & Seminar)	0	0	40	20	40
<b>Total</b>		<b>0</b>	<b>0</b>	<b>40</b>	<b>20</b>	<b>40</b>
<b>Total course credits</b>		<b>37</b>	<b>1</b>	<b>85</b>	<b>80.5</b>	<b>123</b>

\*Note- The students will chose the respective specialization streams in Sem-III. Each specialization has 5 course and one specialization lab. Further, the project phase- I & II will be in line with specialization chosen by the student.

## Stream Electives Theory

<b>Analytical Chemistry</b>		
I.	20MSC611T	Atomic & Molecular Spectroscopy
II.	20MSC612T	Advanced Instrumental Techniques-I
III.	20MSC613T	Advanced Instrumental Techniques-II
IV.	20MSC614T	Electro Analytical and Radio Analytical Methods of Analysis
V.	20MSC615T	Method Development and Validation
<b>Medicinal Chemistry</b>		
I.	20MSC616T	Chemical Biology
II.	20MSC617T	Medicinal Chemistry-I
III.	20MSC618T	Medicinal Chemistry-II
IV.	20MSC619T	Pharmaceutical Chemistry and Biochemistry
V.	20MSC620T	Formulation Development
<b>Industrial Chemistry</b>		
I.	20MSC621T	Paints, pigments & cosmetics
II.	20MSC622T	Polymer Chemistry & Composite Materials
III.	20MSC623T	Materials and Nano Chemistry
IV.	20MSC624T	Fine chemicals (Petrochemicals, oil, soap and pesticides)
V.	20MSC625T	Petroleum Chemistry & Catalysis
<b>Organic Chemistry</b>		
I.	20MSC626T	Reagents and organic synthesis
II.	20MSC627T	Stereochemistry and Photochemistry
III.	20MSC628T	Heterocycles and vitamins
IV.	20MSC629T	Chemistry of Natural Products
V.	20MSC630T	Asymmetric synthesis/catalysis

## Stream Elective Lab

<b>Course Code</b>	<b>Subject</b>
20MSC631P	Analytical Chemistry Lab
20MSC632P	Pharmaceuticals Chemistry Lab
20MSC633P	Industrial Chemistry Lab
20MSC634P	Organic Chemistry Lab

20MSC501T					Organic Chemistry I					
Teaching Scheme					Examination Scheme					
L	T	P	C	Hrs/Week	Theory			Practical		Total Marks
					MS	ES	IA	LW	LE/Viva	
3	0	0	3	3	25	50	25	--	--	100

**COURSE OBJECTIVES**

- To acquire the basic concepts of reactivity and stability of reactive intermediates.
- To understand and analyze the 3D structures of molecules.
- To demonstrate the basic understanding of chirality.
- To explain the basic knowledge of pericyclic reactions and photochemistry.
- To show the reactivity of different types of heterocycles.

**UNIT 1 ORGANIC REACTION MECHANISM AND STUDY OF REACTIVE INTERMEDIATES****10Hrs.**

Aliphatic Nucleophilic Substitution: The SN<sub>2</sub>, SN<sub>1</sub>, mixed SN<sub>1</sub> and SN<sub>2</sub> and SET mechanisms. The S<sub>N</sub>i mechanism. Nucleophilic substitution at an allylic, aliphatic trigonal and a vinyl carbon. Reactivity effects of substrate structure, attaching nucleophile, leaving group and reaction medium. Electrophilic Substitution: Aliphatic: Bimolecular mechanisms: SE<sub>1</sub>, SE<sub>2</sub> and SE<sub>i</sub>. The SE<sub>1</sub> mechanism, electrophilic substitution accompanied by double bond shifts. Effect of substrates, leaving group and the solvent polarity on the reactivity. Aromatic: The arenium ion mechanism, orientation and reactivity, energy profile diagrams. The ortho/para ratio, ipso attack, orientation in other ring systems. Quantitative treatment of reactivity in substrates and electrophiles.

Aromatic Nucleophile Substitution: The S<sub>N</sub>Ar, SN<sub>1</sub>, benzyne and SRN<sub>1</sub> mechanisms. Reactivity; effect of substrate structure, leaving group and attacking nucleophile. Elimination Reactions: The E<sub>2</sub>, E<sub>1</sub> and E<sub>1</sub>cB mechanisms and their spectrum. Orientation of the double bond. Reactivity; effects of substrate structures, attaching base, the leaving group and the medium.

Generation, structure, stability, and reactions involving Carbocations, Carbanions, Radicals, carbenes, carbenoids and nitrenes. The Hammett equation and linear free energy relationship (sigma-rho) relationship, Taft equation.

**UNIT 2 STEREOCHEMISTRY****10Hrs.**

Configurational and conformational isomerism in acyclic and cyclic compounds. Configuration nomenclature D, L, R, S and E, Z nomenclature. Conformational analysis of cycloalkanes, cyclohexenes, cyclohexanones, halocyclohexanones, decalins, decalols, and decalones; effect of conformation on reactivity. Elements of symmetry, chirality, molecules with more than one chiral center, projection formulae (i) Fischer (ii) Sawhorse (iii) Newman (iv) Flying Wedge; threo and erythro isomers, methods of resolution, optical purity, enantiotopic and diastereotopic atoms, groups and faces, stereospecific and stereoselective synthesis. Optical activity in the absence of chiral carbon; Stereochemistry and configuration of allenes, spiranes, alkylidene cycloalkanes, adamantanes, catenanes, biphenyls (atropisomerism), bridged biphenyls, ansa compounds and cyclophanes. Asymmetric induction: Cram's, Prelog's and Horeau's rule

**UNIT 3 INTRODUCTION TO PERICYCLIC AND PHOTOCHEMISTRY****12Hrs.**

Pericyclic Reactions: Molecular orbital symmetry, Frontier orbitals of ethylene, 1,3-butadiene, 1,3,5-hexatriene and allyl system. Classification of pericyclic reactions. Woodward-Hoffmann correlation diagrams. FMO and PMO approach. Electrocyclic reactions - conrotatory and disrotatory motions, 4n, 4n+2 and allyl systems. Cycloadditions - antarafacial and suprafacial additions, 4n and 4n+2 system, 2+2 addition of ketenes, 1, 3 dipolar cycloadditions and cheletropic reactions. Sigmatropic rearrangements - suprafacial and antarafacial shifts of H, sigmatropic shifts involving carbon moieties, 3, 3- and 5, 5-sigmatropic rearrangements. Claisen, Cope and Aza-Cope rearrangements. Ene reaction. Photochemistry: Introduction, Jablonskii diagram, energy pooling, photosensitization, Quantum yields, solvent effects, Stern-Volmer plot, intersystem crossing, delayed fluorescence, photosensitization, and energy transfer reactions.

**UNIT 4 FUNDAMENTALS OF HETEROCYCLIC COMPOUNDS****8 Hrs.**

Synthesis and reactivity of common heterocyclic compounds containing one or two heteroatoms (O, N, S).

Synthesis and reactions of Three membered and four membered Heterocycles i.e. aziridines, oxiranes, thiranes, azetidines, oxitanes and thietanes. Synthesis and reactions of benzopyrroles, benzofurans and benzothiophenes. Synthesis and reactivity of furan, thiophene, pyrrole, pyridine, quinoline, isoquinoline and indole; Skraup synthesis, Fisher indole synthesis.

**COURSE OUTCOMES****40 Hrs**

On completion of the course, student will be able to

CO1 – Understand the basic concepts of organic chemistry. CO2 –

Analyse the three-dimensional structure of a molecule

CO3 – Comment upon the stability and reactivity of various organic compounds. CO4 –

Differentiate between various types of reaction intermediates.

CO5 – Acquire knowledge about basic concepts of the photochemistry. CO6 –

Understand the basic concepts of heterocyclic chemistry

**TEXT/REFERENCE BOOKS**

1. Advanced Organic Chemistry by J. March, John Wiley & Sons, 1992
2. Stereochemistry of Carbon Compounds by E. J. Eliel, McGraw Hill
3. Stereochemistry of Organic Compounds by D. Nasipuri, Wiley, 1994.
4. Organic Chemistry by P.Y. Bruice, Prentice Hall, 1998.
5. Organic Reaction and their Mechanism by P.S. Kalsi, New Age, 1996.
6. Frontier Orbital and Organic Chemical Reactions by I. Fleming, John Wiley, 1976.
7. Heterocyclic Chemistry by T. R. Gilchrist, Longman, 1989.

**END SEMESTER EXAMINATION QUESTION PAPER PATTERN**

Max. Marks: 100

Exam Duration: 3 Hrs

Part A/Question: &lt;Details&gt;

&lt;&gt; Marks

Part B/Question: &lt;Details&gt;

&lt;&gt; Marks

20MSC501P					Organic Chemistry-I Practical					
Teaching Scheme					Examination Scheme					
L	T	P	C	Hrs/Week	Theory			Practical		Total Marks
					MS	ES	IA	LW	LE/Viva	
0	0	3	1.5	3				50	50	100

**COURSE OBJECTIVES**

- Learn safety measures while working in the laboratory
- Learn different separation techniques
- Knowledge about different organic transformations
- Synthesize different organic compounds
- To familiarizes with chemicals and instruments

**LIST OF EXPERIMENTS**

1. Separation of various organic compounds using thin layer chromatography.
2. Separation of the given mixture of compounds using column chromatography.
3. To synthesis Phthalic anhydride using Phthalic acid by sublimation method.
4. To prepare Phthalimide using Phthalic anhydride.
5. Preparation of Cinnamic acid by Perkin's reaction.
6. Preparation of p-Nitro Aniline from p-nitro acetanilide.
7. Preparation of Benzoic acid from Benzaldehyde and Benzyl alcohol by cannizaro reaction.
8. Preparation of Dibenzalacetone from acetone.
9. Preparation of 2, 2'-Dihydroxy, 1, 1'-binaphthyl (BINOL) from 2-naphthol.
10. Preparation of Benzoic acid from Toluene using potassium permanganate

**COURSE OUTCOMES**

On completion of the course, student will be able to

- CO1– Separate various organic compounds  
 CO2– Perform different organic reactions  
 CO3– Prepare various organic compounds  
 CO4– Understand different separation techniques  
 CO5– Comprehend Perkin's reaction  
 CO6– Design different organic transformations

**TEXT/REFERENCE BOOKS**

1. Comprehensive practical organic chemistry: Quantitative analysis by V.K Ahluwalia, Renu Aggarwal; Universities press; ISBN 13: 978 81 7371 273 9
2. A. K. Nad, B. Mahapatra & A. Ghosal, An Advanced Course in Practical Chemistry, New Central, 2007. Vogel's Text Book of Practical Organic Chemistry (5th Edn).
3. Finar, I. L. Organic Chemistry (volume 1), Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).

**SEMESTER EXAMINATION PATTERN****Max. Marks: 100**

LW(Daily lab performance plus journal maintain each 25 marks)  
 LE (Viva-voce plus Lab examination each 25 marks)

**Exam Duration: 3 Hrs**

50 Marks  
 50 Marks

20MSC502T					Inorganic Chemistry I					
Teaching Scheme					Examination Scheme					
L	T	P	C	Hrs/Week	Theory			Practical		Total Marks
					MS	ES	IA	LW	LE/Viva	
3	0	0	3	3	25	50	25	--	--	100

**COURSE OBJECTIVES**

- To acquire the basic knowledge of advanced inorganic chemistry
- To develop the concepts of inorganic rings, chains, cages, clusters frameworks
- To gain the knowledge on molecular materials and learn about their applications
- To develop an insight into the chemistry of transition metals and inner-transition elements
- To attain an understanding of magnetic properties of transition and inner-transition elements
- To understand the basic concepts of bioinorganic chemistry and the application of metals in medicine

**UNIT 1: Inorganic Chains, Rings, Cages, Clusters & Framework.****12 Hrs.**

Introduction; Boranes; Carboranes; Metallocarboranes; Borazines; Phosphazenes; Phosphorus-Oxygen; Phosphorus-Sulfur; Sulfur-Nitrogen Compounds; Silicates; Silicones. Iso- and Hetero-poly anions; Framework Structures; Organic-

Inorganic Hybrid Materials; Porous Materials; Molecular Clusters to Materials; Applications in Energy Storage; Hydrogen Economy; CO<sub>2</sub> Sequestration.

**UNIT 2: Chemistry of Transition Metals.****8 Hrs.**

Nomenclature; Isomerism; Chelate Effect; Macrocyclic Ligands. Bonding in Coordination Complexes: Crystal-Field Theory; d-orbital Splitting in Octahedral, Tetrahedral, Square Planar Geometries; Molecular Orbital Theory; p-bonding; Jahn-Teller effect; Electronic Spectra: d-d transitions; Orgel and Tanabe-Sugano Diagrams; Charge-Transfer Spectra.

**UNIT 3: Magnetic Properties and Inner Transition Elements.****12 Hrs.**

Paramagnetism; Ferro- and Antiferro-magnetism; Diamagnetism; Pascal Constants; Curie Equation; Russell-Saunders's Terms; Determination of Magnetic Susceptibility; Magnetic Properties of First Transition Series Metal Ions and Lanthanides. CFT and its Limitations; Calculations of  $Dq$ ,  $B$  and  $b$ -parameters; Anomalous Magnetic Moment; Magnetic

Exchange Coupling and Spin Crossover.

Comparison of Characteristics of Inner Transition and Transition metals. Magnetic Properties and Absorption Spectra of Lanthanides and Actinides. Lower Oxidation State Compounds. General Chemistry of Actinides.

**UNIT 4: Bioinorganic Chemistry.****8 Hrs.**

Introductions; Oxygen Carriers; Porphyrins; Metalloporphyrins; Structure and Functions of Hemoglobin and Myoglobin; Synthetic Oxygen Carrier Model Systems; Nitrogen Fixation: Biological Nitrogen Fixation; Nitrogenase; Model for Nitrogenase; Metal-N<sub>2</sub> Complexes; Photosynthesis and Chlorophyll. Metal Transport and Storage: Transferrin; Ferritin;

Siderophores; Metals in Medicine.

**COURSE OUTCOMES Max.****40 Hrs**

On completion of the course, student will be able to

**CO1** – Understand the concepts of inorganic rings, chains, cages, clusters frameworks.

**CO2** – Demonstrate the theoretical knowledge of inorganic compounds, molecular materials and evaluate their applications.

**CO3** – Knowledge of transition metals and inner-transition elements.

**CO4** – Apply the theoretical knowledge to interpret the spectroscopic characteristics of transition metal complexes.

**CO5** – Explain the magnetic properties of the transition and inner-transition elements.

**CO6** – Illustrate the importance of bioinorganic chemistry and metals in medicine for diagnostic/therapeutic use.

**TEXT/REFERENCE BOOKS**

1. Inorganic Chemistry: Principles of Structure and Reactivity by J. E. Huheey; E. A. Keiter and R. L. Keiter; 4th ed. Harper Collins 1993
2. Concepts and Models of Inorganic Chemistry by B. E. Douglas; D. H. McDaniel and J. J. Alexander; John Wiley; 1993; 3rd ed.
3. Organotransition metal chemistry; Fundamental concept and applications; A. Yamamoto; John Wiley; 1986.
4. The organometallic Chemistry of transition metals; R.H. Crabtree; John Wiley; 1994.
5. Organometallic chemistry: A unified concept; R C Melhotra; New Age International; 2007
6. Chemistry of the Elements by N. N. Greenwood and A. Earnshaw; Pergamon; 1985.
7. Advanced Inorganic Chemistry by F. A. Cotton; G. W. Wilkinson; 5th edition; John-Wiley & Sons; 1988.
8. Physical Methods in Chemistry by R. S. Drago; Saunders; 1992
9. Organometallic Photochemistry by G. L. Geoffrey and M. S. Wrighton; Academic Press; 1979.
10. Fundamentals of Photochemistry by K. K. Rohatagi-Mukherjee; Wiley Eastern; 1978.
11. Inorganic and Organometallic Photochemistry by M. S. Wrighton; ACS Pub.; 1978.
12. Photochemistry of Co-ordination compounds by V. Balzani and V. Carasiti; Academic Press; 1970.

**END SEMESTER EXAMINATION QUESTION PAPER PATTERN****Max. Marks: 100****Exam Duration: 3 Hrs**

Part A/Question: 10 multiple choice questions 1 mark each

10 Marks

Part B/Question: 10 short answer type questions of 2 marks each with internal choice

20 Marks

Part C/Question: 4 Questions of 15 marks each with internal choice

60 Marks

Part D/Question: 1 Questions of 10 marks with internal choice

10 Marks

20MSC502P					Inorganic Chemistry I Practical					
Teaching Scheme					Examination Scheme					
L	T	P	C	Hrs/Week	Theory			Practical		Total Marks
					MS	ES	IA	LW	LE/Viva	
0	0	3	1.5	3	--	--	--	50	50	100

**COURSE OBJECTIVES**

- To learn experimental techniques for the quantitative estimation of different inorganic samples
- To acquire the skill to separate mixture of ions by chromatography
- To gain practical knowledge of ore analysis
- To develop the skill for alloy analysis
- To demonstrate the skills for spectrophotometric estimation of coordination complexes

1. Separation of Cations and Anions by Ion exchange/ Thin Layer Chromatography.

**2. Ore analysis (At least two)**

- a. Determination of Manganese in pyrolusite
- b. Determination of Copper and iron from chalcopyrite.
- c. Determination of iron from hematite.
- d. Quantitative estimation of CaCO<sub>3</sub> in dolomite

**3. Alloy analysis (At least two)**

- a. Stainless Steel (Fe, Cr and Ni)
- b. Steel or Mild Steel (Fe and Cr)
- c. Bronze (Cu and Zn)
- d. Gun metal (Cu, Sn)
- e. Solder (Pb and Sn)
- f. Nichrome (Fe, Ni, Cr)
- g. Cupronickel (Cu and Ni)

**4. Spectrophotometric Estimation (Any one)**

- a. Colourimetric estimation of Fe(III) (as thiocyanate complex)
- b. Colourimetric estimation of Fe(II) and Fe(III) in a mixture as Fe(II)-1,10-phenanthroline complex.

**5. Quantitative analysis (At least three)**

- a. Gravimetric estimation of Zn(II) as Zn(NH<sub>4</sub>)(PO<sub>4</sub>)
- b. Gravimetric estimation of Cu(II) as CuSCN
- c. Gravimetric estimation of Pb(II) as (Pb)<sub>3</sub>(PO<sub>4</sub>)<sub>2</sub>
- d. Volumetric estimation of Mn(II)/Fe(III)
- e. Volumetric estimation of Cr(VI)/ Fe(III)
- f. Volumetric estimation of Cu(II)/ Fe(III)
- g. Volumetric estimation of Cu(II)/Cr(VI)

**COURSE OUTCOMES**

On completion of the course, student will be able to

**CO1** – Gain an insight into multifarious laboratory techniques for the quantitative analysis of inorganic compounds.

**CO2** – Demonstrate the skills to separate the given mixture of ions by chromatographic techniques.

**CO3** – Practical knowledge and skills for ore analysis.

**CO4** – Determine percent composition of different metals in a given alloy.

**CO5** – Demonstrate the expertise for spectrophotometric estimation of coordination complexes.

**CO6** – Gain an experience in determining the inorganic content by gravimetric and volumetric estimation.

**TEXT/REFERENCE BOOKS**

- 1) A text book of Quantitative Inorganic Analysis – A. I. Vogel
- 2) Experimental Inorganic Chemistry - W. G. Palmer
- 3) The analysis of minerals and ores of the rarer elements – W. R. Schoeller and A.R. Powell, Charles, Griffin and Company Limited.
- 4) EDTA Titrations –F.Laschka

**END SEMESTER EXAMINATION QUESTION PAPER PATTERN**

**Max. Marks: 100**

Laboratory work including maintaining journal book+ mid-sem viva (LW)

End-sem exam and viva (LE/Viva)

**Exam Duration: 3 Hrs**

50 Marks

50 Marks

20MSC503T					Physical Chemistry-I					
Teaching Scheme					Examination Scheme					
L	T	P	C	Hrs/Week	Theory			Practical		Total Marks
					MS	ES	IA	LW	LE/Viva	
3	0	0	3	3	25	50	25	--	--	100

**COURSE OBJECTIVES (04)**

- To familiarize the students with concepts of thermodynamics and thermodynamic properties of macroscopic systems
- To understand the theories of reaction kinetics and factors affecting reaction kinetics
- To understand the basic principles of electrochemistry, inter-phase and their applications,
- To understand the concepts of, surface chemistry and various surface phenomenon and their applications

**Unit 1 Classical Thermodynamics****10 h**

Third law, thermodynamics, need for it, Nernst heat theorem and other forms of stating the third law. Thermodynamic quantities at absolute zero, apparent exceptions to the third law - thermodynamics of systems of variable composition, partial molar properties, chemical potential, relationship between partial molar quantities, Gibbs Duhem equation and its applications (the experimental determination of partial molar properties not included)- thermodynamic properties of real gases, fugacity concept, calculation of fugacity of real gas, activity and activity coefficient, concept, definition, standard states and experimental determinations of activity and activity coefficient of electrolytes.

**Unit 2 Chemical Kinetics****12 h**

Kinetics of complex reactions, Simultaneous reactions - opposing, parallel and consecutive reactions, the steady state approximation, Temperature dependence and Arrhenius law, theories of reaction rates- collision theory, transition state theory RRK and RRKM theories potential energy surfaces, reaction coordinates, reaction probabilities, kinetic isotope effects, factors determining reaction rates in solution, solvent dielectric constant and ionic strength. Chain reactions - linear reactions, branching chains - explosion limits; Rice-Herzfeld scheme; kinetics of free radical polymerization reactions. Enzyme catalysis - rates of enzyme catalysed reactions - effect of substrate concentration, pH and temperature - determination of Michael's parameters, Lineweaver-Burk and Eadie plots Salt effects. Photochemical reactions. Ultrafast reactions

**Unit 3- Electrochemistry****12 h**

Ion transport in solution - migration, convection and diffusion -Fick's laws of diffusion conduction - ion-solvent interaction: Born model and Born equation, enthalpy of ion-solvent interaction and its calculation, Eley-Evan model, solvation number and methods for determination of solvation number, ion association: Bjerrum equation, fraction of ions associated, ion association constant; influence of ionic atmosphere on the conductivity of electrolytes-The Debye Huckel-Onsager equation for the equivalent conductivity of electrolytes - experimental verification of the equation - conductivity at high field and at high frequency - conductivity of non-aqueous solutions-effect of ion association on conductivity. The electrode-electrolyte interface- electrical double layer-electro capillary phenomena, Lippmann equation - the Helmholtz- Perrin - Guoy-Chapmann and Stern models, electro kinetic phenomena relation between current and rate of electrode reaction, current-overpotential relationship, Tafel equation and its importance Tiselius method of separation of protons of proteins - membrane potential.

**Unit 4- Surface Chemistry****10 h**

Surface Phenomena, Gibbs adsorption isotherm, types of adsorption isotherms, solid-liquid interfaces, contact angle and wetting, solid-gas interface, physisorption and chemisorption, Freundlich, derivation of Langmuir and BET isotherms, surface area determination. Kinetics of surface reactions involving adsorbed species, Langmuir-Hinshelwood mechanism, Langmuir- Rideal mechanism, Rideal-Eley mechanism, Surface Films, Langmuir-Blodgett films, self-assembled mono layers, membranes/bilayers, collapse pressure, surface area and mechanism of heterogeneous catalysis, phase transfer catalysis.

**COURSE OUTCOMES (06)****Max. 44 h**

On completion of the course, student will be able to

- CO1 - Apply the concepts of thermodynamic to understand the thermodynamic properties of macroscopic systems  
 CO2 – Interpret reaction rates and propose reaction mechanism with the help of concepts of chemical kinetics  
 CO3- Articulate the factors determining reaction rates and concept of catalysis chemical reaction  
 CO4- Acquire knowledge about theories of surface chemistry and their applications.  
 CO5- Understand the fundamental concept about surface phenomenon and catalysis.  
 CO6- Analyse and apply the principles of electrochemistry in real world problems.

**TEXT/REFERENCE BOOKS**

1. P. W. Atkins, Physical Chemistry, Oxford University Press, 6thEdn., (1998).
2. D. McQuarie, and J. D. Simmen, Physical Chemistry, University Science, 1stEdn., (1998).
3. S. Glasstone, Thermodynamics for Chemists, Affiliated East West Press, (1965).
4. P.W. Atkins, Physical Chemistry, Oxford University Press, 6th Edn., 1998.
5. K. J. Laidler, Chemical Kinetics, Harper and Row Publishers, 3rd Edn., 1987.
6. J. O. M. Bockris and A. K. N. Reddy, Modern Electrochemistry, Plenum Press, 1970

**END SEMESTER EXAMINATION QUESTION PAPER PATTERN****Max. Marks: 100**

Part A/Question: 3 Questions from each unit, each carrying 3 marks  
 Part B/Question: 2 Questions from each unit, each carrying 8 marks

**Exam Duration: 3 h**

36 Marks  
 64 Marks



20MSC503P					Physical Chemistry-I Practical					
Teaching Scheme					Examination Scheme					
L	T	P	C	Hrs/Week	Theory			Practical		Total Marks
					MS	ES	IA	LW	LE/Viva	
0	0	3	1.5	3				50	50	100

**COURSE OBJECTIVES**

- To familiarize with the concept of chemical kinetics and rate law concept.
- To comprehend the factors affecting rate of reaction
- To use the methods of science, in which quantitative, analytical reasoning techniques are used.
- To learn about the properties of polymers and solutions.

**LIST OF EXPERIMENTS**

1. To study the kinetics of ester hydrolysis by acid and base;
2. Determine the order and specific reaction rate of the potassium persulphate-iodide reaction by initial rate method
3. To study primary salt effects in oxidation of iodide ion by persulphate ion.
4. To compare the strengths of two acids by studying acid-catalyzed hydrolysis of an ester.
5. To study the kinetics of iodination of acetone in the presence of acid by initial rate method.
6. Determination of Energy of activation for acid catalyzed hydrolysis of methyl acetate.
7. Polarimetric determination of Concentration of unknown sugar solution
8. To study the kinetics of inversion of cane sugar by optical rotation measurement.
9. Determination of relative strength of acids using reaction kinetics of inversion of cane sugar by polarimetry.
10. To study the iodination of acetone using a colorimeter
11. Partition coefficient of  $\text{NH}_3$  between water and chloroform/ benzoic acid between benzene and water
12. Determination of partition coefficient and equilibrium constant for  $\text{KI} + \text{I}_2 \rightarrow \text{KI}_3$  by solubility product or partition method.
13. Adsorption of oxalic acid and acetic acid on activated charcoal.
14. Study of chain linkages in PVA and its molecular weight determination by viscometry.
15. Determination of partial molar volume of NaCl.

**COURSE OUTCOMES**

On completion of the course, student will be able to

CO1– Explain and apply concepts of chemical kinetics

CO2– Apply the scientific process in the design, conduct, evaluation and reporting of experimental investigations

CO3– Demonstrate the effect of various factors on rate of chemical reaction and its kinetics

CO4– Derive and construct rate equations from mechanistic data and evaluate reaction mechanisms

CO5– Understand the surface phenomenon of adsorption,

CO6– Comprehend the molecular properties of polymers and solutions

**TEXT/REFERENCE BOOKS**

4. J.B.Yadav, *Advanced Practical Physical Chemistry*, Goel Publications, Meerut, 2003.
5. A. I. Vogel, *Fundamentals of Quantitative Analysis*, 5<sup>th</sup> Ed., Addison Wesley longman., 1989.
6. G. Suehla, *Vogel's Qualitative Inorganic Analysis*, 6<sup>th</sup> Ed., Orient Longman, 1989
7. P. Samnani, *Experiments in Chemistry*, Anmol Publications, New Delhi 2007

**SEMESTER EXAMINATION PATTERN**

**Max. Marks: 100**

LW(Daily lab performance plus journal maintain each 25 marks)

LE (Viva-voce plus Lab examination each 25 marks)

**Exam Duration: 3 Hrs**

50 Marks

50 Marks

20MSC504T					Analytical Chemistry I					
Teaching Scheme					Examination Scheme					
L	T	P	C	Hrs/Week	Theory			Practical		Total Marks
					MS	ES	IA	LW	LE/Viva	
2	0	0	2	2	25	50	25	--	--	100

**COURSE OBJECTIVES**

- 1 Gaining the factual knowledge of analytical techniques
- 2 Acquiring basic principles applied for analytical data analysis.
- 3 Learning the fundamental principal of various acid base equilibria and solutions
- 4 Attaining necessary basic knowledge of volumetric and gravimetric concepts for chemical analysis
- 5 Learning the basic experimental techniques of various analytical systems comprising titrations, detection of unknown elements, pH metery.

**UNIT 1 Data Analysis****6 Hrs.**

Mean and standard deviations, reliability of results, confidence interval, comparison of results, comparison of two samples, correlation and regression, correlation coefficient and liner regression

**UNIT 2 Acid Base Equilibria and Buffer Solutions****10 Hrs.**

Acid-base theories, Definition of pH and pH scale (Sorenson and operational definitions), and its significance, Hammett Acidity function, pH at elevated temperatures, pH for aqueous solutions of very weak acid and base, pH for salts of weak acid and weak bases, polyprotic acids. Buffer solutions, buffer capacity, applications of buffers

**UNIT 3 Theory of Volumetric and Gravimetric Analysis:****10 Hrs.**

Introduction, Titrimetric analysis, classifications of reactions in titrimetric analysis, standard solutions, preparation of Standard solutions, primary and secondary standards, Indicators, theory of indicators, Acid–base titrations in non-aqueous media.

Gravimetric Analysis, Impurities in precipitates, Gravimetric calculations, precipitation equilibria (Solubility product, common ion effect, stoichiometry), organic precipitation.

**UNIT 4 Complexometric equilibria:****8 Hrs.**

Introduction, Titration curves, Types of EDTA titrations, Methods of end point Detection Indicators, Applications of Complexometric Titrations.

**COURSE OUTCOMES****Max. 32 Hrs.**

On completion of the course, student will be able to

**CO1** - understand the basic principal of data analysis and will be able to calculate and interpret analytical data.

**CO2** - Student will learn the theoretical aspects of Acid-base equilibria, buffer solutions and can corelate this knowledge withvarious analytical applications.

**CO3** - Student will acquire the knowledge of volumetric and gravimetric principles and will be able to interpret and analysevarious chemical compounds.

**CO4** – Students can describe the technique to analyse the chemical complexes by advance complexometric fundamentals.

**CO5** - Students will be able to explain the working principal of pH metry and calculations based on pH of various chemicals.

**TEXT/REFERENCE BOOKS**

1. G. H. Gefferyetal, Vogel's Text Book of Quantitative Chemical Analysis, ELBS Edn, 1989
2. D. A. Skoog, D.M. West, F.J Holler, S.R Crouch, Fundamentals of Analytical Chemistry, 8th edition, Thomson Brooks Cole, 2004
3. F. Rouessac and A. Rouessac, Chemical Analysis: Modern Instrumentation
4. Methods and Techniques, 2nd edn, John Wiely and Sons
5. D. A. Skoog, E. J. Holler, S. R. Crouch, Principles of Instrumental Analysis, 6th edition, Thomson Brooks Cole, 2007
7. Instrumental Methods of Analysis: Chatwal and Anand
8. Instrumental Methods of Inorganic Analysis (ELBS): A.I. Vogel
9. Chemical Instrumentation: A Systematic approach- H.A. Strobel.

**END SEMESTER EXAMINATION QUESTION PAPER PATTERN****Max. Marks: 100****Exam Duration: 3 Hrs**

Part A/Question: 10 multiple choice questions 1 mark each

10 Marks

Part B/Question: 10 Questions of 2 marks each with internal choice

20 Marks

Part C/Question: 4 Questions of 15 marks each with internal choicePart

60 Marks

D/Question: 1 Questions of 10 marks with internal choice

10 Marks

20MSC504P					Analytical Chemistry I Practical					
Teaching Scheme					Examination Scheme					
L	T	P	C	Hrs/Week	Theory			Practical		Total Marks
					MS	ES	IA	LW	LE/Viva	
0	0	3	1.5	3				25	25	100

**COURSE OBJECTIVES**

- 1 Learning the basic experimental techniques in the laboratory for multifarious analytical techniques
- 2 Gaining experimental knowledge to determine of %age purity of given inorganic sample and organic pharmaceutical samples
- 3 Analysis of the quality of waste water by analytical techniques
- 4 Estimation of inorganic ions by solvent extraction technique and EDTA titrations
- 5 Separation of mixture of organic content by thin layer chromatography

1. Determination of sodium carbonate and sodium bicarbonate in washing soda.
2. Determination of available chlorine in bleaching powder.
3. Determination of %age purity of given sample of Isoniacid.
4. Determination of sulphate in water sample.
5. Determination of %age purity of given sample of Analgin tablet.
6. Determination of %age of Asprin in the given tablet.
7. Determination of saponification value of oil.
8. Determination of iodine value of oil.
9. Determination of iron by chloride extraction by solvent extraction process.
10. Determination of chemical oxygen demand.
11. Simultaneous estimation of chromium (III) and iron (III) by EDTA titration.
12. Separation of aminoacids/ dyes/ drugs by TLC.

**COURSE OUTCOMES**

On completion of the course, student will be able to

**CO1** – Student will get an insight into the laboratory technique for the various analytical techniques

**CO2** - Student will learn the experimental analytical technique to determine % purity of desired compound present in the given raw material.

**CO3** - Student will acquire the knowledge of determination of chemical oxygen demand in the given sample of waste water.

**CO4** – Students will gain experience in determining the inorganic content by solvent extraction technique and EDTA titrations

**CO5** - Students will be able separate given organic mixture TLC technique.

**TEXT/REFERENCE BOOKS**

1. Analytical Chemistry Practice, John H. Kennedy, Saunders College Publishing, Second Edition 1990.
2. Vogels Textbook of Quantitative Chemical Analysis, 6th Edition, 2002.
3. Comprehensive Experimental Chemistry; V. K. Ahluwalia, New Age Publications, 1997
4. Analytical Chemistry: Theory and Practice; R. M. Varma, CBS Publishers, 1994
5. A. K. Nad, B. Mahapatra & A. Ghosal, An Advanced Course in Practical Chemistry, New Central, 2007. Vogel's Text Book of Practical Organic Chemistry (5th Edn).

**END SEMESTER EXAMINATION QUESTION PAPER PATTERN****Max. Marks: 100**

Laboratory work including manitaning journal book+ mid-sem viva (LW)  
End-sem exam and viva (LE/Viva)

**Exam Duration: 3 Hrs**

50 Marks  
50 Marks

20MSC505T					Environmental and Green chemistry					
Teaching Scheme					Examination Scheme					
L	T	P	C	Hrs/Week	Theory			Practical		Total Marks
					MS	ES	IA	LW	LE/Viva	
2	0	0	2	2	25	50	25	--	--	100

#### COURSE OBJECTIVES

- To develop the fundamental understanding about aquatic and atmospheric chemistry.
- To provide the knowledge about the experimental methods in environment chemistry.
- To develop the fundamental knowledge about green chemistry and its importance.
- To provide the awareness about the greener chemicals and approaches.

#### Unit 1: Aquatic and atmospheric chemistry

7h

Aquatic chemistry principles of sedimentation, coagulation, precipitation, concept of solubility product, filtration and adsorption process, photochemical oxidants, smog formation, acid rain, nuclear accidents, global warming, carbon sequestration, toxic chemicals in environment, trace metal characteristics in relation to toxicity, biochemical effects of trace elements, biochemical effects of nitrogen oxides, sulphur dioxide, nitrate, fluoride, carcinogens, methyl isocyanate.

#### Unit 2: Experimental methods in environment chemistry

6h

Introduction and sampling techniques: Sample preparation, preservation and processing of air, water and soil samples; precipitation, fractional distillation, solvent extraction, air sampling equipments, particulate matter, its measurement and practical importance, characterization of water quality - alkalinity, hardness, electrical conductivity, pH, chlorides, fluoride, nitrates, origin and treatments of industrial wastes

#### Unit 3: Green chemistry and importance

7h

Introduction to green chemistry, importance of green chemistry, natural and synthetic processes, twelve principles of green chemistry, concept of atom economy with examples, role of solvents in green chemistry, organic and aqueous solvents, water as green solvent, solvent less reactions, industrial hazards and safety precautions, types of hazards, hazard assessment in chemical industry, green synthesis examples: Ibuprofen, adipic acid, ammonia, sulfuric acid.

#### Unit 4: Greener chemicals and approaches

6h

Properties and use of Ionic liquids, advantages of ionic liquids, biocatalyst and enzymes, different types of biocatalysts and their functions, alternative energy sources for green chemistry, microwave synthesis; advantages with example, sonochemical synthesis: mechanism and examples; combinatorial synthesis: different approaches and examples.

#### COURSE OUTCOMES

##### On completion of the course, student will be able to

- CO1 - Understand the basic principles of aquatic chemistry.  
 CO2 - Acquire knowledge about the chemical processes occurring in the environment.  
 CO3 –Understand and learn the fundamentals to monitor the air and water quality.  
 CO4 – Explain the definition of green chemistry and characterizing chemical reactions in terms of green chemistry.  
 CO5 – Acquire knowledge about the industrially important green chemical processes.  
 CO6 - Develop the knowledge on the green chemicals and greener synthesis approaches.

#### References

1. Environment Chemistry, Garry W. vanlon & Stephen J. Duffy, Oxford University press, third edition, (2011)
2. Chemistry for Environmental Engineering and Science, C.N. Sawyer, PL McCarty, G.F. Parkin, Tata Mc. Graw-Hill Edition, 2003.
3. Environmental Engineering, Principles and Practices, N.S. Varandani, Pearson publications.
4. Sheldon, R.A., Arends, I., and Hannefed, U., Green Chemistry and Catalysis, Wiley-VCH Verlag GmbH and Co. (2007).
5. Handbook of green chemistry and technology by Clark J, WILEY (2014)

20MSC506T					Organic Chemistry II					
Teaching Scheme					Examination Scheme					
L	T	P	C	Hrs/Week	Theory			Practical		Total Marks
					MS	ES	IA	LW	LE/Viva	
3	0		3	3	25	50	25	--	--	100

**COURSE OBJECTIVES**

- To acquire the basic understanding of reagents.
- To understand numerous name reactions involved in organic synthesis.
- To demonstrate the disconnection approach.
- To explain the basic concepts of natural product chemistry.

**UNIT 1 OXIDATION/REDUCTION AND OTHER REAGENTS****12 Hrs.**

Osmium tetroxide, DDQ, selenium dioxide,  $\text{Ti}(\text{NO}_3)_3$ , CAN,  $\text{MnO}_2$ ,  $\text{Ag}_2\text{CO}_3$ , Hypervalent iodine(V) (Dess-Martin reagent), Oppenauer oxidation ( $\text{Al}(\text{O}^i\text{Pr})_3$ ),  $\text{NaIO}_4$ , Tetrapropyl ammonium peruthenate. Organic peroxides (Sharpless epoxidation,

Baeyer Villiger oxidation), PCC, PDC, Dimethyl sulfoxide (Moffatt oxidation, Swern oxidation). Catalytic hydrogenation (Pt, Pd, Fe, Ni, Rh, Ru catalysed), Clemmensen reduction, Wolff Kishner reduction, Reduction with diimide ( $\text{NH}_2\text{-NH}_2$ ) and Birch reduction.  $\text{NaBH}_4$ ,  $\text{NaBH}_3\text{CN}$ ,  $\text{LiAlH}_4$ , DIBAL-H, Applications of hydroboration. Mechanism of metal hydride reduction of saturated and unsaturated carbonyl compounds, acids, esters and nitriles. Addition of Grignard reagents, organozinc, and organolithium reagents to carbonyl and unsaturated carbonyl compounds, Lithium Organocuprates, ylides of sulfur, phosphorous and nitrogen. Organosilanes, Organostannes reagents.

**UNIT 2 ADVANCED NAME REACTIONS****8 Hrs.**

Detailed study of Neber, Prins, Bouveault Blanc Reaction, Appel reaction, Vilsmeier-Haack Reaction, Tishchenko Reaction, Fukuyama reaction, McMurry reaction, Jones Oxidation, Wilkinson reaction, Woodward and Prevost Reaction, Oxymercuration-Demercuration reaction. Cross coupling reactions: Stille, Suzuki, Sonogashira, Heck, Negishi, Hiyama, Kumada couplings. Mitsunobu reaction, Buchwald Hartwing reaction, Swern oxidation reaction, Michael addition, Darzen's glycidic ester synthesis, Mannich reaction, Dickmann reaction, Witting reaction, Knoevenagel reaction. Multicomponent reactions: Olefin metathesis, Passerine reaction, Ugi reaction, Phase transfer catalysis.

**UNIT 3 RETEROSYNTHESIS AND DISCONNECTION APPROACH****10 Hrs.**

An introduction to Synthons and synthetic equivalents, disconnection approach, functional group interconversions. One group C-X and two group disconnections in 1,2, 1,3, 1,4 & 1,5- difunctional compounds. Retro- synthesis of Alkene, acetylenes and aliphatic nitro alcohols and carbonyl compounds, amines, the importance of the order of events in organic synthesis, chemoselectivity, regioselectivity. Diels Alder reaction, Michael addition and Robinson annulation.

**UNIT 4 NATURAL PRODUCTS - ALKALOIDS AND TERPENOIDS****10 Hrs.**

Alkaloids: Phenyl ethyl amine, quinine, nicotine, peptides, nucleoside and nucleotide structure, synthesis, biogenesis. Terpenoids: Isoprene rules, acyclic monoterpenoids, central geraniolneral, linalool monocyclic monoterpenoids; terpineol, structure elucidation, synthesis and biogenesis. Higher terpenoids: sesqui-, di-, sester-, tri-, tetra- terpenoids.

**40 Hrs.****COURSE OUTCOMES**

On completion of the course, student will be able to

- CO1– Understand various reagents involved in different chemical transformation. CO2– Acquire knowledge about various advanced reagents  
 CO3– Understand the advanced name reactions and their applications.  
 CO4– Apprehend the synthesis and application of different types of reagents. CO5– Plan different organic synthesis.  
 CO6– Understand the chemistry of natural products.

**TEXT/REFERENCE BOOKS**

7. A guide book to mechanism in Organic chemistry (Orient-Longmens)- Peter Sykes.
8. Organic reaction mechanism (Benjamin) R. Breslow.
9. Organic Synthesis, The Disconnection Approach, Stuart Warren.
10. Simonson: Terpenes.
11. Manskey and Holmes: Alkaloids.

**END SEMESTER EXAMINATION QUESTION PAPER PATTERN****Max. Marks: 100****Exam Duration: 3 Hrs**

Part A/Question:

Part B/Question:

20MSC506P					Organic Chemistry-II Practical					
Teaching Scheme					Examination Scheme					
L	T	P	C	Hrs/Week	Theory			Practical		Total Marks
					MS	ES	IA	LW	LE/Viva	
0	0	3	1.5	3				50	50	100

**COURSE OBJECTIVES**

- Learn safety measures while working in the laboratory.
- Knowledge about different laboratory reagents and multistage synthesis.
- Learn how to handle hazardous chemicals with all the safety measures.
- Application of organic chemistry for industrial and domestic use.
- Learn advanced laboratory techniques.

**LIST OF EXPERIMENTS**

1. Extraction of Natural product (5 different extractions)
2. Multistage synthesis of organic compounds (4 different synthesis)
3. Introduction to the important/sensitive organic reactions/Reagents (10 different sensitive reactions/reagents)
4. Introduction to the advanced laboratory techniques (2 techniques)
5. Synthesis of Dyes & pigments (7 dyes)
6. Synthesis of Drugs (4 drugs)
7. Estimation of functional groups (6 estimations)
8. Introduction to the Analytical and Instrumental Techniques (2 Instrumental techniques)
9. Separation and identification of mixtures (4 mixtures)
10. Identification of compounds by spectroscopy

**COURSE OUTCOMES**

On completion of the course, student will be able to

- CO1– Extract natural products from organic compounds  
 CO2– Design multistage synthesis  
 CO3– Separate organic compounds mixtures  
 CO4– Understand different separation techniques  
 CO5– Estimate different functional groups  
 CO6– Identify the structure of the organic compound by spectroscopy

**TEXT/REFERENCE BOOKS**

1. Vogel A. I., Furniss B.S., Hannaford A.J., Smith P.W.G., Tatchell A. R., "Vogel's Textbook of Practical Organic Chemistry", 5th Ed., Prentice Hall, 1996. John Wiley & Sons Inc
2. Modern projects and experiments in organic chemistry: Mini scale and Williamson micro scale, second edition by Jerry R. Mohrig et al; W.H Freeman and company press; ISBN: 0-7167-3921-6
3. B.S. Fumiss, A.J. Hannaford, V. Rogers, P.W.G. Smith and A.R. Tatchell, "Text book of Practical Organic Chemistry", LBS, Singapore, 1994

**SEMESTER EXAMINATION PATTERN**

**Max. Marks: 100**

LW(Daily lab performance plus journal maintain each 25 marks)  
 LE (Viva-voce plus Lab examination each 25 marks)

**Exam Duration: 3 Hrs**

50 Marks  
 50 Marks

20MSC507T					Inorganic Chemistry II					
Teaching Scheme					Examination Scheme					
L	T	P	C	Hrs/Week	Theory			Practical		Total Marks
					MS	ES	IA	LW	LE/Viva	
3	0	0	3	3	25	50	25	--	--	100

**COURSE OBJECTIVES**

- To understand the basic concepts of inorganic reaction mechanism
- To gain the knowledge of organometallic chemistry
- To learn the importance of organometallic chemistry for industrial applications
- To attain an understanding of inorganic photochemistry
- To develop the theoretical knowledge on nuclear chemistry

**UNIT 1: Inorganic Reaction Mechanism.****10 Hrs.**

Introduction to Inorganic Reaction Mechanism; Substitution in Octahedral and Square Planar Complexes; Lability; Trans-effect; Conjugate Base Mechanism; Racemisation; Electron Transfer Reactions: Inner Sphere and Outer Sphere Mechanism; Marcus theory.

**UNIT 2: Organometallic Chemistry.****10 Hrs.**

18-electron Rule; Metal Carbonyls; Nitrosyls; Carbonyl Hydrides; Isolobal Analogy; Dioxygen and Dinitrogen Compounds; Metal Alkyls; Carbenes; Carbynes; Alkenes; Alkynes; and Allyl Complexes. Hydrides; Metallocenes; Metal Arene Complexes; Carbonylate Anions; Agostic Interaction; Oxidative Addition and Reductive Elimination; Insertion and Elimination Reactions; Homogeneous and Heterogeneous Catalysis; Fluxional Molecules; Metal-Metal bonding.

**UNIT 3: Inorganic Photochemistry.****10 Hrs.**

Introduction to Inorganic Photochemistry; Photochemical Laws and Photochemical Kinetics; Photochemical Reactions: Substitution, Decomposition and Fragmentation, Rearrangement, and Redox Reactions; Electronic absorption spectra of Metal Complexes; Characteristics of the Electronically Excited States of Inorganic Compounds; Photophysical Processes; Photosensitization; Photo-electrochemistry of Excited State Redox Reactions.

**UNIT 4: Nuclear Chemistry.****10 Hrs.**

Radioactive Decay Processes: Multipole Radiation and Selection Rules; Isomeric Transition; Internal Conversion and Auger Effect; Nuclear Structure; Nuclear Energy Levels; Nuclear Models; Nuclear Reactions; Labelling; Nuclear Reactors; Radioanalytical Techniques.

Nuclear Processes in Geology, Geochemistry & Astrophysics: Ages of Rocks and Minerals; Age of earth-Radioactive Dating; Threshold; Nuclear Reactions in Stars and Nucleogenesis; Nuclear Fusion and Stellar Energy (Cosmo chemistry).

**Max. 40 Hrs.****COURSE OUTCOMES**

On completion of the course, student will be able to

**CO1** – Understand different types of inorganic reactions and their mechanism.

**CO2** – Demonstrate the theoretical knowledge of organometallic chemistry.

**CO3** – Illustrate the importance of organometallic chemistry towards current industrial applications. **CO4** –

Explain different photophysical and photochemical processes of inorganic compounds.

**CO5** – Apply the concept of inorganic photochemistry in predicting their potential applications.

**CO6** – Learn the advanced concepts of nuclear chemistry and applications thereof.

**TEXT/REFERENCE BOOKS**

1. The organometallic Chemistry of transition metals, R.H. Crabtree, John Wiley, 1994.
2. Organometallic chemistry: A unified concept, R C Melhotra, New Age International, 2007
3. G. L. Geoffrey and M. S. Wrighton, Organometallic Photochemistry, Academic Press, 1979.
4. K. K. Rohatagi-Mukherjee, Fundamentals of Photochemistry, Wiley Eastern, 1978.
5. M. S. Wrighton, Inorganic and Organometallic Photochemistry, ACS Pub., 1978.
6. H. J. Arnikar, Essentials of Nuclear chemistry, 4th Ed., Wiley-Eastern Ltd. New Delhi.
7. G. Friedlander, J. W. Kennedy, E. S. Macias and J. M. Miller, Nuclear and Radiochemistry, 3rd Ed., John-Wiley & Sons, New York.

**END SEMESTER EXAMINATION QUESTION PAPER PATTERN****Max. Marks: 100****Exam Duration: 3 Hrs**

Part A/Question: 10 multiple choice questions 1 mark each

10 Marks

Part B/Question: 10 short answer type questions of 2 marks each with internal choice

20 Marks

Part C/Question: 4 Questions of 15 marks each with internal choice

60 Marks

Part D/Question: 1 Questions of 10 marks with internal choice

10 Marks

20MSC507P					Inorganic Chemistry II Practical					
Teaching Scheme					Examination Scheme					
L	T	P	C	Hrs/Week	Theory			Practical		Total Marks
					MS	ES	IA	LW	LE/Viva	
0	0	3	1.5	3	--	--	--	50	50	100

**COURSE OBJECTIVES**

- To understand synthetic inorganic complexes
- To acquire the practical knowledge of qualitative verification of the spectrochemical series
- To gain the practical knowledge of studying optical isomerism of coordination complexes
- To gain an experience in equilibrium studies of inorganic reactions by different methods
- To develop the skills for handling air and moisture sensitive compounds

**1. Synthesis and Characterization of inorganic compounds (Melting point, IR, UV-vis, Magnetic Moment, Conductivity, Cyclic voltammetry etc.) [At least three]**

- a. Reinkey's salt
- b.  $[\text{Co}(\text{NH}_3)_6]\text{Cl}_3$
- c.  $[\text{Co}(\text{NH}_3)_5\text{Cl}]\text{Cl}_2$
- d.  $[\text{Ni}(\text{en})_2]\text{Cl}_2$
- e.  $\text{K}_3[\text{Fe}(\text{ox})_3]$
- f.  $\text{K}_3[\text{Cr}(\text{ox})_3]$
- g.  $[\text{Co}(\text{NH}_3)_6]\text{Cl}_3$
- h.  $[\text{Cu}(\text{NH}_3)_4(\text{SO}_4)(\text{H}_2\text{O})]$
- i. Chrome alum  $[\text{K}_2\text{SO}_4, \text{Cr}_2(\text{SO}_4)_3, 24\text{H}_2\text{O}]$

2. Comparison of the electronic spectra of  $[\text{Ni}(\text{H}_2\text{O})_6]^{2+}$ ,  $[\text{Ni}(\text{NH}_3)_6]^{2+}$  and qualitative verification of the spectrochemical series.

3. Synthesis and characterization of  $[\text{Co}(\text{en})_3]\text{Cl}_3$ . Separation of its optical isomers and determination of their optical rotation by using polarimeter.

**4. Equilibrium studies on inorganic reactions [At least two]**

- a. Determination of composition of Fe(III)-sulfosalicylate complex in solution by Mole-Ratio method.
- b. Determination of composition of Fe(II)-1,10-phenanthroline complex in solution by Mole-Ratio method.
- c. Determination of composition of Fe(III)-sulfosalicylate complex in solution by Slope-Ratio method.
- d. Determination of composition of Fe(II)-1,10-phenanthroline complex in solution by Slope-Ratio method.
- e. Determination of composition of Fe(III)-sulfosalicylate complex in solution by Job's method of continuous variation.
- f. Determination of composition of Fe(II)-1,10-phenanthroline complex in solution by Job's method of continuous variation.

**5. Handling of air and moisture sensitive compounds.****COURSE OUTCOMES**

On completion of the course, student will be able to

- CO1 – Develop the skills for synthesis and purification of inorganic complexes.  
 CO2 – Learn the skills for characterization of inorganic complexes by different physicochemical techniques.  
 CO3 – Demonstrate the practical skills for qualitative verification of the spectrochemical series.  
 CO4 – Gain an experience in studying optical isomerism of coordination complexes.  
 CO5 – Demonstrate the practical knowledge for equilibrium studies of inorganic reactions by different methods.  
 CO6 – Understand the handling of air and moisture sensitive compounds.

**TEXT/REFERENCE BOOKS**

1. A Text book of quantitative Inorganic Analysis – A. I. Vogel
2. Standards methods of Chemical Analysis-F. J. Welcher.
3. Experimental Inorganic Chemistry – W. G. Palmer.
4. Manual on Water and Waste Water Analysis, NEERI- Nagpur D. S. Ramteke and C. A. Moghe
5. Inorganic synthesis- King.
6. Synthetic Inorganic Chemistry-W. L. Jolly.
8. Synthesis and Technique in Inorganic Chemistry: A Laboratory Manual, Gregory S. Girolami, Thomas B. Rauchfuss and Robert J. Angelici. University Science Books.
9. Synthetic methods of organometallic and inorganic chemistry ed. by Wolfgang A. Herrmann, Georg Thieme Verlag, New York, 1997, Vol 7 and 8.

**END SEMESTER EXAMINATION QUESTION PAPER PATTERN**

Max. Marks: 100

Laboratory work including maintaining journal book+ mid-sem viva (LW)

End-sem exam and viva (LE/Viva)

Exam Duration: 3 Hrs

50 Marks

50 Marks



20MSC508T					Physical Chemistry-II					
Teaching Scheme					Examination Scheme					
L	T	P	C	Hrs/Week	Theory			Practical		Total Marks
					MS	ES	IA	LW	LE/Viva	
3	0	0	3	3	25	50	25	--	--	100

**COURSE OBJECTIVES (-04)**

- Conceptualize the fundamental principles of the properties of matter, energy quantization, its application,
- To develop the fundamental understanding about the classical and statistical models of thermodynamics.
- To acquire knowledge about concepts of photochemistry and photochemical processes
- Understand the symmetry properties of molecules and application of group theory in understanding the molecular properties based on symmetry.

**Unit I Quantum Chemistry****12 h**

The failures of classical physics, Bohr's quantum theory, Wave particle duality, Operator algebra, Linear and Hermitian operators, Quantum mechanical postulates, Schrodinger equation for a particle in one and three dimensional boxes, Rigid rotator and simple harmonic oscillator, Schrodinger equation for hydrogen atom and its solution-Derivation of Eigen function and Eigen value for hydrogen atom. Term symbols, LS and JJ coupling. The origin of electronic quantum numbers and physical significance - radial probability density-significance of magnetic quantum number with respect to angular momentum. Hydrogen molecule ion and hydrogen molecule-Pauli's exclusion principle. Born Oppenheimer approximation, Mulliken designation of molecular orbitals. MO theory of bonding, MO treatment of H-bonded systems, ethylene, butadiene and benzene. Approximation methods: Perturbation and variation method, wave functions for many electron atoms – Hartree-Fock SCF method, Slater orbital

**Unit 2 Statistical Thermodynamics****10 h**

Statistical view of entropy. Laws of thermodynamics from statistical considerations. Molecular view of temperature and heat capacity. Derivation of Maxwell Boltzmann distribution law – partition functions and their calculation. Expressions for thermodynamic quantities in terms of partition functions-translational, rotational, vibrational and electronic contributions to the thermodynamic properties of perfect gases, Intermolecular forces in imperfect gases. Thermodynamic quantities in terms of partition functions. Statistical mechanics of simple gases and solids. Kinetic theory of gases. Equilibrium constant, mean energies and heat capacities in terms of partition functions. Bose-Einstein and Fermi-Dirac statistics. Use of Statistical Thermodynamics in understanding molecular interaction in liquids.

**Unit 3 Photochemistry****10 h**

Absorption and emission of radiation, Franck Condon principle decay of electronically excited states, Jablonski diagram, radiative and non-radiative processes, fluorescence and phosphorescence, spin-forbidden radiative transitions, inter conversion and intersystem crossing. Theory of energy transfer - resonance and exchange mechanism, triplet-triplet annihilation, photosensitization and quenching. Spontaneous and induced emissions. Einstein transition probability- inversion of population - laser and masers. Flash photolysis: Chemi and thermo luminescence.

**Unit 4 Group Theory****12 h**

Elements of group theory, definition, group multiplication tables, conjugate classes, conjugate and normal subgroups, symmetry elements and operations, point groups, assignment of point groups to molecules, Matrix representation of geometric transformation and point group, reducible and irreducible representations, construction of character tables, bases for irreducible representation, direct product, symmetry adapted linear combinations, projection operators. Orthogonality theorem - its consequences. Symmetry aspects of molecular orbital theory, planar  $\pi$ -systems, symmetry factoring of Huckel determinants, solving it for energy and MOs for ethylene and 1,4-butadiene, sigma bonding in  $Ax_n$  molecules, hybridization, tetrahedral, octahedral, square planar, trigonal planar, linear, trigonal bipyramidal systems, hybrid orbitals as linear combination of AOs, electronic spectra, selection rule, polarization electron dipole transition, electronic transitions in formaldehyde, butadiene, configuration interaction, symmetry types of normal molecules, symmetry coordinates, selection rules for fundamental vibrational transition.

**Max. 44 h****COURSE OUTCOMES (06)**

On completion of the course, student will be able to

CO1- Understand the properties of matter and the wave-particle duality

CO2 - Apply statistical models to understand the thermodynamic properties of macroscopic systems CO3 - apply the concept of quantization of energy and its modes

CO4- Investigate the photochemical processes and apply of principles of photochemistry to real life phenomenon CO5-Relate symmetry of the molecules to their properties

CO6-Apply group theory and character table to analyse the molecular properties

**TEXT/REFERENCE BOOKS**

1. A. K. Chandra, Introductory Quantum Chemistry, Tata McGraw Hill, 1994
2. C. McClelland, Statistical Thermodynamics, Chapman and Hall, (1973).
3. F. A. Cotton, Chemical Applications of Group Theory, Wiley Eastern, 1991.
4. L. K. Nash, Elements of Classical and Statistical Thermodynamics, Addison-Wesley, (1970).
5. K. K. Rohatgi - Mukerjee, Fundamentals of Photochemistry, Wiley (1992).

**END SEMESTER EXAMINATION QUESTION PAPER PATTERN****Max. Marks: 100****Exam Duration: 3 h**

Part A/Question: 3 Questions from each unit, each carrying 3 marks

36 Marks

Part B/Question: 2 Questions from each unit, each carrying 8 marks

64 Marks

20MSC508P					Physical Chemistry-II Practical					
Teaching Scheme					Examination Scheme					
L	T	P	C	Hrs/Week	Theory			Practical		Total Marks
					MS	ES	IA	LW	LE/Viva	
0	0	3	1.5	3				50	50	100

**COURSE OBJECTIVES**

- To understand the concepts of electrochemistry for analytical purpose.
- To use the methods of science, in which quantitative, analytical reasoning techniques are used.
- To learn learn depth concepts about electrochemistry.
- To demonstrate the application of electrochemical methods in

**LIST OF EXPERIMENTS**

1. Conductometric titration of mixture of acids and precipitation titration (KCl Vs AgNO<sub>3</sub>) using conductivity bridge.
2. Determination of the capacitance of electrochemical interfaces, formal potential and diffusion coefficient of [Fe(CN)<sub>6</sub>]<sup>3-</sup> by cyclic voltammetry.
3. Determination of redox potential of Fe<sup>2+</sup>/Fe<sup>3+</sup> system by potentiometry.
4. Determination of strength of strong and weak acids in a given mixture conductrometrically,
5. Determination of ratio of Potassium Dicromate, chromate in a supplied mixture conductometric titrations.
6. Determination of cell constant of a cell and study the effect of dilution on equivalent conductance of strong/weak electrolytes.
7. Determination of equivalent conductance, degree of dissociation and dissociation constant of a weak acid like acetic acid.
8. Determination of percentage composition of a given acid mixture by pH metry.
9. Conducometric measurement of degree of hydrolysis of a salt.
10. Conductometric titration of a weak acid with strong base/mixture of strong and weak acid with strong base and weak acid with weak base.
11. Potentiometric titration of polyprotic acids with strong base/mixture of strong and weak acid with strong base.
12. Determination of pKa of weak acid/base/Determination of dissociation constants, pK1 and pK2 of a dibasic by potentiometry.
13. Determination of the isotherm for a three component system
14. To determine the critical micelle concentration of Sodium lauryl sulphate from the measurement of conductivities at different concentration
15. Determination of pKA and isoelectric point of an amino acid.

**COURSE OUTCOMES**

On completion of the course, student will be able to

CO1– Apply the scientific process in the design, conduct, evaluation and reporting of experimental investigations

CO2–Derive essential mathematical relationships in kinetics and electrochemistry.

CO3- Define central parts of electrochemical cells and electrochemical equipment

CO4-Integrate qualitative and quantitative concepts of physical chemistry

CO5-Demonstrate procedures and instrumental methods applied in analytical and practical tasks of physical chemistry;

CO6-Solve problems in physical chemistry by using appropriate methodologies;

**TEXT/REFERENCE BOOKS**

4. C. W. Garland, J. W. Nibler, & D. P. Shoemaker, *Experiments in Physical Chemistry*, 8<sup>th</sup> Ed., McGraw – Hill, New York, 2003.
5. J. Mendham, R. C. Denney, J. B. Barnes & M. J. K. Thomas, *Vogel's Textbook of Quantitative Chemical Analysis*, 6<sup>th</sup> Ed., Pearson Education, New Delhi, 2003.
6. V.D. Athawale and P. Mathur, *Experimental Physical Chemistry*, 1<sup>st</sup> Edition, New Age International Publications, New Delhi 2001.
7. J.B.Yadav, *Advanced Practical Physical Chemistry*, Goel Publications, Meerut, 2003.

**SEMESTER EXAMINATION PATTERN**

**Max. Marks: 100**

LW(Daily lab performance plus journal maintain each 25 marks)

LE (Viva-voce plus Lab examination each 25 marks)

**Exam Duration: 3 Hrs**

50 Marks

50 Marks

20MSC509T					Analytical Chemistry II					
Teaching Scheme					Examination Scheme					
L	T	P	C	Hrs/Week	Theory			Practical		Total Marks
					MS	ES	IA	LW	LE/Viva	
2	0	0	2	2	25	50	25	--	--	100

**COURSE OBJECTIVES**

- 1 Acquisition the fundamental knowledge of advance analytical methods
- 2 Learning the basic principles of spectroscopic techniques.
- 3 Understanding and acquiring the necessary basic knowledge of chromatographic separation working of various chromatographic techniques
- 4 Attaining necessary basic knowledge of extraction procedures for practical application in various fields
- 5 Learning the basic electrochemical techniques and attaining the fundamental knowledge of potentiometry.

**UNIT 1 Separation Techniques****8 Hrs.**

Types of separation techniques, solid (SLE), liquid liquid extraction (LLE), Technique for solvent extraction: batch extraction and continuous extraction, Extraction of lighter type or heavier type liquid, Working Methodology and Applications of extraction LLE, SPE, SPME, solid- liquid extraction factors influencing.

**UNIT 2 Chromatography****10 Hrs.**

Fundamentals of chromatography, Definition of resolution, capacity factor, selectivity factor, dead time and dead volume. Types of chromatography depending upon mobile phase, instrumentation and separation TLC, HPTLC, Ion exchange, types of resin, working methodology and application of TLC, HPTLC and Ion exchange, instrumentation and working methodology and applications of HPLC & GC (Gas Chromatography), types of columns, packed columns, capillary columns, bonded phase columns.

**UNIT 3 Introduction to Spectroscopy****12 Hrs.**

Interaction between Electromagnetic Radiation and Matter: Introduction to Electromagnetic Radiation, Interaction of Electromagnetic Radiation with Matter  
Introduction to Atoms and Atomic Spectroscopy, Molecules and Molecular Spectroscopy: Rotational Transitions in Molecules, Vibrational Transitions in Molecules, Electronic Transitions in Molecules.  
Absorption Laws: Beer Law  
Methods of Calibration: Calibration with Standards, Method of Standard Additions, Internal Standard Calibration Optical Systems Used in Spectroscopy: Radiation Sources, Wavelength Selection Devices, Filters, Monochromator Resolution Required to Separate Two Lines of Different Wavelengths, Detectors, Single-Beam and Double-Beam Optics

**UNIT 4 Electrochemical techniques****8 Hrs.**

Potentiometry - electrode systems, potentiometric titrations and applications

**Max. 36 Hrs.****COURSE OUTCOMES**

On completion of the course, student will be able to

CO1 - understand the basic principal of various separation techniques and will be able to distinguish and propose the appropriate technique for different types of analysis.

CO2 - Student will acquire the fundamental knowledge of spectroscopy and will be able to understand the principle behind spectroscopic instruments.

CO3 - Learn various type of chromatographic techniques and will acquire the basic knowledge of the instrumentation involved in these techniques.

CO4 - Students will learn methods of calibration of instruments involved in analytical chemistry and will be able to understand the basic optical systems of instruments.

CO5 - Students will be able to explain the working principal of potentiometric analysis and will be able to describe the working principle of electrodes in potentiometric techniques.

**TEXT/REFERENCE BOOKS**

1. Introduction to Spectroscopy by D.L. Pavia, G. M. Lampman, G. S. Kriz, Harcourt College Publisher, NY, 2001
2. Organic Spectroscopy by William Kemp, ELBS 3rd Ed. 1994.
3. Modern Analytical Chemistry, David Harvey, McGraw Hill, 2000.
4. Organic Spectroscopy, Kemp W. 5. Treatise on Analytical Chemistry: Vol I to VII – I. M. Kolthoff
5. Spectroscopic identification of organic compounds- R.M. Silverstein and G. C. Bassler
6. Spectroscopic methods in organic chemistry- D.H. Williams and I. Fleming 8. Absorption spectroscopy of organic molecules- V.M. Parikh
7. Applications of spectroscopic techniques in Organic chemistry- P. S. Kalsi

**END SEMESTER EXAMINATION QUESTION PAPER PATTERN**

Part A/Question: 10 multiple choice questions 1 mark each	10 Marks
Part B/Question: 10 Questions of 2 marks each with internal choice	20 Marks
Part C/Question: 4 Questions of 15 marks each with internal choice	60 Marks
Part D/Question: 1 Questions of 10 marks with internal choice	10 Marks

20MSC509P					Analytical Chemistry II Practical					
Teaching Scheme					Examination Scheme					
L	T	P	C	Hrs/Week	Theory			Practical		Total Marks
					MS	ES	IA	LW	LE/Viva	
0	0	3	1.5	3	25	50	25	25	25	100

**COURSE OBJECTIVES**

- 1 Learning the basic experimental techniques like ion-exchange, solvent extraction, titrimetric methods
- 2 Gaining experimental knowledge to determine cation or anion content by ion-exchange chromatography
- 3 Estimation of organic content by spectrophotometric methods
- 4 Quantitative analysis of organic content by titrimetric methods
- 5 Determining the inorganic content in the water sample

1. Determination of cation content in hard water by ion exchange chromatography.
2. Ion-exchange separation of cations and anions
3. To determine the amount of each para nitro-phenol and meta nitro-phenol from the given mixture by spectrophotometric titration using standard NaOH solution at  $\lambda_{\text{max}} = 280 \text{ nm}$
4. Solvent extraction of transition metal ions
5. Estimation of the purity of oxalic acid employing standard Ce(IV) solution
6. Redox titrations of determination of ascorbic acid
7. Simultaneous determination of metal ions by spectrophotometry
8. Determination of total alkalinity of soda ash.
9. Determination of nitrite Using NEDA in drinking water samples.
10. Determination of Cr (VI) using Diphenyl carbazide
11. To determine the stoichiometry and stability constant of ferric salicylic acid complex by Job's method and mole ratio method
12. To determine the indicator constant and isobestic point of an indicator

**COURSE OUTCOMES**

On completion of the course, student will be able to

- CO1** – Student will get an insight into the laboratory techniques like ion-exchange, solvent extraction and titrimetric methods
- CO2** - Student will learn the experimental analytical technique to determine inorganic and organic content by ion-exchange chromatography.
- CO3** - Student will acquire the knowledge of determination organic content by spectrophotometric methods.
- CO4** – Students will gain experience in determining the organic content titrimetric methods
- CO5** - Students will be able to determine the inorganic content in water sample.

**TEXT/REFERENCE BOOKS**

1. Analytical Chemistry Practice, John H. Kennedy, Saunders College Publishing, Second Edition 1990.
2. Vogel's Textbook of Quantitative Chemical Analysis, 6th Edition, 2002.
3. Comprehensive Experimental Chemistry; V. K. Ahluwalia, New Age Publications, 1997
4. Analytical Chemistry: Theory and Practice; R. M. Varma, CBS Publishers, 1994
5. A. K. Nad, B. Mahapatra & A. Ghosal, An Advanced Course in Practical Chemistry, New Central, 2007. Vogel's Text Book of Practical Organic Chemistry (5th Edn).

**END SEMESTER EXAMINATION QUESTION PAPER PATTERN****Max. Marks: 100**

Laboratory work including maintaining journal book+ mid-sem viva (LW)  
End-sem exam and viva (LE/Viva)

**Exam Duration: 3 Hrs**

50 Marks  
50 Marks

20MSC510T					Theoretical & Computational Chemistry					
Teaching Scheme					Examination Scheme					
L	T	P	C	Hrs/Week	Theory			Practical		Total Marks
					MS	ES	IA	LW	LE/Viva	
2	1	0	3	3	25	50	25	--	--	100

**COURSE OBJECTIVES**

- The objective of unit I is to ensure that students learn the basic of UNIX and LINUX programming.
- The objective of unit II is to ensure that students learn about molecular mechanics and how it is implemented into chemistry.
- The objective of unit III is to ensure that students learn how electronic structure calculations can be used as an adjunct to their experimental research.
- The objective of unit IV is to ensure that students understand the role of cheminformatics in drug design process.

**Unit I INTRODUCTION****4 hours**

Introduction to the LINUX and UNIX operating system, LINUX/UNIX commands, Difference in UNIX and LINUX operating systems, Comparison of LINUX operating system with windows.

**Unit 2 ELECTRONIC STRUCTURE THEORY-I****16 hours**

Molecular mechanics: Introduction, Basic theory, Concept of potential energy surface. Force field and its components (stretch- Morse Potential, bend, out-of-plane bending, torsional, van der Waals and electrostatic energy).

Electronic structure methods: Basics of electronic structure calculations, Semi-empirical methods and Ab-initio methods, Advantages of Semi-empirical methods.

**Unit 3 ELECTRONIC STRUCTURE THEORY-II****10 hours**

Density functional methods: Basic theory, building geometry, Basis set, functional's, Notation, Level of theory, Optimization and computable properties like absorption, energy, optimized bond lengths, bond angles, dihedral angles, charge calculations.

**Unit 4 CHEMINFORMATICS IN DRUG DESIGN****10 hours**

Computer-aided drug discovery: Classification of CADD, Ligand-based drug design, Structure-based drug design, Virtual screening.

Ligand based drug design: Basic concept, Pharmacophore modelling and QSAR (brief overview), common softwares for implementing ligand-based drug design.

Structure-based drug design: Basic concept, Pharmacophore modelling and Molecular docking (brief overview), common softwares for implementing structure-based drug design.

**COURSE OUTCOMES**

Upon completion of the course, student will be able to CO1 – Understand the types of operating systems.

CO2 – Explain the concept of molecular mechanics and its implementation.

CO3 – Describe the role of electronic structure calculations in defining the experimental research. CO4 – Explain the role of CADD in drug discovery process.

CO5 – Describe the use of different computational softwares.

CO6 – Utilize the softwares to evaluate the structural parameters related to small organic compounds.

**REFERENCE BOOKS:**

1. Linux Fundamentals by Paul Cobbault, Publication date 2015-05-24 CEST.
2. Online tutorial pdf: [https://www.tutorialspoint.com/unix/unix\\_tutorial.pdf](https://www.tutorialspoint.com/unix/unix_tutorial.pdf) (UNIX computer operating system by tutorialspoint)
3. Computational Chemistry: A Practical Guide for Applying Techniques to Real-World Problems. David C. Young Copyright (2001 John Wiley & Sons, Inc.)
4. Exploring Chemistry with electronic structure methods, 2nd edition, James V. Foresman.
5. Chemoinformatics in Drug Discovery: Methods and Principles in Medicinal Chemistry, Vol. 23, edited by Tudor I. Oprea.
6. Computational Drug Design: A Guide for Computational and Medicinal Chemists, By D. C. Young.
7. The Practice of Medicinal Chemistry, 4<sup>th</sup> edition, edited by Camille Georges Wermuth, David Aldous Pierre Raboisson, Didier Rognan.

**SEMESTER EXAMINATION PATTERN****Max. Marks: 100****Exam Duration: 3 Hrs**

Part A/Question: 10 questions of 2 marks each with internal choice

20 Marks

Part B/Question: 8 questions of 10 marks each with internal choice

80 Marks

20MSC510P					Theoretical & Computational Chemistry- Practical					
Teaching Scheme					Examination Scheme					
L	T	P	C	Hrs/Week	Theory			Practical		Total Marks
					MS	ES	IA	LW	LE/Viva	
0	0	2	1	2	--	--	--	50	50	100

**COURSE OBJECTIVES**

- The objective of the practical session is to ensure that students learn the practical aspects of electronic structure calculations of chemical compounds and modelling of bio-molecular structures.

**ELECTRONIC STRUCTURE THEORY PRACTICALS (Any 4 practical's)**

1. Geometry construction: Linear and ring systems, setting up and running calculations.
2. Energy calculation, Molecular orbital visualization and atomic charges, dipole and higher dipole moments, calculating conformer energy.
3. Frequency calculation, IR, RAMAN & NMR spectra, thermal energy correction and calculation.
4. Isomerization energy calculation, stability calculation, enthalpy of isomerization.
5. Basis set dependence and its limit, potential energy surface and locating stationary points.
6. Use of some softwares to study electronic structure properties like optimized bond lengths, bond angles, dihedral angles and energy.
7. Exercise on modelling of small molecules using Argus lab: water, methane, benzene, cyclohexane: chair and boat form.

**CADD THEORY PRACTICAL (Any 4 practical's)**

8. Advanced visualizing softwares and 3D representation with CHIMERA or any visualization software.
9. Coordinate generation and interconversion.
10. Superimposition of proteins using CHIMERA or Discovery studio.
11. Virtual Screening using drug-likeness properties.
12. Molecular docking.

**COURSE OUTCOMES**

Upon completion of the course, student will be able to

CO1 – Construct the linear and ring systems using softwares.

CO2 – Can explain the structural properties parameters retrieved during electronic structure calculations. CO3 – Describe the role of electronic structure calculations in defining the experimental research.

CO4 – Utilize the visualization softwares to evaluate the structure of proteins. CO5 –

Describe the conversion of chemical structure in different formats.

CO6 – Can superimpose the proteins with the software or manually.

**REFERENCE BOOKS:**

3. Computational Chemistry: A Practical Guide for Applying Techniques to Real-World Problems. David C. Young Copyright (2001) John Wiley & Sons, Inc.)
4. Exploring Chemistry with electronic structure methods, 2nd edition, James V. Foresman.
5. Chemoinformatics in Drug Discovery: Methods and Principles in Medicinal Chemistry, Vol. 23, edited by Tudor I. Oprea.
6. Computational Drug Design: A Guide for Computational and Medicinal Chemists, By D. C. Young.
7. The Practice of Medicinal Chemistry, 4th edition, edited by Camille Georges Wermuth, David Aldous Pierre Raboisson Didier Rognan.

**SEMESTER EXAMINATION PATTERN**

**Max. Marks: 100**

**Exam Duration: 3 Hrs**

LW (Daily lab performance plus journal maintain each 25 marks)

50 Marks

LE (Viva-voce plus Lab examination each 25 marks)

50 Marks

20MSC626T					Reagents and Organic Synthesis					
Teaching Scheme					Examination Scheme					
L	T	P	C	Hrs/Week	Theory			Practical		Total Marks
					MS	ES	IA	LW	LE/Viva	
3	0	0	3	3	25	50	25	--	--	100

**COURSE OBJECTIVES**

- To study various lanthanides-based reagents
- To understand numerous name reactions involved in various organic transformation.
- To explain the basic knowledge of modern spectroscopic techniques.
- To train in interpreting individual spectra and sets of spectra obtained by different spectroscopic techniques.

**UNIT 1 LANTHANIDES BASED REAGENTS****9Hrs.**

General properties and use of Lanthanides, Lanthanide metal compounds at different oxidation states in synthesis. Study of reagents from (i) Cerium (ii) Samarium (iii) Ytterbium

**UNIT 2 MODERN ORGANIC SYNTHETIC REACTIONS****11Hrs.**

Aza-Cope and Aza-Wittig reactions, Baylis-Hillman reaction, BINAL and BINAP assisted reactions, click reaction, Julia- Lythgoe olefination, Mukayama aldol reaction, Peterson's stereoselective olefination, selected total synthesis.

**UNIT 3 PRINCIPLES AND APPLICATION OF UV-VISIBLE AND IR SPECTROSCOPY FOR ORGANIC COMPOUNDS****9Hrs.**

UV-VISIBLE SPECTROSCOPY: Various electronic transitions - Effect of solvent on electronic transitions - Ultraviolet bands for carbonyl compounds, unsaturated carbonyl compounds, dienes, conjugated polyenes aromatic and heterocyclic compounds. Fieser Woodward rules for conjugated dienes and carbonyl compounds. IR: Characteristic vibrational frequencies of alkanes, alkenes, alkynes, aromatic compounds, alcohols, ethers, phenols and amines. Effect of hydrogen bonding and solvent effect on vibrational frequencies, overtones, combination bands and Fermi resonance. Interpretation of spectroscopic (UV and IR) data, as applied to organic system.

**UNIT 4 PRINCIPLES AND APPLICATION OF NMR AND MASS SPECTROMETRY FOR ORGANIC COMPOUNDS****11Hrs.**

NUCLEAR MAGNETIC RESONANCE SPECTROSCOPY:  $^1\text{H}$ -,  $^{13}\text{C}$ -,  $^{19}\text{F}$ -,  $^{15}\text{N}$ -, and  $^{31}\text{P}$ -NMR, Introduction to 2D- NMR techniques: COSY, HMQC and HECTOR Spectra. MASS: Theory, instrumentation and modifications; Unit Mass and molecular ions; recognition of  $\text{M}^+$  ions, General fragmentation rules; McLafferty rearrangements. Interpretation of spectroscopic (NMR and mass) data, as applied to organic system.

**40Hrs****COURSE OUTCOMES**

On completion of the course, student will be able to

CO1 – Acquire knowledge about various lanthanides-based reagents

CO2 – Understand the basic concepts of advanced organic reagents and reactions

CO3 – Understand various organic transformations

CO4 – Investigate and determine the structure of typical organic chemical compounds using spectroscopic techniques.

CO5 – Identify organic compounds by analysis and interpretation of spectral data.

CO6 – Apply the concepts of spectroscopy in industrial application.

**TEXT/REFERENCE BOOKS**

1. T. Imamoto, Lanthanides in Organic synthesis, Academic Press, 1994.
2. Carruthers, W. Modern Methods of Organic Synthesis, Cambridge University Press, 1971.
3. Kemp, W. Organic Spectroscopy 3rd Ed., W. H. Freeman & Co, 1991.
4. Silverstein, R. M., Bassler, G. C. & Morrill, T. C. Spectroscopic Identification of Organic Compounds, John Wiley & Sons, 1992.

**END SEMESTER EXAMINATION QUESTION PAPER PATTERN****Max. Marks: 100**

Part A/Questions: 10 questions of 3 marks

Part B/ Questions: 7 questions of 10 marks each with internal choice

**Exam Duration: 3 Hrs**

30 Marks

70 Marks



20MSC627T					Stereochemistry and photochemistry					
Teaching Scheme					Examination Scheme					
L	T	P	C	Hrs/Week	Theory			Practical		Total Marks
					MS	ES	IA	LW	LE/Viva	
3	0	0	3	3	25	50	25	--	--	100

### COURSE OBJECTIVES

- To understand the Molecular Symmetry & Chirality importance of stereo chemistry.
- To provide knowledge about the compounds containing Nitrogen, Sulphur and Phosphorus.
- To develop skills for various isomerism and stereo selective, specific synthesis and its application in organic chemistry
- To develop the fundamental knowledge about organic photochemical reactions.
- Knowledge on different types of photochemical reactions.

#### Unit 1: Stereochemistry-I

10 h

Molecular Symmetry & Chirality: Symmetry operations and symmetry elements ( $C_n$  &  $S_n$ ). Criteria for Chirality. Desymmetrization, Stereochemistry of the compounds containing Nitrogen, Sulphur and Phosphorus. Asymmetric synthesis. Stereochemistry of fused, bridged, and caged ring systems, resolution of enantiomers,

#### Unit 2: Stereochemistry-II

10 h

Prochirality, enantiotopic and diastereotopic groups and faces, The Hammett relationship, stereochemistry and mechanism. Stereoelectronic and steric principles in reactions: Substitution, elimination and addition; selectivity and specificity. Importance of stereochemistry in real life: some examples

#### Unit 3: Photochemistry-I

10 h

Photochemical energy Franck Condon Principle, Jablonski diagram singlet and triplet states, dissipation of photochemical energy, photosensitization, quenching, quantum efficiency and quantum yield, experimental methods of photochemistry. Photochemistry of carbonyl compounds n- $\pi^*$  transitions Norrish type I and Norrish type II cleavages, Paterno-Buchi reaction.

#### Unit 4: Photochemistry-II

10 h

Photochemical reduction, substitution reaction, cis-trans isomerism, photochemistry of butadiene, di-pi methane rearrangement and related processes, Photochemistry of aromatic compounds - Excited state of benzene its 1,2-1,3 1-4 additions, photo Fries rearrangements

### COURSE OUTCOMES

#### On completion of the course, student will be able to

- CO1 - Understand the Molecular Symmetry & Chirality importance of stereo chemistry.  
 CO2-Enable to illustrate and appraise about the provide knowledge about the compounds containing Nitrogen, Sulphur and Phosphorus.  
 CO3. Illustrate the importance of various isomerism and stereo selective, specific synthesis and its application in organic chemistry  
 CO4 - Understand the fundamentals and principles of organic photochemistry.  
 CO5 – Acquire knowledge about the experimental methods and reaction progresses in photochemical reactions  
 CO6 - Develop the knowledge on different types of photochemical reactions.

### TEXT/REFERENCE BOOKS

1. J. Clayden, N. Greeves and S. Warren, **Organic Chemistry** 2nd edition (Oxford University Press, 2012) [ISBN 0199270295](#) (with useful [extra chapters](#)).
2. M. J. T. Robinson, **Organic Stereochemistry** (Oxford Chemistry Primer, no. 88) (Oxford University Press, 2000) [ISBN 0198792751](#) (affordable, technically thorough guidebook).
3. E. L. Eliel and S. H. Wilen, **Stereochemistry in Organic Compounds** (Wiley, 1994) [ISBN 0471016705](#) (a comprehensive reference text).
4. Stereochemistry of Organic Compounds by D. Nasipuri, Wiley, 1994.
5. Advanced Organic Chemistry: Reactions Mechanisms and Structure by Jerry March, WILEY-INTERSCIENCE A JOHNWILEY & SONS, INC., PUBLICATION.
6. Reaction Mechanism in Organic Chemistry, S.M. Mukherji and S. P. Singh, Trinity press.
7. Molecular reactions and Photochemistry by Charles Dupey and O. Chapman, Prentice Hall.
8. Principles of Molecular Photochemistry, Nicholas J. Turro V. Ramamurthy J. C. Scaiano

20MSC628T					Heterocycles and Vitamins					
Teaching Scheme					Examination Scheme					
L	T	P	C	Hrs/Week	Theory			Practical		Total Marks
					MS	ES	IA	LW	LE/Viva	
3	0	0	3	3	25	50	25	--	--	100

**COURSE OBJECTIVES**

- To understand the definition, basic concepts, importance of Heterocycles
- To develop skills for various heterocycle synthesis and its application in organic chemistry
- To acquire the basic knowledge of vitamins
- To understand the biosynthesis of vitamins.

**UNIT 1 HETEROCYCLES - I****10 h**

Five and six membered heterocyclics with two hetero atoms. Synthesis, reactivity, aromatic character and importance of the following heterocycles: Pyrazole, Imidazole, Oxazole, Thiazole, Isoxazole, Isothiazole, Pyridazine, Pyrimidine, Pyrazine, Oxazine, thiazine, benzimidazole, benzoxazole and benzthiazole. Heterocyclics with more than two hetero atoms. Synthesis, reactivity, aromatic character and importance of the following and their applications in organic synthesis. Heterocycles: 1,2,3-triazoles, 1,2,4-triazoles, Tetrazoles, 1,2,4-oxadiazole, 1,3,4-oxadiazole, 1,2,5-oxadiazole, 1,2,3-thiadiazoles, 1,3,4-thiadiazoles, 1,2,5-thiadiazoles, 1,2,3-triazine, 1,2,4-triazine, 1,3,5-triazine, tetrazines. Synthesis and importance of purines and pteridines. Synthesis of Caffeine, theobromine and theophylline.

**UNIT 2 HETEROCYCLES – II****10 h**

Nomenclature of bicyclic and tricyclic fused systems; Introduction to the chemistry of azepines, diazepines, oxepines, thiepins and their aza-analogues; Phosphorus and selenium containing heterocycles. Cyclazines. Larger ring and other Heterocycles: structure, stability and reactivity of Azepines, Oxepines and Thiepins. Synthesis of Diazepines rearrangements of 1, 2 - diazepines. Synthesis of Benzoazepines, Benzodiazepines, Benzooxepines, Benzothiepins, Azocines and Azonines. Synthesis of selenophenes, Tellerophenes, Phospholes and Boroles.

**UNIT 3 VITAMINS – I****10 h**

Introduction, structure, and classification of common vitamins. Biological importance of vitamins. Chemistry, absorption & transport, sources, function and deficiency of both fat soluble and water-soluble vitamins.

**UNIT 4 VITAMINS – II****10 h**

BIOSYNTHESIS OF VITAMIN A, E, B1 (THIAMIN), AND B2 (RIBOFLAVIN)

**40 h****COURSE OUTCOMES**

On completion of the course, student will be able to

- CO1 – Understand the basic concepts, importance of Heterocycles
- CO2 – Illustrate the importance of various heterocycle synthesis and its application in organic chemistry
- CO3 – Evaluate the synthesis, properties and application of various industrial heterocyclic compound
- CO4 – Understand the basic concepts of Vitamins
- CO5 – Learn the function and deficiency of vitamins
- CO6 – Understand the biosynthesis of vitamins

**TEXT/REFERENCE BOOKS**

1. Morrison, R. N. & Boyd, R. N. Organic Chemistry, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
2. Bahl, A. (2005). A text book of organic chemistry. S. Chand.
3. Graham Solomons and Craig B. Fryhle, Organic Chemistry, Eighth Edition John Wiley and Sons, 2004.
4. Lubert Stryer, Biochemistry, 6th Edition, W. H. Freeman and Company, 2007.

**END SEMESTER EXAMINATION QUESTION PAPER PATTERN****Max. Marks: 100****Exam Duration: 3 Hrs**

Part A/Question: &lt;Details&gt;

&lt;&gt; Marks

20MSC629T					Chemistry of Natural Products					
Teaching Scheme					Examination Scheme					
L	T	P	C	Hrs/Week	Theory			Practical		Total Marks
					MS	ES	IA	LW	LE/Viva	
3	0	0	3	3	25	50	25	--	--	100

**COURSE OBJECTIVES**

- To acquire the basic concepts of natural products chemistry.
- To determine and analyze the structure and stereochemistry of natural products.
- To demonstrate the basic knowledge of natural product synthesis.
- To understand biosynthesis of natural products.
- To apply the concepts of natural product chemistry in real life/pharmaceutical and industrial sector.

**UNIT 1 TERPENOIDS AND CAROTENOIDS****10 h**

Structure determination, stereochemistry, biosynthesis and synthesis of the following representative molecules: Menthol, and  $\beta$ -Carotene.

**UNIT 2 ALKALOIDS AND PLANT PIGMENTS****10 h**

Alkaloids: Structure, stereochemistry, synthesis and biosynthesis of Ephedrine and Morphine.

Plant Pigments: Occurrence, nomenclature and general methods of structure determination; Isolation and synthesis of anthocyanins.

**UNIT 3 STEROIDS****10 h**

Basic skeleton and stereochemistry, Structure and synthesis of cholesterol, Steroid hormones, Chemical tests for steroids.

**UNIT 4 PEPTIDES, PROTEINS AND NUCLEIC ACIDS****10 h**

Structure, synthesis, biogenesis of peptides, proteins, nucleosides, nucleotides; DNA and RNA.

**40 h****COURSE OUTCOMES**

On completion of the course, student will be able to

CO1 – Learn the basic concepts of natural products chemistry. (occurrence, isolation, general properties, classification etc.)

CO2 –Determine structure of the given natural products. (chemical/spectroscopic)

CO3 –Understand the stereochemistry of the given natural products.

CO4 –Develop theoretical knowledge about natural products synthesis.

CO5 –Understand the biogenesis of natural products.

CO6 –Apply the concepts of natural products chemistry in real life. (drug design, natural dyes, metabolism etc.)

**TEXT/REFERENCE BOOKS**

1. Finar, I. L. Organic Chemistry (volume 2), Dorling Kindersley (India) Pvt. Ltd. (Pearson Education). (available in library)
2. Agarwal, O. P. Organic Chemistry Natural Products. Krishnan Prakashan. (vol 1 and vol 2).
3. Cseke, L.J. (2006). Natural Products from plants. CRC Press, Taylor and Francis, 2nd edition, US. (available online)
4. Dewick, P.M. (2009). Medicinal Natural Products: A Biosynthetic Approach. Willey & Sons, 3rd edition, UK. (available online)
5. Thomson, R.H. (2008). The Chemistry of Natural Products, Springer, 1st edition. (1993 edition available online)
6. D. L. Nelson, M. M. Cox (2017), Lehninger Principles of Biochemistry, W. H. Freeman, 7<sup>th</sup> edition. (available online)

**END SEMESTER EXAMINATION QUESTION PAPER PATTERN****Max. Marks: 100****Exam Duration: 3 Hrs**

Part A/Questions: 10 questions of 3 marks

30 Marks

Part B/ Questions: 7 questions of 10 marks each with internal choice

70 Marks

20MSC630T					Asymmetric Synthesis/Catalysis					
Teaching Scheme					Examination Scheme					
L	T	P	C	Hrs/Week	Theory			Practical		Total Marks
					MS	ES	IA	LW	LE/Viva	
3	0	0	3	3	25	50	25	--	--	100

**COURSE OBJECTIVES**

- To develop a fundamental understanding of asymmetric synthesis.
- To convey the importance of enantiomerically pure organic compounds.
- To develop effective strategies to control stereochemical relationships.
- To explain the basic knowledge of asymmetric catalysis.

**UNIT 1 PRINCIPLES OF ASYMMETRIC SYNTHESIS****10 h**

Introduction and terminology. Topocity in molecules. Homotopic, Stereoheterotopics (enantiotropic and diastereotopic) groups and faces – Symmetry, substitution and addition criteria. Prochirality nomenclature: Pro – R, Pro – S, Re and Si.

**UNIT 2 SELECTIVITY IN SYNTHESIS****10 h**

Stereospecific reactions, Stereoselective reactions, Conditions of Stereoselectivity: Symmetry and transition state criteria, kinetic and thermodynamic control. Methods for inducing enantio and diastereoselectivity. Analytical methods: Techniques for determination of Enantioselectivity. Specific rotation, Chiral HPLC.

**UNIT 3 METHODOLOGY OF ASYMMETRIC SYNTHESIS****10 h**

CLASSIFICATION OF ASYMMETRIC REACTIONS INTO (1) SUBSTRATE CONTROLLED (2) CHIRAL AUXILIARY CONTROLLED (3) CHIRAL REAGENT CONTROLLED AND (4) CHIRAL CATALYST CONTROLLED.

**UNIT 4 ASYMMETRIC CATALYSIS****10 h**

Metal mediated catalysis – asymmetric hydrogenation; Noyori's BINAP – Sharpless epoxidation, dihydroxylation, aminohydroxylation of alkenes, Organocatalysis – Proline mediated aldol reaction and further expansion in the field of Organocatalysis.

**40 h****COURSE OUTCOMES**

On completion of the course, student will be able to

- CO1 – Understand the basic principles of asymmetric synthesis
- CO2 – Develop effective strategies to control stereochemical relationships
- CO3 – Acquire knowledge of classification of asymmetric synthesis
- CO4 – Fabricate efficient and elegant syntheses of target core structures in a stereocontrolled manner
- CO5 – Understand the importance of enantiomerically pure organic compounds
- CO6 - Understand the basic concepts of metal catalysis and organocatalysis

**TEXT/REFERENCE BOOKS**

1. Stereochemistry of Organic Compounds by D. Nasipuri, Wiley, 1994.
2. Catalysis in Asymmetric Synthesis by Vittorio Caprio, Jonathan M. J. Williams, Wiley, 2009.
3. Catalytic Asymmetric Synthesis by Iwao Ojima, Wiley, 2013.
4. Fundamentals of Asymmetric Catalysis by Marisa C. Kozlowski, Patrick J. Walsh, 2008.

**END SEMESTER EXAMINATION QUESTION PAPER PATTERN****Max. Marks: 100****Exam Duration: 3 Hrs**

Part A/Question: &lt;Details&gt;

&lt;&gt; Marks

20MSC634P					Organic Chemistry Stream Elective Lab					
Teaching Scheme					Examination Scheme					
L	T	P	C	Hrs/Week	Theory			Practical		Total Marks
					MS	ES	IA	LW	LE/Viva	
0	0	3	1.5	3				50	50	100

**COURSE OBJECTIVES**

- Knowledge about different multistage organic transformations
- Learn regio-selective and chemo-selective Principles
- Extract different natural products
- Estimate vitamin C in tablets
- Learn Lambert's Beer's Law with the help of U.V. visible spectrophotometer

**LIST OF EXPERIMENTS**

1. Stereospecific preparation of trans-cyclohexane-1,2-diol via bromohydrin and epoxide formation.
2. Multistage synthesis (benzaldehyde  $\longrightarrow$  chalcone  $\longrightarrow$  chalcone epoxide) and their characterization by UV, IR and Melting point
3. Fischer Indole synthesis: Synthesis of Tetra Hydro carbazole.
4. Steam distillation of essential oil from lemon peel.
5. Extraction of anthocyanins and their application as pH indicator.
6. To verify Lambert's Beer's Law with the help of U.V. visible spectrophotometer
  - (a) To determine  $\lambda$  max of a given organic sample (Allura red or  $\beta$ -carotene).
  - (b) To determine the concentration of unknown sample (Allura red or  $\beta$ -carotene) with the help of U.V. visible spectrophotometer.
7. Verification on the photo-catalytic decomposition of organic dye (e.g. methyl orange)
8. Extraction of natural dyes (chlorophyll and betalain dyes) and determination of their UV-vis absorption peaks.
9. Green methods of synthesis (microwave induced)
  - (i) Synthesis of Schiff's base from aniline and p-anisaldehyde in the presence of lime juice
  - (ii) Synthesis of coumarin by Knoevenagel reaction using salicylaldehyde and ethyl acetate in the presence of a base.
10. Interpretation of spectral data of organic compounds (Minimum 4 spectral analysis)
11. Process for preparation of Vitamin C and method for determination of vitamin C in tablets.

**COURSE OUTCOMES**

On completion of the course, student will be able to

- CO1– Understand phase transfer catalysis  
 CO2– Perform multistage organic reactions  
 CO3– Extraction of natural products  
 CO4– Understand Lambert's Beer's Law with the help of U.V. visible spectrophotometer  
 CO5– Comprehend Green methods of synthesis  
 CO6– Prepare and determine Vitamin C in tablets

**TEXT/REFERENCE BOOKS**

1. Comprehensive practical organic chemistry: Quantitative analysis by V.K Ahluwalia, Renu Aggarwal; Universities press; ISBN 13: 978 81 7371 273 9
2. A. K. Nad, B. Mahapatra & A. Ghosal, An Advanced Course in Practical Chemistry, New Central, 2007. Vogel's Text Book of Practical Organic Chemistry (5th Edn).
3. Finar, I. L. Organic Chemistry (volume 1), Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).

**SEMESTER EXAMINATION PATTERN****Max. Marks: 100****Exam Duration: 3 Hrs**

LW(Daily lab performance plus journal maintain each 25 marks)

50 Marks

LE (Viva-voce plus Lab examination each 25 marks)

50 Marks

20MSC621T					Paints, Pigments & Cosmetics					
Teaching Scheme					Examination Scheme					
L	T	P	C	Hrs/Week	Theory			Practical		Total Marks
					MS	ES	IA	LW	LE/Viva	
3	0	0	3	3	25	50	25	--	--	100

**COURSE OBJECTIVES**

- To learn the basic concepts of paints, pigments, dyes and cosmetics.
- To understand the formulation and structure-activity relationship of different paints, pigments and cosmetics.
- To demonstrate the knowledge of natural pigment extraction and dye synthesis.
- To evaluate the safety, efficacy and physiological effect of synthetic and herbal cosmetics.
- To apply the theoretical concepts in design and formulation of paints and cosmetics.

**UNIT 1 PIGMENTS & DYES****7 Hrs.**

Introduction to dyes and natural pigments: history, nomenclature and classification. Colour and chemical constitution: chromophores, auxochromes, hypsochromic and bathochromic shift. Concepts of fluorescence and phosphorescence. Extraction of natural pigments. Classification of dyes. Synthesis, properties and application of representative azo dyes. Synthesis, properties and application of representative fluorescent and laser dyes.

**UNIT 2 PAINTS****7 Hrs.**

Introduction to paints, surface coating compounds. Paints and pigments-formulation, composition and related properties. Oil paint. Thinners. Enamels. Emulsifying agents. Special paints (Heat retardant, Fire retardant, Eco-friendly paint, Plastic paint).

**UNIT 3 CHEMISTRY OF COSMETICS****7 Hrs.**

Introduction to cosmetics and cosmetology: definition, history and application. Anatomy of skin and hair with respect to cosmetology. Classification of cosmetics. Physiological effects of cosmetics. Introduction to cosmeceuticals: definition, classification, chemicals, mechanism of action. Introduction to oral care, skin, nail and hair care products: classification, properties, working mechanism, and formulation. Chemistry and function of materials used in cosmetics and cosmeceuticals.

**UNIT 4 MODERN TRENDS IN COSMETICS****7 Hrs.**

Study of representative cosmetic products. Introduction to herbal cosmetics. Safety and testing of cosmetics. Regulatory and quality control of cosmetics. Modern developments in cosmetic chemistry. Cosmetic surgery and related studies.

**28 Hrs.****COURSE OUTCOMES**

On completion of the course, student will be able to

- CO1 – Learn the basic concepts and application of pigments and dyes.
- CO2 – Demonstrate the knowledge on extraction of natural pigments and synthesis of selected dyes.
- CO3 – Understand composition, formulation and application of paints.
- CO4 – Develop theoretical knowledge on the formulation and working mechanism of various classes of cosmetics and cosmeceuticals.
- CO5 – Evaluate safety, efficacy and physiological effects of cosmetic products.
- CO6 – Analyse the modern trends and development in cosmetology.

**TEXT/REFERENCE BOOKS**

1. The Chemistry of Synthetic Dyes, Vol. I to VII by Venkataraman, Academic Press, New York.
2. Dyes and their intermediates by E. N. Abrahart.
3. Handbook of Synthetic Dyes and Pigments, Vol. I & II by K. M. Shah.
4. Industrial Dyes by Klans Hunger, Germany by Wiley-VCH.
5. Chemistry and Technology of the Cosmetics and Toiletries Industries by D.F. Williams, Springer International Edition.
6. Organic chemistry for cosmetic chemists by Anthony J. O'Lenick Jr.; Thomas G. O'Lenick, Carol Stream, IL: Allured Publishing, © 2008.
7. Beginning Cosmetic Chemistry by Schueller and Romanowsk, Allured Pub Corp; 3rd edition, 2008.
8. Handbook of cosmetic science and technology by Barel AO, Paye M, Maibach HI. CRC Press; 2014.

**END SEMESTER EXAMINATION QUESTION PAPER PATTERN****Max. Marks: 100**

Part A/Question: &lt;Details&gt;

Part B/Question: &lt;Details&gt;

**Exam Duration: 3 Hrs**

&lt;&gt; Marks

&lt;&gt; Marks

20MSC622T					Polymer Chemistry & Composite Materials					
Teaching Scheme					Examination Scheme					
L	T	P	C	Hrs/Week	Theory			Practical		Total Marks
					MS	ES	IA	LW	LE/Viva	
3	0	0	3	3	25	50	25	--	--	100

**COURSE OBJECTIVES**

- Students should understand and differentiate the main categories of composite materials and cite the distinguishing features of each.
- Students should understand the principles of the matrix and disperse phases and their behaviors on the characteristics, geometry/distribution, and properties of the constituent phases.
- Students should be able to gain the in-depth knowledge of types of polymers, different methods of synthesis, their properties and applications.
- Students should be able to understand the concept of characterization of polymeric materials.

**UNIT 1 INTRODUCTION TO POLYMERS****10 h**

Classification of Polymers; Degree of Polymerization. General Characteristics of Chain Growth Polymerization; Alkene Polymerization by Free Radical, Cationic and Anionic Initiators; General Characteristics of Step Growth Polymerization; Synthesis of Polymers by Step Growth Polymerization: Polyesters, Polyamides, Polycarbonates, Polysulphones, Polyphenyl Oxides and Polysiloxanes, Ring-opening Polymerization of Ethers and Lactones, glass transition temperature  $T_g$

**10 h****UNIT 2 FUNCTIONAL POLYMERS, POLYMERIC MATERIALS AND THEIR APPLICATIONS**

Conducting polymers, polymer catalysts, photoresponsive polymers, ionomers (PTFE, etc.) and packaging applications of ionomers, biopolymers

**UNIT 3 INTRODUCTION TO COMPOSITE MATERIALS****10 h**

Definition of composites, history of composites, classification of composites, properties of fiber-reinforced and particulate composites: advantages of composites, disadvantages of composites, applications of composites

**UNIT 4 TYPES OF COMPOSITES, THEIR PROCESSING PROPERTIES AND APPLICATIONS****10 h**

**Polymer Matrix Composites (PMC):** Glass Fiber–Reinforced Polymer (GFRP) Composites, Carbon Fiber–Reinforced Polymer (CFRP) Composites. Processing, properties and applications of PMC

**Metal Matrix Composites (MMC):** Types of Metal Matrix Composites, Important Metallic Matrices, Aluminium alloys, Titanium Alloys, Magnesium Alloys, Copper Alloys, Intermetallic Compounds. Processing, properties and applications of PMC.

**Ceramic Matrix Composites (CMC):** Processing of CMC, properties and applications of CMC.

**COURSE OUTCOMES**

On completion of the course, student will be able to

- CO1 – Be able to understand polymerization and classification of polymers, their unique properties and applications.
- CO2 – Be able to understand synthesis methods and mechanisms of various polymerization techniques
- CO3 – Be able to understand and define composite materials and the principles for the classification of composite materials.
- CO4 – Be able to understand the concepts of reinforcements in matrix materials and the fundamental properties underlying the formation of composites.
- CO5 – Be able to understand the relation between the disperse phase and matrix materials in order to visualize enhancement in the properties of the new composites.

**TEXT/REFERENCE BOOKS**

1. Chawla, Krishan K. Composite materials: science and engineering. Springer Science & Business Media, 2012.
2. Callister Jr, William D., and David G. Rethwisch. Fundamentals of materials science and engineering: an integrated approach. John Wiley & Sons, 2012.
3. Balasubramanian, M. Composite materials and processing. CRC press, 2013.
4. Text Book of Polymer Science By F. W. Billmeyer
5. Introduction to Polymers by R. J. Young and P. A. Lovell
6. Polymer Chemistry by G. Challa
7. Principles of Polymerization by George Odian
8. Mathews and Rawlings, Composite materials: Engineering and Science, Chapman and Hall.
9. Clyne, T. W., and Derek Hull. An introduction to composite materials. Cambridge university press, 2019.

Pandit Deendayal Upadhyay University					Materials & Nano Chemistry					
Teaching Scheme					Examination Scheme					
L	T	P	C	Hrs/Week	Theory			Practical		Total Marks
					MS	ES	IA	LW	LE/Viva	
3	0	0	3	3	25	50	25	--	--	100

#### COURSE OBJECTIVES (04)

- To familiarize with the concepts of materials and nanochemistry and their size and shaped dependent properties
- To provide the knowledge about the various strategies for the synthesis of nanomaterials
- To understand the different techniques for characterization of nanomaterials
- To evaluate the role of nanomaterials in various applications associated to real world problems

#### UNIT -1: Nanomaterials and Nanochemistry

Introduction to Nanomaterials, classifications of nanomaterials, Surface area to volume ratio, Quantum Confinement, Size and shape Dependent Chemical and Physical Properties: Electrical, optical, catalytic, thermodynamic, electrical and structural, electrochemical, mechanical, etc. Bulk and Nanoporous materials, Nanocomposite and Hybrid materials. Incorporation of heteroelements [10]

#### UNIT -2: Synthetic methods for nanomaterials

Bottom-up and top-down approach, wet chemical synthesis (Sol-gel, hydrothermal, thermal decomposition, chemical precipitation, micro-emulsion), Chemical and Physical methods (Grinding, Ball milling, PLD, Lithography), Thin and Thick films, Chemical Vapour Deposition (CVD), Spin coating-Epitaxy, Templated self-assembly and Electrochemical approaches [10]

**UNIT-3:** Characterization of Nanostructured Materials X-ray diffraction, X-ray photoelectron spectroscopy (XPS), Raman Spectroscopy; Thermal analysis (TGA/DTA/DSC), BET surface area, Scanning Electron Microscope (SEM)) Transmission electron microscopy (TEM), Atomic Force Microscopy (AFM), Elemental analysis: CHNS, AAS, ICP-OES. [10]

#### UNIT-4: Applications of Nanomaterials

Nanomaterials as catalyst, Nanomaterials for energy storage and conversion, Batteries, Supercapacitors, Fuel cells, Water splitting and solar cell; Electrochemical device/Cell fabrication and measurements techniques; Nanosensors; Environmental remediation, nanotechnology based water treatment strategies. [10]

Max. 40 h

#### COURSE OUTCOMES (06)

On completion of the course, student will be able to

- CO1 – Understand the concepts of materials and nanochemistry
- CO2 – Articulate the size and shape dependent chemical and physical properties of nanoscale materials
- CO3 – Develop understanding for synthesis of nanomaterials
- CO4 – Acquire knowledge about characterization of nanomaterials.
- CO5 – Understand the fundamental concept and learn about the applications of nanoscale materials
- CO6 – Analyse and apply the principles of nanochemistry in real world problems.

#### TEXT/REFERENCE BOOKS

1. C. N. R. Rao, A. Muller, A. K. Cheetham (Eds), The chemistry of nanomaterials: Synthesis, properties and applications, Wiley VCH Verlag GmbH & Co, Weinheim, 2004.
2. Nanoparticles: From theory to applications – G. Schmidt, Wiley Weinheim 2004.
3. Ghuzang G.Cao, Nanostructures and Nanomaterials: Synthesis, properties and applications, Imperial College Press, 2004
4. Introduction to Nanoscience by Gabor L. Hornyak, Joydeep Dutta, Harry F. Tibbals, Anil K. Rao. CRC Press, 2008.
5. Nanotechnology: Importance and Application by M.H. Fulekar, IK International, 2010.

#### END SEMESTER EXAMINATION QUESTION PAPER PATTERN

Max. Marks: 100

Part A/Question: 3 Questions from each unit, each carrying 3 marks

Part B/Question: 2 Questions from each unit, each carrying 8 marks

Exam Duration: 3 h

36 Marks

64 Marks



20MSC624T					Fine chemicals (Petrochemicals, oil, soap and pesticides)					
Teaching Scheme					Examination Scheme					
L	T	P	C	Hrs/Week	Theory			Practical		Total Marks
					MS	ES	IA	LW	LE/Viva	
3	0	0	3	3	25	50	25			100

**COURSE OBJECTIVES**

1. To acquire the fundamental knowledge of fine chemicals of industrial importance.
2. Learning the chemical composition manufacturing and applications of fats, oils and soaps in industries.
3. To understand and acquire the necessary basic knowledge, chemical composition and manufacturing of pesticides.
4. Attaining basic knowledge and applications of fine chemicals, pharmaceuticals and biochemical reagents.
5. Learning the basics of the manufacturing and applications of heavy organic chemicals in industries.

**Unit I: Fats, Oils and soaps: (8h)**

Chemical composition of fats and oils; Essential oils, surfactants and emulsifying agents, Hydrogenation, oxidation and auto-oxidation, polymerization, hydrolysis, esterification, interesterification, sulfonation, amidation, methathesis and co-metathesis, pyrolysis etc.; Present status of soap and detergent industries; Raw materials for soap industry and their selection; Kinetics and Phase reactions in soap boiling, various types of soaps and applications; Chemistry and technology of synthetic detergents (anionic, cationic, non-ionic, and amphoteric), detergent additives.

**Unit II: Pesticides: (8h)**

General introduction to pesticides (natural and synthetic), benefits and adverse effects, changing concepts of pesticides, structure activity relationship, synthesis and technical manufacture and uses of representative pesticides in the following classes: organochlorines (DDT, gammexene); organophosphates (malathion, parathion); carbamates (carbofuran and carbaryl); quinones (chloranil), anilides (alachlor and butachlor).

**Unit III: Fine chemicals: (8h)**

Manufacture of following with reference to: (i) raw material, (ii) production process, (iii) quality control, (iv) hazards and safety, (v) effluent management. Sodium borohydride, lithium aluminium hydride, sodium ethoxide, paracetamol, chloramphenicol; sulphonamides; sulphamethoxazol, sulphacetamide, trimethoprim; acyclovir, phenobarbital, diazepam, glyceryl trinitrate, dapson, AZT-Zidovudine; Biochemical reagents – ninhydrin, tetrazolium blue, 1, 2-naphthoquinone-4-sulphonate.

**Unit IV: Heavy organic chemicals: (8h)**

Manufacture of following with reference to: (i) raw material, (ii) flow chart, (iii) effluent management. (iv) uses; propargyl alcohol, 1, 4- butanediol, vinyl chloride, pyridines, picolines, phthalic anhydrides, glycerol, sorbitol, chloroform, Ethanolamine; Industrial solvents – DMF, DMSO, sulfolane, alkyl pyrrolidone, THF, dioxane

**COURSE OUTCOMES**

On completion of the course, student will be able to

- CO1 - Understand the basic techniques about the chemical composition and manufacturing of fats and oils, and their applications.  
 CO2- Get an insight into the basic techniques used for the synthesis and of soaps and detergents and their applications.  
 CO3 - Acquire the fundamental knowledge about the synthesis of pesticides in industries and their applications.  
 CO4 - Learn various techniques for the synthesis, quality control, hazards and safety measures employed for the synthesis of fine chemicals.  
 CO5 – Acquire new knowledge about synthesis, quality control, hazards and safety measures employed in synthesis of important pharmaceuticals and biochemical reagents.  
 CO6 - Understand the synthesis, quality control, hazards and safety measures used for the synthesis of valuable heavy organic chemicals and industrial solvents.

**Recommended texts:**

1. Vermani, O. P.; Narula, A. K. (2004), Industrial Chemistry, Galgotia Publications Pvt. Ltd., New Delhi.
2. Bhatia, S. C. (2004), Chemical Process Industries, Vol. I & II, CBS Publishers, New Delhi.
3. Gupta, P.K.; Gupta, S.K. (2011), Pharmaceuticals and Cosmetics, Pragati Prakashan
4. Industrial Chemistry part 1&2 by Krishna Prakashan, by B K Sharma
5. E. Stocchi: Industrial Chemistry, Vol-I, Ellis Horwood Ltd. UK
6. Roger's Manual of Industrial Chemistry, C.C. Furnas (Edition), 6th edition, Vol.I, D. Van Nostrand Company, Inc.
7. Engineering Chemistry, 4th Edition, V.P. Mehta, Jain Brothers, New Delhi.
8. Engineering Chemistry, by P.C. Jain and M. Jain.

**END-SEMESTER EXAMINATION QUESTION PAPER PATTERN**

<u>Max. Marks: 100</u>	<u>Exam Duration: 3 Hrs</u>
Part A	25 Marks
Part B	25 Marks
Part C	25 Marks
Part D	25 Marks

20MSC625T					Petroleum Chemistry & Catalysis					
Teaching Scheme					Examination Scheme					
L	T	P	C	Hrs/Week	Theory			Practical		Total Marks
					MS	ES	IA	LW	LE/Viva	
3	0	0	3	3	25	50	25			100

### COURSE OBJECTIVES

1. To acquire the fundamental knowledge of catalysis and petroleum products.
2. Learning the methods of preparation of catalysts.
3. To understand and acquire the necessary basic knowledge of catalyst characterization.
4. Attaining basic knowledge of catalytic reactors used in industry.
5. Learning the industrial application of catalysts and application of petroleum chemistry.

#### Unit I: Introduction to Petroleum Chemistry (7h)

Properties and General Characteristics of Hydrocarbon, Composition, Molecular types in Petroleum.

Characterization and Analytical Techniques for Crude Oil: Physical properties, Thermal properties, Electrical properties, Optical properties, Chromatographic techniques, Spectroscopic methods (Principles and Applications of UV Visible, IR, and NMR Spectroscopy), Characterization of formation water. SARA Separation methods, Metals and Heteroatoms in Heavy crude oil.

#### Unit II: Catalysis: Fundamentals, Preparation & Characterization: (7h)

Introduction to Catalysis, Definition, Classification, Properties of catalysts, Preparation of catalysis - Laboratory Techniques, Industrial methods, Transition models, Dual functional catalysts, Zeolites, Enzymes, Solid Catalysts, Powder Catalysts, Pellets, Composition, Active ingredients.

Surface area measurements, BET Theory, Pore size distribution, Porosimetry Chemisorption, Crystallography and surface analysis techniques, XRD, Surface acidity and toxicity, Activity, Life time, Bulk density, Thermal stability

#### Unit III: Applications of Petroleum Chemistry: (7h)

Processing and Refining of crude oil: Processing and Refining of crude oil: Distillation, Sweetening and Cracking (basic concepts), Reforming, Isomerization, Alkylation processes, Polymerization processes, Solvent process, Knocking, Octane number and Cetane number, Additives to improve the quality of Diesel and Petrol, Catalysis and Applications of Catalysts (like Zeolite and other catalysts) in separation processes and also in petroleum industries.

#### Unit IV: Catalytic Reactors & Industrial Application of Heterogeneous Catalysts (7h)

Industrial reactor types, theoretical background, design and operation of reactors, strategy and considerations in reactor design, evaluation of reactor performance, Catalyst deactivation, types of deactivation and regeneration. Industrial applications of catalyst, Catalysis and green chemistry, phase transfer catalysis and bifunctional catalysis.

### COURSE OUTCOMES

On completion of the course, student will be able to

- CO1 - Understand the basic fundamentals behind catalysis & petroleum chemistry.
- CO2- Get an insight into the different methods of catalyst preparation.
- CO3 – Analyse and correlate the physicochemical properties of catalysts.
- CO4 – Correlate the evolution and properties of crude oil and further petroleum products.
- CO5 – Understand the use of catalytic reactors in various chemical industries
- CO6 – Have depth knowledge of industrial applications of catalysis in petroleum industry.

#### Recommended texts:

1. Elements of Chemical Reaction Engineering, Fourth Edition, H. Scott Fogler.
2. Chemical Reactor Analysis and Design, G. F. Froment, K. B. Bischoff
3. Green Chemistry and Catalysis, Roger Arthur Sheldon , Isabel Arends.
4. Petroleum Refining Processes, James Speight, Baki Ozum. Methods and Procedures for Catalyst Characterization, Jerzy Haber<sup>1</sup>, Jochen H. Block, Bernard Delmon
5. Speight, J. G - The Chemistry and Technology of Petroleum
6. George A. Olah & Arpad Molnar – Hydrocarbon Chemistry
7. Speight, J. G. - Handbook of Petroleum Analysis
8. William D. McCain - The Properties of Petroleum Fluids

20MSC633P					Industrial Chemistry Stream Elective Lab					
Teaching Scheme					Examination Scheme					
L	T	P	C	Hrs/Week	Theory			Practical		Total Marks
					MS	ES	IA	LW	LE/Viva	
0	0	3	1.5	3				50	50	100

**COURSE OBJECTIVES**

- To learn synthesis and characterization of pigments
- To learn analysis of commercial cosmetic products
- To learn synthesis and characterization of nanomaterials
- To acquire hands on experience on polymer synthesis
- To learn use of gas chromatography for sample analysis
- To test various properties of oils and fats

**LIST OF EXPERIMENTS**

1. Preparation and characterization of red/yellow/white/green pigment. (Any one amongst Fe<sub>3</sub>O<sub>4</sub>/Chrome yellow/ZnO, PbCl<sub>2</sub>/Malachite)
2. Testing photostability of commercial sunscreens by absorption spectroscopy.
3. Extraction and chromatographic analysis of commercial hair dyes (by TLC/LC).
4. Analysis of oils and fats (iodine value, saponification value, acid value).
5. Estimation of hardness of water by titration with soap solution.
6. Synthesis and characterization of nanomaterials using wet chemical methods (any one): Metal Oxides/Metal Hydroxides/Metal Sulphides/Hybrid Composites
7. Synthesis and characterizations of metal nanoparticles (Any one): Ag/Au/Pt/Pd
8. Bulk Polymerization of MMA with AIBN
9. Emulsion Polymerization of Styrene
10. Analysis of mixture of hydrocarbons by gas chromatography
11. To find the flash and fire point of the given oil sample
12. To determine the viscosity of a given oil sample and also the effect of temperature on viscosity

**COURSE OUTCOMES**

On completion of the course, student will be able to

CO1– Prepare and characterize pigments

CO2– Analyse purity and stability of commercial cosmetic products by spectroscopic/chromatographic techniques

CO3– Prepare and characterize different types of nanomaterials

CO4– Synthesize polymers by different processes

CO5– Analyse mixture of hydrocarbons by gas chromatography

CO6– Evaluate important quality parameters of oils and fats

**TEXT/REFERENCE BOOKS**

- 1.

**SEMESTER EXAMINATION PATTERN**

**Max. Marks: 100**

LW(Daily lab performance plus journal maintain each 25 marks)

LE (Viva-voce plus Lab examination each 25 marks)

**Exam Duration: 3 Hrs**

50 Marks

50 Marks

20MSC611T					Atomic & Molecular Spectroscopy					
Teaching Scheme					Examination Scheme					
L	T	P	C	Hrs/Week	Theory			Practical		Total Marks
					MS	ES	IA	LW	LE/Viva	
3	0	0	3	3	25	50	25	--	--	100

**COURSE OBJECTIVES**

- To comprehend advanced spectroscopy as a tool for molecular structure determination
- Attaining basic principles applied for mass spectrometry measurements
- To estimate how chemical reactions like fragmentation in mass assist in spectral analysis
- To acquire the knowledge of basic theory of nuclear magnetic resonance spectroscopy and able to interpret basic NMR spectra
- To learn the fundamental principle of photoelectron spectroscopy

**UNIT 1 Fundamentals of Mass spectrometry****10 Hrs.**

Introduction of mass spectrometry- Basic terminology, Principle of a mass spectrometer Formation and acceleration of ions, Behavior of ions in electric and magnetic fields, Ion focusing, The Mass Spectrometer, High-Resolution Mass Spectrometry

Instrumentation: Ionization Methods, Chemical Ionization; Electron Ionisation (EI), Electrospray Ionisation (ESI), Desorption Ionization, Modes of ionization (positive, negative), mass analyser and detectors Detectors, data acquisition, vacuum systems:

Interpretation of mass spectra: Molecular and Fragment Ions, The Base Peak, The Molecular or Parent Ion (M+), The (M + 1)+ Ion Formation of Adducts, Isotopic Fragments; Depicting Mass Spectral Data; The Molecular or Parent Ion; Predicting the Formation of M+; The Nitrogen Rule; Metastable Ions; Doubly Charged Ions; The General Fragmentation Process; The Fragmentation of a Hypothetical Molecule

**UNIT 2 Mass spectrometry: Data Analysis & Structure Elucidation****10 Hrs.**

The Analysis of Mass Spectra: Identifying the Molecular Ion; The Fragmentation of M+; Determining the Molecular Ion from the Fragments; General Rearrangement; Skeletal Rearrangement; The McLafferty Rearrangement; The Loss of Neutral Fragments; Atomic Weight Determinations; The Isotopes of Carbon; Calculating Relative Intensities; The Experimental Determination of the Carbon Number; Compounds Containing Bromine and/or Chlorine; Compounds Containing Sulfur,

Structural Elucidation: The Fragmentation Patterns of- Straight-Chain Alkanes, Branched Alkanes, Cycloalkanes, Unsaturated Hydrocarbons, Alkyl Halides, Phenyl Halides, Benzyl Halides, Alcohols and Phenols, Problems in Mass Spectrometry: Some General Suggestions for Interpreting Mass Spectra

**UNIT 3 Proton Nuclear magnetic resonance spectroscopy****12 Hrs.**

Introduction to NMR: Theory: Nuclear spin quantum number, properties of the nuclei, Magnetic moment of a nucleus, Fundamental NMR equation, Larmor precession, spin-spin and spin lattice relaxations,

Instrumentation & Chemical Shift: Sample Handling, Shielding, Deshielding and Chemical Shift, Standard for proton NMR, Tetramethylsilane (TMS) as reference compound, Advantages of TMS as a reference compound, Measurement of Chemical Shift: NMR Scale,  $\delta$  (or ppm) and  $\tau$  scale, Factors Affecting chemical Shift: Electronegativity-inductive effect, Anisotropic effects, Hydrogen bonding, van der Waals deshielding

Interpretation & Applications of NMR: Number of PMR Signals: Equivalent and Non-equivalent Protons, Peak Area and Proton counting, Spin-Spin Splitting: Spin-Spin coupling, Multiplicity-Number of Component Peaks (Lines) in Multiplet, Relative Intensities of Component Peaks (Lines) of a Multiplet, Analysis (Interpretation) of NMR Spectra, Applications of PMR Spectroscopy.

**UNIT 4 Photoelectron spectroscopy****8 Hrs.**

Introduction to Photoelectron spectroscopy: The photoelectric effect, Origin of X-ray spectra, Energy levels in atom, electron binding (ionization) energy, UV photoelectron spectroscopy, Principle & Instrumentation X-ray photoelectron spectroscopy: Chemical shifts in XPS, Chemical shifts and oxidation states, Analytical applications of XPS, Auger electron spectroscopy: Auger process, mechanism of emission of an Auger electron, Auger Transitions: ionization, relaxation and emission, nomenclature for Auger transitions: ABB transitions, AAB transitions, Coster-Kronig transitions, Examples of Auger Processes, Kinetic Energies of Auger Electrons.

**COURSE OUTCOMES****Max. 40 Hrs**

On completion of the course, student will be able to

CO1- Estimate molecular weight by using mass spectra and

CO2- Able to understand various mass spectrometric parameters

CO3- Elucidate chemistry of fragmentation reactions in mass spectrometry

CO4- understand and differentiate between XPS, UPS and Auger spectroscopy and can demonstrate their practical application

CO5- Interpret the basic  $^1\text{H}$ NMR spectra, differentiate equivalent and non-equivalent protons and identify the splitting of NMR peak by analysing the chemical formulae.

CO6- Conceptualize the role of electron, proton and atomic mass, in magnetic resonance spectroscopy, photoelectron spectroscopy and mass spectrometry

**TEXT/REFERENCE BOOKS**

1. Donald L. Pavia, Gary M. Lampman, George S. Kriz, Introduction to Spectroscopy
2. Yadav, L. D. S. (2013). *Organic spectroscopy*. Springer Science & Business Media.
3. C. N. Banwell, E. M. McCash, Fundamentals of molecular spectroscopy
4. Peter Atkins, Julio de Paula, Physical Chemistry
5. William Kemp, Organic Spectroscopy
6. D. A. Skoog, D. M. West, Principles of Instrumental Analysis

**END SEMESTER EXAMINATION QUESTION PAPER PATTERN****Max. Marks: 100****Exam Duration: 3 Hrs**

Part A/Question: 10 multiple choice questions 1 mark each

10 Marks

Part B/Question: 10 Questions of 2 marks each with internal choice

20 Marks

Part C/Question: 4 Questions of 15 marks each with internal choice

60 Marks

Part D/Question: 1 Questions of 10 marks comprising a figure of an instrument for Labelling and identifying its various parts

10 Marks

20MSC612T					Advanced Instrumental Techniques-I					
Teaching Scheme					Examination Scheme					
L	T	P	C	Hrs/Week	Theory			Practical		Total Marks
					MS	ES	IA	LW	LE/Viva	
3	0	0	0	3	25	50	25	--	--	100

**COURSE OBJECTIVES**

- Gaining the practical knowledge of microscopic techniques.
- Acquiring basic principles applied for spectroscopic measurements.
- Attaining necessary basic knowledge of chromatographic separation and difference in various kind of chromatographic techniques
- Gaining the factual knowledge of surface analysis techniques
- Learning the basic instrumentations of various analytical techniques comprising instruments used in surface analysis, spectroscopic analysis, thermal analysis and chromatographic analysis

**UNIT 1: Advanced Microscopy Techniques in Modern Science****10 Hrs.****Optical Microscopy**

Introduction to Light Microscopy; Principles of Geometrical Optics and Snell's Law; Understanding Magnification and Resolution in Light Microscopy; In-depth Analysis of Instrumentation in Light Microscopy; Functions and Significance of Key Components in Optical Microscopy Exploring Different Microscopy Modes: Bright-field, Dark-field, and Phase Contrast

**Electron Microscopy**

Principles and Fundamentals of Electron Microscopy; Electron Behavior in Microscopy and its Applications; Resolution Enhancement in Electron Microscopy; Comprehensive Study of Electron Microscopy Instrumentation; Scanning Electron Microscopy (SEM): Electron Sources, Lens, and Imaging Mechanisms; Detailed Analysis of SEM Components and its Pros and Cons; Transmission Electron Microscopy (TEM): Working Principles and Components; Advantages and Limitations of Transmission Electron Microscopy

**Atomic Force Microscopy (AFM)**

Exploring the Working Principle of Atomic Force Microscopy; Types of AFM: Contact Mode, Non-contact Mode, and Tapping Mode; Achieving High Resolution in Atomic Force Microscopy

**Unit 2: Optical techniques in Spectroscopy****12 Hrs****Introduction to Infrared Spectroscopy**

Fundamentals of IR Spectroscopy: Electromagnetic Spectrum, Spectroscopic Analysis; Infrared Regions and Molecular Vibrations; Calculating Molecular Vibrations and Identifying Infrared Active Modes; Absorption Considerations in IR Spectroscopy; Application of IR Spectroscopy in Various Fields

**FTIR Instrumentation and Operation**

Basic Principles of FTIR Instruments; Components of FTIR Instruments: IR Source, Interferometer, Beam Splitter, Mirrors, and Detector; Functioning of FTIR Instrument and Advantages: Speed, Sensitivity, Simplicity, and Internal Calibration; Sample Preparation Techniques: Liquid, Solution, Nujol Mull, KBr Disc, Attenuated Total Reflectance (ATR); ATR Crystal Materials, ATR Instrumentation, and Practical Applications

**Introduction to UV/VIS Spectroscopy**

Basics of UV/VIS Spectroscopy: Measurement Principle and Lambert-Beer Law; Role of UV/VIS Spectroscopy in Analytical Chemistry; Importance of UV/VIS Spectra: Qualitative and Quantitative Analysis; Spectrophotometer Design: Comparison, Scanning vs. Array Spectrophotometers

**Optical Pathways and Applications**

Understanding Optical Pathways: Single Beam and Double-Beam Configurations; Cuvette-Based UV/VIS Spectroscopy and Its Applications; Fixed Wavelength Spectroscopy and Concentration Determination; Scanning Spectroscopy, Kinetics, and Time-Dependent Measurements

**Accurate and Precise UV/VIS Measurements**

Factors Influencing Accurate UV/VIS Measurements: Solvent, Sample Concentration, Wavelength; Analysis of Mixtures and Strategies for Improved Precision; Micro-Volume Based UV/VIS Spectroscopy Techniques

**Unit 3: Fundamentals and Applications of Chromatographic Techniques****10 Hrs****Introduction to Chromatographic Techniques**

Overview and Classification of Chromatographic Techniques; Understanding Principles and Efficiency of Chromatographic Methods

**Mechanisms of Separation in Chromatography**

Exploring Adsorption, Partition, and Ion Exchange Separation Mechanisms

**Development of Chromatograms**

Techniques for Chromatogram Development: Frontal, Elution, and Displacement Methods

**Qualitative and Quantitative Analysis in Chromatography**

In-depth Analysis of Chromatographic Methods for Qualitative and Quantitative Studies; Study of Liquid Chromatography (LC), Gel Permeation Chromatography (GPC), Thin Layer Chromatography (TLC), Gas Chromatography (GC), and High Performance Liquid Chromatography (HPLC)

**Instrumentation and Applications of Chromatographic Techniques**

Exploration of Instrumentation in Gas Chromatography (GC), Gel Permeation Chromatography (GPC), and High Performance Liquid Chromatography (HPLC); Real-world Applications for GC, GPC, and HPLC

**Unit 4: Surface analysis Instruments****8 Hrs**

BET surface area technique- Brunauer-Emmett-Teller (BET) theory, the physical adsorption of gas molecules on a solid surface, BET equations, measurement of the total Surface area, specific surface area of materials, Porosity - pore volume, pore radius, sample preparation and experimental setup, Applications and shortcomings of BET

**COURSE OUTCOMES**

On completion of the course, student will be able to

CO1 - Understand the basic principal of microscopy will be able to explain the working mechanism of electron microscopy.

CO2 – Student will be able to understand the topographic techniques available for surface analysis

CO3 - Student will learn the theoretical aspects of FTIR and can explain the instrumentation of FTIR for material characterization.

CO4- Student will acquire the knowledge of advance instrumentation for UV/Vis and RAMAN techniques and will be able to understand their working principal and applications .

CO5 - Learn various type of chromatographic techniques and will acquire the basic knowledge of the instrumentation involved in these techniques.

CO6 – Students can describe the technique to analyse surface area and can differentiate between topographic techniques and surface area analysis

**TEXT/REFERENCE BOOKS**

1. Vogel, Arthur I: A Test book of Quantitative Inorganic Analysis (Rev. by G.H. Jeffery and others) 5th Ed. The English Language Book Society of Longman.
2. Willard, Hobert H. et al.: Instrumental Methods of Analysis, 7th Ed. Wardsworth Publishing Company, Belmont, California, USA, 1988.
3. Christian, Gary D; Analytical Chemistry, 6th Ed. John Wiley & Sons, New York, 2004.
4. Harris, Daniel C: Exploring Chemical Analysis, Ed. New York, W.H. Freeman, 2001.

5. Robinson, James W., Eileen Skelly Frame, and George M. Frame II. Undergraduate instrumental analysis. CRC press, 2014.
6. Srivastava. A.K. and Jain, P.C., "Instrumental Approach to Chemical Analysis", 4th Edition, S Chand and Company Ltd, New Delhi, 2012. 2.
7. Chatwal. G. R., Anand, Sham K., "Instrumental Methods of Chemical Analysis" 5th Edition, Himalaya Publishing House, 2005.

**END SEMESTER EXAMINATION QUESTION PAPER PATTERN**

**Max. Marks: 100**

**Exam Duration: 3 Hrs**

Part A/Question: 10 multiple choice questions 1 mark each

10 Marks

Part B/Question: 10 Questions of 2 marks each with internal choice

20 Marks

Part C/Question: 4 Questions of 15 marks each with internal choice

60 Marks

Part D/Question: 1 Questions of 10 marks comprising a figure of an instrument for

10 Marks

Teaching Scheme					Examination Scheme					
L	T	P	C	Hrs/Week	Theory			Practical		Total Marks
					MS	ES	IA	LW	LE/Viva	
3	0	0	3	3	25	50	25	--	--	100

**COURSE OBJECTIVES**

- To gain the factual knowledge of X-Ray analysis techniques and basic instrumentation techniques based on X-ray
- To learn the fundamental principles of various thermal techniques
- To acquire basic principles applied for magnetic resonance measurements
- To attain necessary basic knowledge of Raman analysis
- To learn the basic instrumentations of various analytical techniques comprising instruments used in surface analysis, spectroscopic analysis, and thermal analysis

**UNIT 1: X-Ray Diffraction Techniques**

Principles of Diffraction- Origin of X-Ray Spectra, Energy Levels in Atoms, Moseley's Law, X-Ray Methods, X-Ray Absorption Process, X-Ray Fluorescence Process, X-Ray Diffraction Process.

X-Ray Diffraction- Single-Crystal X-Ray Diffractometry, Crystal Structure Determination, Powder X-Ray Diffractometry, Applications of XRD, Analytical Limitations of XRD

X-Ray Photoelectron Spectroscopy- Basics principles of XPS, application of XPS 10 Hrs.

**UNIT 2 Thermal Techniques 10 Hrs.**

Thermogravimetry- TGA Instrumentation, Analytical Applications of Thermogravimetry, Derivative Thermogravimetry, Sources of Error in Thermogravimetry

Differential Thermal Analysis- DTA Instrumentation, Analytical Applications of DTA

Differential Scanning Calorimetry- Basics principles of DSC, Difference between DSC and DTA, DSC Instrumentation, Applications of DSC.

**UNIT 3 Electron Spin Resonance (ESR) technique 10 Hrs.**

Introduction, Theory, ESR Absorption Positions: The g Factor, Instrumentation, Working of an ESR Spectrometer, Sample Handling, Sensitivity of an ESR Spectrometer, Multiplet Structures in ESR Spectroscopy, Interpretation of ESR Spectra, Applications of ESR Spectroscopy

**UNIT 4 Raman Spectroscopy 10 Hrs.**

Principles of Raman Scattering, Raman Instrumentation, Applications of Raman Spectroscopy Introduction, Raman Effect and Origin of Raman Spectroscopy, Theories of Raman Effect and Raman Spectroscopy, Zero-Point Energy, Vibrational Raman Spectra, Pure Rotational Raman Spectra, Types of Molecules and Rotational Raman Spectra, Vibrational-Rotational Raman Spectra, Polarization of Raman Lines, Rule of Mutual Exclusion, Instrumentation, Sample Handling, Applications of Raman Spectroscopy

**Max. 40 Hrs.****COURSE OUTCOMES**

On completion of the course, student will be able to

CO1 - Understand the basic principal of surface analysis and will be able to explain the working mechanism of XPS.

CO2 - Learn the theoretical aspects of X-ray and can differentiate various X-ray instrumentation techniques for material characterization.

CO3 - Acquire the knowledge of advance instrumentation techniques based on various thermal techniques. CO4 - Describe the technique to analyse ESR spectrum various molecules

CO5 - Explain the working principal of Raman.

CO6 - Learn various type of surface analysis and molecular analysis techniques and will acquire the basic knowledge of the instrumentation involved in these techniques.

**TEXT/REFERENCE BOOKS**

1. Vogel, Arthur I: A Test book of Quantitative Inorganic Analysis (Rev. by G.H. Jeffery and others) 5th Ed. The English Language Book Society of Longman.
2. Willard, Hobert H. et al.: Instrumental Methods of Analysis, 7th Ed. Wardsworth Publishing Company, Belmont, California, USA, 1988.
3. Christian, Gary D; Analytical Chemistry, 6th Ed. John Wiley & Sons, New York, 2004.
4. Harris, Daniel C: Exploring Chemical Analysis, Ed. New York, W.H. Freeman, 2001.
5. Robinson, James W., Eileen Skelly Frame, and George M. Frame II. Undergraduate instrumental analysis. CRCpress, 2014.
6. Srivastava. A.K. and Jain, P.C, "Instrumental Approach to Chemical Analysis", 4th Edition, S Chand and Company Ltd, New Delhi, 2012. 2.
7. Chatwal. G. R., Anand, Sham K., "Instrumental Methods of Chemical Analysis" 5th Edition, Himalaya Publishing House, 2005.

**END SEMESTER EXAMINATION QUESTION PAPER PATTERN****Max. Marks: 100****Exam Duration: 3 Hrs**

Part A/Question: 10 multiple choice questions 1 mark each

10 Marks

Part B/Question: 10 Questions of 2 marks each with internal choice

20 Marks

Part C/Question: 4 Questions of 15 marks each with internal choice

60 Marks

Part D/Question: 1 Questions of 10 marks comprising a figure of an instrument for labelling and identifying its various parts

10 Marks

Pandit Deendayal Ji University					Electroanalytical and Radio Analytical Methods of Analysis					
Teaching Scheme					Examination Scheme					
L	T	P	C	Hrs/Week	Theory			Practical		Total Marks
					MS	ES	IA	LW	LE/Viva	
3	0	0	3	3	25	50	25	--	--	100

#### COURSE OBJECTIVES

- To understand the role of electrochemistry in use of electroanalytical techniques.
- To understand the importance of radioanalysis.
- To gain knowledge about the principles of potentiometry, amperometry and coulometry.
- To attain basic knowledge of voltammetry, polarography and electrochemical impedance spectroscopy.
- To learn the basic principles and techniques for radioactive/radiolabelled chemical's analysis.

#### Unit I: Introduction to Electroanalytical techniques

[8h]

Introduction to electroanalytical techniques, electrochemical cells, electrode potentials, ion-selective electrodes and sensors; Faradaic and Non-Faradaic Processes: charging currents, double layer theory -structure of double layer, point of zero charge, polarized and non-polarized electrodes; Rates of Electrode Reactions: overpotentials and cell resistances, mass transport control (Nernst-Planck Equation), Current-voltage relationship; Evaluation and Calculation; Application to Inorganic and Organic Trace analysis

#### Unit II: Electroanalytical techniques I

[12h]

Potentiometry: Thermodynamics and Cell EMF Values; measuring cell potential; half-cells, and Nernst equation; reference electrodes; potential determining processes at phase boundaries; two immiscible phases; potentials at electrolyte- electrolyte boundaries-conductance and transference & Henderson equation for liquid junction potentials.

Amperometry: Principle, typical applications, amperometric titrations, chronoamperometry and chrono-potentiometry. Coulometry: Operating cell at fixed applied potential, Electrolysis at constant working electrode potential, Coulometric methods of analysis, Faraday's laws of electrolysis, coulometric titrations, controlled potential coulometry, (Amperostatic coulometry)-Apparatus and applications, advantages and limitations.

#### Unit III: Electroanalytical techniques II

[10h]

Controlled potential techniques, Ilkovic Equation, dc polarography, ac polarography, differential pulse polarography, square wave voltammetry, stripping voltammetry, linear sweep voltammetry, cyclic voltammetry, hydrodynamic (rotating disk) voltammetry, Applications of polarography and voltammetry for chemical analysis, electrochemical impedance spectroscopy-principle and applications.

#### Unit IV: Radioanalytical Methods of Analysis

[10h]

Activation analysis: Neutron activation analysis, principle, technique, steps involved in neutron activation analysis. Radiochemical and instrumental methods of analysis, important applications of NAA; Isotope dilution analysis: Principle, types of isotope dilution analysis, typical applications of isotope dilution analysis; Radiometric titration: Principle, techniques based on complex formation and precipitation, radiometric titration curves for estimation of ions from their mixture.

Total 40 h

#### COURSE OUTCOMES

On completion of the course, student will be able to

CO1 – Learn the foundation principles applied to electroanalytical analysis and radioanalysis.

CO2 – Understand the fundamentals of potentiometry, amperometry and potentiometry.

CO3 – Apply the fundamental knowledge of electrochemistry and electroanalytical technique to select the appropriate characterization method.

CO4 – Analyze the fundamentals and applicability of voltammetry, polarography and EIS for different redox systems. CO5 – Evaluate the use of various types of radioanalytical techniques.

CO6 – Formulate schemes for chemical sample analysis using radioanalytical and electrochemical techniques.

#### TEXT/REFERENCE BOOKS

- Introduction to instrumental analysis by R. D. Broun, Mc Graw Hill (1987).
- Instrumental methods of chemical analysis by H. Willard, L. Merritt, J.A. Dean and F.A. Settle. Sixth edition CBS (1986).
- Fundamentals of analytical chemistry by D. A. Skoog, D. M. West and H. J. Holler sixth edition (1992) and Principles of Instrumental Analysis Skoog, West, Niemann.
- Cyclic Voltammetry and frontiers of electrochemistry by N. Noel and K.I. Vasu IBH, New Delhi (1990).
- Principle of Activation Analysis- P. Kruger, John Wiley and sons.
- Nuclear Analytical Chemistry – J. Tolgyessy and S. Verga vol. 2, university Park press.
- Radiochemistry and Nuclear Chemistry- Gregory Choppin, Jan-Olov Liljenzin, Jan Rydberg, Christian Ekberg, Fourth Edition • 2013, Elsevier Inc.
- Radiochemistry and Nuclear methods – W.D. Ehmann and D.E. Vance, John Wiley and Sons.
- Nuclear and Radiochemistry: Fundamentals and Applications, Third, Revised Edition, Editor(s): Jens-Volker Kratz, Karl Heinrich Lieser, First published: 30 August 2013.

#### END-SEMESTER EXAMINATION QUESTION PAPER PATTERN

Max. Marks: 100

Exam Duration: 3 Hrs

Part A/Question: 10 multiple choice questions 1 mark each

10 Marks

Part B/Question: 10 Questions of 2 marks each with internal choice

20 Marks

Part C/Question: 4 Questions of 15 marks each with internal choice

60 Marks

Part D/Question: 1 Question of 10 marks comprising a figure of an instrument for labelling and identifying its various parts

10 Marks



Pandit Deendayal Upadhyay University					Method Development and Validation School of Energy Technology					
Teaching Scheme					Examination Scheme					
L	T	P	C	Hrs/Week	Theory			Practical		Total Marks
					MS	ES	IA	LW	LE/Viva	
3	0	0	3	3	25	50	25	--	--	100

### COURSE OBJECTIVES

- To gain the fundamental knowledge of advance data analysis, correlation, and regression analysis
- To learn the basic principles for regulatory requirements for analytical method validation
- To understand and acquire the necessary basic knowledge of qualification of instruments; installation, operation, and performance qualification of analytical equipment.
- To attain detailed insight into accuracy and precision role in method validation
- To learn the basic calibration of instrument including the Limit of Detection (LOD) and Limit of Quantification (LOQ).

#### UNIT 1 Data Analysis

10Hrs.

Sampling (Statistics of Sampling), Standardization and Calibration: Analytical samples and methods; Sampling; Automated Sample Handling; Standardization and Calibration; Correlation and Regression Analysis, Linear Regression; Detection Limits; How to efficiently use MS Excel and Origin in data analysis (Slope, Intercept, and Coefficient of Determination) Calibration of analytical balance and pH meter; role of quantification limit and specificity; Limit of Detection (LOD) and Limit of Quantification (LOQ); Robustness and method validation; Ruggedness of chromatographic method; Ruggedness of sample preparation procedure; Calibration versus Qualification versus Validation

#### UNIT 2 Method Development and Validation-I: Spectroscopic and Thermal Techniques

12 Hrs.

Qualification: Overview of qualification of instruments; installation, operation, and performance qualification of analytical equipment; method validation for UV-Visible Spectrophotometer, IR Spectrophotometer, Spectrofluorometer, TGA, DSC, DTA, qualitative and quantitative method validation; parameters of validation; statistics in validation; detailed discussion on accuracy and precision role in method validation; protocols and interpretation.

#### UNIT 3 Method Development and Validation-II: Chromatographic

12 Hrs.

Qualification: Overview of qualification of instruments; installation, operation, and performance qualification of analytical equipment; method validation for HPTLC, GC, HPLC; qualitative and quantitative method validation; parameters of validation; statistics in validation; detailed discussion on accuracy and precision role in method validation; protocols and interpretation.

#### UNIT 4 Method Development and Validation-III Electroanalytical techniques

10 Hrs.

Qualification: Overview of qualification of instruments; installation, operation and performance qualification of analytical equipment; method validation for electroanalytical techniques like voltametric techniques (cyclic voltammetry, liner sweep voltammetry), pulse techniques (SWV and DPV), frequency response analysis (FRA); qualitative and quantitative method validation; parameters of validation; statistics in validation; detailed discussion on accuracy and precision role in method validation; protocols and interpretation.

### COURSE OUTCOMES

On completion of the course, student will be able to

- CO1 - understand the basic principles of advance data analysis including various statistical tests.  
 CO2 - acquire the fundamental knowledge of correlation and regression analysis including linear regression.  
 CO3 - learn various type of principles for regulatory requirements for analytical method validation.  
 CO4 - learn methods necessary to interpret the qualification of instruments; installation, operation, and performance qualification of analytical equipment.  
 CO5 - explain the accuracy and precision role in method validation.  
 CO6- explain the basic calibration of instrument including the Limit of Detection (LOD) and Limit of Quantification (LOQ).

### TEXT/REFERENCE BOOKS

- Valid Analytical Methods and Procedures, Chris Burgess & J J Wilson, 2001
- Analytical Method Validation and Instrument Performance Verification, Chung Chow Chan, Herman Lam, Y.C. Lee, Xue-Ming Zhang, 2004
- Modern Analytical Chemistry, David Harvey, McGraw Hill, 2000.
- Quality Assurance and Quality Control in the Analytical Chemical Laboratory: A Practical Approach, Charles H. Lochmüller, Duke University, 2009
- G. H. Geffery et al, Vogel's Text Book of Quantitative Chemical Analysis, ELBS Edn, 1989
- D. A. Skoog, D.M. West, F.J Holler, S.R Crouch, Fundamentals of Analytical Chemistry, 8th edition, Thomson Brooks Cole, 2004
- F. Rouessac and A. Rouessac, Chemical Analysis: Modern Instrumentation
- Methods and Techniques, 2nd edn, John Wiely and Sons
- D. A. Skoog, E. J. Holler, S. R. Crouch, Principles of Instrumental Analysis, 6th edition,

### END SEMESTER EXAMINATION QUESTION PAPER PATTERN

Max. Marks: 100

Exam Duration: 3 Hrs

Part A/Question: 10 multiple choice questions 1 mark each	10 Marks
Part B/Question: 10 Questions of 2 marks each with internal choice	20 Marks
Part C/Question: 4 Questions of 15 marks each with internal choice	60 Marks
Part D/Question: 1 Questions of 10 marks with internal choice	10 Marks

Pandit Deendayal Upadhyay University					Analytical Chemistry III School of Energy Technology					
Teaching Scheme					Examination Scheme					
L	T	P	C	Hrs/Week	Theory			Practical		Total Marks
					MS	ES	IA	LW	LE/Viva	
0	0	3	1.5	3				50	50	100

#### COURSE OBJECTIVES

- To learn the basic experimental techniques like chromatography, titrimetric, spectrophotometric methods
- To gain experimental knowledge to separate ions by paper chromatographic method
- To estimate organic content in food products
- To perform quantitative analysis of elements/ions by voltammetry, amperometry
- To perform quantitative analysis by conductometric method

1. Determining the Concentration of Citric Acid in Commercially Available Cold Drink Using Titration
2. Analysis of COD and DO in Waste Water Sample
3. Paper Chromatographic technique for separation of metal ions
4. Titration for Quantitative estimation of metal ions/complexes using conductometry
5. Spectrophotometric Analysis of a Mixture: Caffeine and Benzoic Acid in a Soft Drink
6. Determination of the Solubility Product Constant of AgCl
7. Amperometric titration of Pb(II) with potassium dichromate solution
8. Determination of Cu, Pb and Cd in Water Sample by Differential Pulse Anodic Stripping Voltammetry (DPASV)
9. Determination of Diffusion current of  $K_3Fe(CN)_6$  by Cyclic voltammetry
10. Determination of active ingredients using a tablet disintegrator
11. Separation of complex organic mixture (eg. BTX) using GC
12. Separation of amino acids by using HPLC

#### COURSE OUTCOMES

On completion of the course, student will be able to

**CO1** – Learn the basic experimental techniques like chromatography, titrimetric, spectrophotometric methods

**CO2** – Gain experimental knowledge to separate ions by paper chromatographic method

**CO3** – Estimate organic content in food products by titrimetric method

**CO4** – Perform quantitative analysis of commercial products by spectrophotometric method

**CO5** – Perform quantitative estimation by conductometric method

**CO6** – Develop the skills for electrochemical analysis for quantitative estimation (voltammetry, amperometry)

#### TEXT/REFERENCE BOOKS

1. Analytical Chemistry Practice, John H. Kennedy, Saunders College Publishing, Second Edition 1990.
2. Vogels Textbook of Quantitative Chemical Analysis, 6th Edition, 2002.
3. Comprehensive Experimental Chemistry; V. K. Ahluwalia, New Age Publications, 1997
4. Analytical Chemistry: Theory and Practice; R. M. Varma, CBS Publishers, 1994
5. A. K. Nad, B. Mahapatra & A. Ghosal, An Advanced Course in Practical Chemistry, New Central, 2007. Vogel's Text Book of Practical Organic Chemistry (5th Edn).

#### END SEMESTER EXAMINATION QUESTION PAPER PATTERN

##### Max. Marks: 100

Laboratory work including maintaining journal book+ mid-sem viva (LW)

End-sem exam and viva (LE/Viva)

##### Exam Duration: 3 Hrs

50 Marks

50 Marks

Pandit Deendayal Energy University Teaching Scheme					Intellectual Property Rights School of Energy Technology Examination Scheme					
L	T	P	C	Hrs/Week	Theory			Practical		Total Marks
					MS	ES	IA	LW	LE/Viva	
2	0	0	2	2	25	50	25	--	--	100

#### COURSE OBJECTIVES (04)

- To familiarize the students with concepts of thermodynamics and thermodynamic properties of macroscopic systems
- To understand the theories of reaction kinetics and factors affecting reaction kinetics
- To understand the basic principles of electrochemistry, inter-phase and their applications,
- To understand the concepts of, surface chemistry and various surface phenomenon and their applications

#### Unit 1

8 h

Introduction to Intellectual Property Rights: Patents & publications. Understanding Intellectual Property Rights (IPRs), Protecting IPRs: Patents, Copyrights, Trademarks, Industrial designs, Protection of IC Layout design, Geographical Indication, Protection of undisclosed information (Trade secrets), History of Intellectual Property (IP) system, development of IP laws in India, evolution of IPR regime. Overview of IPR Regime. International conventions and treaties on IPR and Patents: Paris convention, drawback of the Paris convention and Patent cooperation treaty (PCT).

#### Unit 2

7 h

Procedure in PCT filing and advantages of PCT. WTO/GATT system and the Uruguay round, Organization of WTO and its agreements, Pillars of GATT. Emergence of TRIPS and enforcement procedure under TRIPS. Compulsory licensing of a patent and Doha declaration. Hatch Waxman Act, antitrust concerns and the case for generic drug manufacturers. WIPO and promotion of creative and innovative activity. Important case studies related to IPRs.

#### Unit 3

6 h

Patents Law, Patent drafting and filing: Introduction to Patents, Patentability of an invention. Importance of Patent Policy, Patent Legislation in India, Patent Act-1970 and subsequent amendments to Patents Act (1999, 2002 and 2005). Specifications, types of specifications and contents of specifications.

#### Unit 4

9 h

Claims and types of claims. Drafting claims of an invention and description of invention. Procedure for filing a Patent Application. Opposition of grant of a Patent. Patent infringement and abuse of patent. Patent Licensing and its significance. Important case studies related to patents. Hands-on in drafting patent application.

Max. 30 h

#### COURSE OUTCOMES (06)

On completion of the course, student will be able to

- CO1 - Apply the concepts of thermodynamic to understand the thermodynamic properties of macroscopic systems
- CO2 – Interpret reaction rates and propose reaction mechanism with the help of concepts of chemical kinetics
- CO3- Articulate the factors determining reaction rates and concept of catalysis chemical reaction
- CO4- Acquire knowledge about theories of surface chemistry and their applications.
- CO5- Understand the fundamental concept about surface phenomenon and catalysis.
- CO6- Analyse and apply the principles of electrochemistry in real world problems.

#### TEXT/REFERENCE BOOKS

1. International intellectual property and the common law world Ed. by Charles E F Rickett and W Austin Graeme: Hart Publishing, 2000.
2. Intellectual property in the new technological age, Robert P Merges, Peter S Menell and Mark A Lemley, 2nd Edition, Aspen Law and Business, 2000.
3. Gearing up for patents: The Indian Scenario, Prabudhha Ganguli, Universities Press (India) Ltd. 1998.
4. Intellectual Property Rights under WTO: Tasks before India, T. Ramappa, Wheeler Publishing, 2000.
5. Patent Office Manual, Department of Industrial Policy and Policy Protection, Government of India, New Delhi.