

**H.H. THE RAJAH'S COLLEGE (AUTONOMOUS)**

**PUDUKKOTTAI-622 001**

**PG & RESEARCH DEPARTMENT OF CHEMISTRY**

**M.Sc., CHEMISTRY**

**COURSE STRUCTURE UNDER CBCS**

**FOR THE STUDENTS ADMITTED FROM THE ACADEMIC YEAR**

**2018 – 2019 ONWARDS**



**M.Sc., CHEMISTRY - SYLLABUS**

<b>PROGRAM SPECIFIC OUTCOMES for M. Sc. Chemistry program</b>	
After Successful completion of the Degree, students can	
<b>PSO1</b>	Get solid foundation in different fields of chemistry which are required to solve chemical, technical and environmental problems.
<b>PSO2</b>	Develop the skills to select, design and apply appropriate techniques, resources and tools to complex research activities with an understanding of the limitations.
<b>PSO3</b>	Comprehend and write effective reports and documentation, make effective presentations.
<b>PSO4</b>	Communicate effectively on complex activities with the scientific community and with society.
<b>PSO5</b>	preparation and ability to engage in independent and life-long learning in the context of scientific and technological change.

<b>PROGRAM OUTCOMES for M. Sc. Chemistry program</b>	
After Successful completion of the Degree	
<b>PO1</b>	Students acquire the advanced knowledge in different branches of chemistry and understand all the theories, essential facts, core concepts, principles and postulates relating to the chemistry.
<b>PO2</b>	Students can identify, formulate, analyse and solve complex problems using the basic principles of chemistry.
<b>PO3</b>	Students understand the role of chemistry in day to day life
<b>PO4</b>	Students can apply the knowledge and ability to synthesize, separate and characterize compounds using laboratory and instrumentation techniques.
<b>PO5</b>	Equipping students to develop analytical and problem skills to articulate the scientific and technical information to enter into industries, higher research program and the job market.
<b>PO6</b>	Creating awareness of the impact of chemistry on the environment, society and to contribute present and future perspectives of scientific community
<b>PO7</b>	Acquire the knowledge towards the role of chemistry in industries and to create passion to become entrepreneur.

**H. H. THE RAJAH'S COLLEGE (Autonomous B<sup>+</sup>), PUDUKKOTTAI**  
**PG & RESEARCH DEPARTMENT OF CHEMISTRY**  
**CBCS – COURSESTRUCTURE**  
**FOR M.Sc. CHEMISTRY (2018-2019 Onwards)**

COURSES	NO. OF PAPERS	CREDIT
<b>CORE COURSES</b>	14	70
<b>ELECTIVE COURSES</b>	3	15
<b>EDC</b>	1	05
<b>TOTAL</b>	18	90

**CBCS – COURSES PATTERN**  
**FOR M.Sc. CHEMISTRY (2018-2019 Onwards)**

PART	CODE	COURSE	TITLE	HRS	MARKS		TOTAL	CREDIT
					Int.	Ext.		
<b>I SEMESTER</b>								
III	18PCH1	CC-I	Organic Chemistry-I	6	25	75	100	5
III	18PCH2	CC-II	Inorganic Chemistry-I	6	25	75	100	5
III	18PCH3P	CP-III	Inorganic Practical-I*	6				
III	18PCH4P	CP-IV	Organic Practical-I*	6				
III	18PCHE1	EC-I	Photochemistry and Pericyclic Reaction(OR) Special topics in Organic synthesis	6	25	75	100	5
			Total	30			300	15
<b>II SEMESTER</b>								
III	18PCH5	CC-V	Physical Chemistry-I	6	25	75	100	5
III	18PCH6	CC-VI	Inorganic chemistry-II	6	25	75	100	5
III	18PCH3P	CP-III	Inorganic Practical-I	6	40	60	100	5
III	18PCH4P	CP-IV	Organic Practical-I	6	40	60	100	5
III	18PCHE2	EC-II	Nanomaterials and Green Chemistry(OR) Medicinal and Pharma- ceutical Chemistry	3	25	75	100	5
III	18PCHEDI	EDC-I	Supramolecular Chemistry	3	25	75	100	5
			Total	30			600	30

PART	CODE	COURSE	TITLE	HRS	MARKS		TOTAL	CREDIT
					Int.	Ext.		
<b>III SEMESTER</b>								
III	18PCH7	CC-VII	Organic Chemistry-II	6	25	75	100	5
III	18PCH8	CC-VIII	Physical Chemistry-II	6	25	75	100	5
III	18PCH9	CC-IX	Inorganic Chemistry-III	6	25	75	100	5
III	18PCH13P	CP-XIII	Physical chemistry practical-I*	6				
III	18PCHE3	EC-III	Physical methods in chemistry(OR)Corrosion Science	6	25	75	100	5
			Total	30			400	20
<b>IV SEMESTER</b>								
III	18PCH10	CC-X	Organic chemistry-III	6	25	75	100	5
III	18PCH11	CC-XI	Physical chemistry-III	6	25	75	100	5
III	18PCH12	CC-XII	Organic Spectroscopy	6	25	75	100	5
III	18PCH13P	CP-XIII	Physical chemistry practical-I	6	40	60	100	5
III	18PCH14	PW-I	Project work	6			100	5
			Total	30			500	25

**Finalized (for the I to IV Semester) in the**  
**BOARD OF STUDIES MEETING HELD ON 28-06-2018**  
**&**  
**APPROVED BY THE ACADEMIC COUNCIL ON 06-10-2018**

# **SEMESTER – I**

**CC-I – ORGANIC CHEMISTRY-I****Course objectives:**

1. *To understand the Nomenclature, Reaction intermediates and Electronic effect*
2. *To know the determination of reaction mechanism*
3. *To learn the aromaticity and chemistry of heterocyclic compounds*
4. *To learn stereochemistry of organic compounds*
5. *To study the optical isomerism, Conformation of Acyclic compounds and Dynamic stereochemistry*

**UNIT – I****Nomenclature and reaction intermediates**

Nomenclature - Naming of linear and branched alkanes, alkenes, polyenes and alkynes with and without functional groups by IUPAC nomenclature- aromatic and hetero aromatic systems- nomenclature of heterocycles having not more than two hetero atoms such as oxygen, nitrogen and sulphur- nomenclature of alicyclic, bicyclic and tricyclic compounds.

Reactive intermediates: free radicals-carbenes, nitrenes, -carbanions- carbonations and arynes- generation, stability, structure and reactivity-nonclassical carbocations.

Electronic effects: inductive effect, resonance effect, hyperconjugation (Baker-Nathan effect)-hydrogen bonding (inter and intra molecular).

**UNIT – II****Determination of Reaction mechanisms**

Thermodynamic and kinetic aspects of organic reactions, energy profile diagrams – intermediate versus transition states, isotopic effects – kinetic and non kinetic methods of determining reaction mechanism, product analysis and its importance. Cross over experiments – isotopic labeling studies – stereo chemical studies – substituent effects.

Correlation analysis: linear free energy relationship – Hammett equation – significance of sigma and rho-applications. Taft, Swain-Scott, Grunwald – Winstein equations and their applications, classification of solvents.

**UNIT – III****Aromaticity and Heterocyclic compounds:**

**Aromaticity:** Huckel's theory of Aromaticity, concept of homoaromaticity and antiaromaticity Aromatic character in five, six, seven and eight membered rings – other



systems with aromatic sextets – Huckel’s rule – Craig’s rule – NMR concept of aromaticity and antiaromaticity – systems with 2,4,8 and 10 electrons – systems with more than 10 electron (annulenes) , Mobius Aromaticity– Alternant and non-alternant hydrocarbons. Chemistry of cyclopentadienyl anion – Fullerenes, Azulene, Tropolones, Sydnones and Annulenes. Bonding properties of system with  $(4n+2)$  and  $4n \pi$  electrons.

**Heterocyclic Compounds:** Structure - synthesis and reactions of the following systems – indole, isoindole, quinoline, isoquinoline, oxazoles, carbazole, imidzole, thiozole, chromones, pyridines, pyrimidines, pyridazine, pyrazoles and pyrazines.

## UNIT – IV

### Stereo chemistry – I

Optical isomerism: principles of symmetry- concept of chirality- optical purity - elements of symmetry and chirality- Newmann, Sawhorse, Fisher and flying wedge notations- representation and inter-conversions.-types of molecules exhibiting optical activity- configurational nomenclature- D and L, & R-S nomenclature- of acyclic and cyclic chiral compounds- stereo chemistry of allenes and spirenes- biphenyls (atropisomerism)- stereochemistry of ansa compounds- cyclophanes and trans cyclo alkenes- definition of terms like prochirality, enantiotopic and diastereotopic groups / faces- asymmetric synthesis-Cram’s rule.

## UNIT – V

### Stereochemistry II

Geometrical isomerism: E and Z nomenclature- determination of configuration of the geometrical isomers. Configuration of cyclic and bicyclic ring systems: Cis and trans nomenclature of three, four, five six membered substituted cyclic systems-configuration of cyclohexane- mono and di substituted cyclohexanes- decalins.

Dynamic stereo chemistry :Quantitative correlation between conformation and reactivity- Winstein, Eliel equation- Curtin-Hammet principle- conformation, reactivity and mechanism of cyclic systems- saponification of an ester, esterification of an alcohol, chromic acid oxidation of cyclohexanols- neighboring group participation, deamination of 2-amino cyclohexanol- stereo specific and stereoselective reactions.

### Course outcome:

*Student understood the knowledge about:*

- 1. The Nomenclature, Reaction intermediates and Electronic effect*
- 2. The determination of reaction mechanism*

3. *The Hammett, Taft, Swain-Scott equations*
4. *The aromaticity and chemistry of heterocyclic compounds*
5. *The stereochemistry of organic compounds*
6. *The stereochemistry of optical isomerism, conformation of acyclic compounds and Dynamic stereochemistry*
7. *The stereo-specific and stereo-selective reactions*
8. *The configuration of cyclic and bicyclic system*

## References

### Unit-I

1. Fundamentals of Organic Reaction Mechanisms- J.M.Harris and C.C. Wamser, John Wiley & Sons, Inc. 1976.
2. R Panico, W H Powell, L Jean and C Ridcher, Agenda of nomenclature of organic compounds, 1993.
3. R S Cahn and O L Dermer, Introduction to chemical nomenclature, 5<sup>th</sup> Edition, Butterworth, 1979.

### Unit-II

4. P J Carratt, Aromaticity, McGraw Hill, 1971
5. Advanced Organic Chemistry, Part A & B, F.A.Carey and Sundberg, III Edn. Plenum Press, 1990.
6. Organic Chemistry, S.H.Pine, J.B. Hendrickson, D.J.Cram and G.S.Hammond, IV Edn. McGraw-Hill Company 1980.
7. Jerry March, Advanced Organic Chemistry, 4<sup>th</sup> Edition, Wesley, 1999.

### Unit-III

8. Mechanism and Theory in Organic Chemistry – T.H. Lowry and K.S. Richardson, Harper and Row, NY 1976.
9. Organic Reactions and Mechanisms, P.S.Kalsi, II Edn. New Age International Publishers, 2000.

### Unit-IV & V

10. D.Nasipuri, Stereochemistry of organic compounds.
11. I L Finar, Organic Chemistry, Vol.I and II.
12. P S Kalsi, Stereochemistry conformation and mechanism.

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## Course Outcome Vs Programme Outcome

	PO1	PO2	PO3	PO4	PO5	PO6	PO7
CO1	9	6	6	3	9	6	6
CO2	9	6	6	6	9	6	6
CO3	9	6	6	6	9	6	6
CO4	9	9	6	9	9	6	6
CO5	9	6	6	6	6	6	6

Level of correlation: 9 – High; 6 – Medium; 3 – Low; and 0- no correlation.

**CC-II – INORGANIC CHEMISTRY – I****Course objectives:**

1. To learn the concept of Acids and bases
2. To know the crystal structures and radius ratio
3. To study about the Nuclear chemistry
4. To learn the detail artificial radioactivity
5. To know the organometallics and various catalysts

**UNIT – I****Acids and Bases**

Bronsted and Lewis acids and bases, pH, pKa, acid-base concept in non-aqueous media, buffer solution, Protonic acids – Proton Affinities – Differentiating and leveling solvents – acidic Behavior of the Binary hydrides – strength of oxyacids – Hydrolysis – Amphoteric oxides – Non protonic Concepts of Acid – Base reactions – Lux concept – Solvent Ion theory of Acids and Bases – Liquid Ammonia, Acetic acid, Bromine trifluoride, Dinitrogen, Soft-Acid-Base strength and Hardness and softness – Symbioses – Theoretical bases of Hardness and Softness – electro negativity and Hardness and softness.

**UNIT – II****Solid state**

Ionic Bond, Crystal Structure and Advanced Covalent Bonding : Radius ratio rules – calculation of some limiting Radius ratio Values for C.N.3 (Planner triangle), C.N.4 (Tetrahedral) C.N.6 (Octahedral).

**Classification of Ionic Structure**

AX, AX<sub>2</sub>, AX<sub>3</sub> types. AX type (ZnS, NaCl, CaCl<sub>2</sub>) Structures only. AX<sub>2</sub> type, fluorite, rutile, betacrystobalite (structure only). layer Structure – CdI<sub>2</sub>, Nickel arsenide Structures – Lattice energy, Born Lande equation derivation – important points arising from Born Lande equation – Schohttky defect and Frenkel defect — Metal excess defect – F centres and interstitial ions – extra interstitial negative ions – Band theory of solids – insulators, semiconductors and super conductors. Walsh Diagram.

**UNIT – III****Nuclear Chemistry**

Nuclear properties-Nuclear spin and moments, origin of nuclear forces, features of the liquid drop and the shell models of the nucleus; Modes of radioactive decay-orbital electron capture, nuclear isomerism, internal conversion; Detection and determination of activity – Cloud chamber, nuclear emulsion, Bubble chamber, GM, Scintillation and Cherenkov

counters. Nuclear reactions-Types, reaction cross section, Q-value, threshold energy, compound nuclear theory, high energy nuclear reactions, nuclear fission and fusion reactions as energy sources, direct reactions, photonuclear and thermo nuclear reactions, Stellar energy, synthesis of elements.

## UNIT – IV

### Artificial Radioactivity

Nuclear reaction – transmutation – stripping and pick up, fission products and fission yields, fusion, spallation and fragmentation reactions scattering reactions – nuclear cross section – Q – value-nuclear reactors (functioning) – charged particle accelerators – neutron sources – gamma ray and X-ray sources. Radioactive techniques – tracer technique neutron activation and isotopic dilution analysis, counting techniques such as G.M. ionization and proportional counter. Applications of nuclear science in agriculture and biology. Radiation risks and medical benefits – natural and manmade isotopes.

## UNIT – V

### Organometallic Chemistry & Catalysis

Carbon donors - Alkyls and Aryls-preparation and properties; Carbonyls -18 electron rule, isolobal concept - application to structure of carbonyls (simple and polynuclear); Nitrosyls - bridging and terminal nitrosyls, bent and linear nitrosyls; dinitrogen complexes; Chain Carbon donors - Olefins, acetylene and allyl complexes - synthesis, structure and bonding; Cyclic Carbon donors - Metallocene - synthesis, structure and bonding (Ferrocene only).

Hydrogenation of olefins (Wilkinson's catalyst); hydroformylation of olefins using Cobalt or Rhodium catalysts (oxo process); Oxidation of olefins to aldehydes and ketones (Wacker process); polymerization (Ziegler-Natta catalyst); Cyclooligomerization of acetylene using Nickel catalyst (Reppé's catalyst); polymer bound catalysts.

### Course outcome:

*Student understood the knowledge about:*

1. *The uses of pH scale*
2. *The structures drawing of the complexes*
3. *The awareness of power plants*
4. *The atomic energy resources*
5. *The preparation of man made isotopes*
6. *The applications of nuclear science in agriculture and biology*

7. *The carbon donors and carbonyls*
8. *The hydrogenation, hydroformylation and oxidation process*

## References

### Unit-I

1. W.Kain and B.Schwederski, *Bioinorganic Chemistry, Inorganic Elements in the Chemistry of Life*, John Wiley & Sons, New York.
2. James E.Huheey, Ellen A.Keiter and Richard L.Keiter, *Inorganic Chemistry : Principles of structure and Reactivity*, 4<sup>th</sup>edn, Wesley, New York.
3. Shriver and Atkins, *Inorganic Chemistry*, III edn, Oxford, 1999.

### Unit-II

4. Badie E. Douglas, 'Concepts and models in Inorganic Chemistry', Indian Edition, 1970, Oxford and IBH publishing Co., New Delhi.
5. J.D.Lee, *A New concise Inorganic Chemistry*, 4<sup>th</sup> Edition, ELBS, 1995.

### Unit-III & IV

6. G.Friedlander, J.W.Kennedy and J.M.Miller, *Nuclear and Radiochemistry*.
7. Keith F.Purchell and John. C.Kotz, *Inorganic Chemistry*, Saunders Golden Sunburst Series, W.B.Saunders Company, Philadelphia.

### Unit-V

8. Cotton and Wilkinsin, *Advanced Inorganic Chemistry*, 5<sup>th</sup> Edition, John Wiley & Sons, New York.

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### Course Outcome Vs Programme Outcome

	PO1	PO2	PO3	PO4	PO5	PO6	PO7
CO1	9	9	6	6	9	6	6
CO2	9	6	6	6	9	6	6
CO3	6	6	6	6	6	9	6
CO4	6	6	6	6	6	6	6
CO5	6	9	6	6	6	6	6

**Level of correlation: 9 – High; 6 – Medium; 3 – Low; and 0- no correlation.**

## CHOICE-I

SUBJECT CODE: 18PCHE1

6 Hrs / 5 Credits

### EC1 –PHOTOCHEMISTRY AND PERICYCLIC REACTION

#### Course objectives:

1. To study the photo-physical processes and experimental techniques in photochemistry
2. To learn the various types of photochemical reactions
3. To know the photochemistry of alkenes and carbonyl compounds
4. To study the molecular orbital symmetry, molecular orbital approaches
5. To learn the cyclo-addition and various photochemical rearrangements

#### UNIT – I

##### Photophysical processes

Photo physical processes in electronically excited molecules – Radiation less transitions –Jablonski diagram -- Internal conversion and intersystem crossing. Fluorescence emission – Fluorescence and structure. Triplet states and phosphorescence emission – Photo physical kinetics unimolecular processes – Stern-Volmer equation. Photochemical techniques- Experimental techniques in photo chemistry –Chemical actinometry–Ferrioxalate, uranyl oxalate, photochromic , Reinecke's salt actinometers – Lasers and their applications.

#### UNIT – II

##### Photochemical reactions

Photo reduction and related reactions Norrish type I and type II reactions Photo oxidation and Photo oxygenation Nature and importance of singlet oxygen quenching on Fluorescence by oxygen. Cyclo addition reactions Photo dimerisation, oxetane formation – Woodward – Hoffman rules, Chemiluminescence.

#### UNIT – III

##### Organic photochemistry

Photochemistry of alkenes and carbonyl compounds; Photooxygenation; Photochemistry of aromatic compounds; Photochemical isomerisation, addition and substitution; Photo-Fries rearrangement of ethers and anilides; Barton reaction, Hoffmann-Loeffler-Freytag reaction, di- $\pi$ -methane rearrangement; Singlet molecular oxygen reactions; Photo-cleavages.

#### UNIT – IV

##### Pericyclic reactions I

Molecular orbital symmetry, frontier orbitals of ethylene, 1,3 butadiene, 1,3,5-hexatriene, allyl system, classification of pericyclic reactions, FMO approach, Woodward-Hoffman correlation diagram method and perturbation of molecular (PMO) approach for the

explanation of pericyclic reactions under thermal and photochemical conditions, electrocyclic reactions: conrotatory and disrotatory motions ( $4n$ ) and ( $4n+2$ ), allyl systems and secondary effects.

## Unit-V

### Pericyclic reactions II

Cycloadditions: antarafacial and suprafacial additions, notation of cycloadditions, ( $4n$ ) and ( $4n+2$ ) systems with a greater emphasis on ( $2+2$ ) and ( $4+4$ ), cycloadditions, ( $2+2$ ), additions of ketones secondary effects of substituents on the rates of cycloadditions and chelotropic reactions, FMO approach and perturbation of molecular (PMO) approach for the explanation of sigmatropic rearrangements under thermal and photochemical conditions, suprafacial and antarafacial shifts of hydrogen, sigmatropic shift involving carbon moieties, retention and inversion of configuration, ( $3,3$ ) and ( $5,5$ ) sigmatropic rearrangements, Claisen and Cope rearrangements, fluxional tautomerism, aza-Cope rearrangements.

### Course outcome:

*Student understood the knowledge about:*

1. *The photo-physical processes and experimental techniques in photochemistry*
2. *The various types of photochemical reactions*
3. *The photochemistry of alkenes and carbonyl compounds*
4. *The molecular orbital symmetry, molecular orbital approaches*
5. *The cyclo-addition and various photochemical rearrangements*

### References

#### Unit-I, II&III

1. K K. Rohatgi Mukherjee, Fundamentals of photo chemistry. Wiley Eastern Ltd. 1988.
2. N J Turro, Molecular photochemistry, New York, W A Benjamin, 1966.
3. S. Arunachalam, Inorganic photochemistry, Kala Publications.

#### Unit-IV&V

4. J. Clayden, N. Greeves, S. Warren and P. Wothers, Organic Chemistry, 1st Ed., Oxford University Press, 2001.
5. M.B. Smith & J. March, March's Advanced Organic Chemistry, 5th Ed., John Wiley & Sons, New York, 2001.
6. F.A. Carey and R.A. Sundberg, Advanced Organic Chemistry, Part A and Part B, 5th Ed., Kluwer Academic/Plenum Publishers, New York, 2004
7. P. G. M. Wuts, Greene's Protective Groups in Organic Synthesis, 5th Ed., Wiley, 2014.

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### Course Outcome Vs Programme Outcome

	<b>PO1</b>	<b>PO2</b>	<b>PO3</b>	<b>PO4</b>	<b>PO5</b>	<b>PO6</b>	<b>PO7</b>
<b>CO1</b>	9	6	9	6	9	9	6
<b>CO2</b>	9	6	9	6	9	9	6
<b>CO3</b>	9	6	9	6	9	9	6
<b>CO4</b>	6	6	9	6	9	9	6
<b>CO5</b>	6	6	9	6	9	9	6

**Level of correlation: 9 – High; 6 – Medium; 3 – Low; and 0- no correlation.**



## CHOICE-II

### EC-I-SPECIAL TOPICS IN ORGANIC SYNTHESIS

#### Course objectives:

1. To know the asymmetric oxidation and reduction, stereo selective reactions
2. To learn about the Lewis, Enamine and Bronsted catalysis
3. To study the different types of NHC and their synthesis
4. To learn the advantages and disadvantages of biocatalysts
5. To know the different types of biocatalytic reactions and it uses

#### UNIT-I

##### Asymmetric synthesis

Asymmetric synthesis: chiral auxiliaries, methods of asymmetric induction, substrate, reagent and catalyst controlled reactions, determination of enantiomeric and diastereomeric excess, enantio-discrimination, resolution – optical and kinetic, asymmetric oxidation [epoxidation: Sharpless, Jacobsen, Shi], dihydroxylation (Sharpless)], asymmetric reduction (Noyori, Corey, Pfaltz), stereoselective aldol reactions (Cram's rule and Felkin-Anh models), auxiliary controlled stereoselection: Evans oxazolidones.

#### UNIT-II

##### Organocatalysis-I

Introduction to organocatalysis, Lewis base catalysis, iminium catalysis, enamine catalysis, Lewis acid catalysis, Bronsted acid and base catalysis, examples.

#### UNIT-III

##### Organocatalysis-II

Carbenes as organocatalysts, types of different NHCs and their synthesis, NHC catalysed umpolung, NHC catalyzed transesterification reactions, homo and cross benzoin type reactions, Stetter reaction, enolate chemistry, homoenolate derived reactions, addition to ketenes and analogs, oxidative NHC catalysis, cooperative catalysis with metal catalysts, cooperative catalysis with other organocatalysts.

#### UNIT-IV

##### Biocatalysis in organic synthesis-I

Introduction to biocatalysts, advantages and disadvantages of biocatalysts, isolated enzymes vs. whole cell systems, brief overview of structure of enzymes, mechanistic aspects of enzymecatalysis, classification and nomenclature, coenzymes, enzyme sources,

biocatalysed hydrolytic reactions, hydrolysis of amides, esters, epoxides and nitriles, biocatalytic reduction reactions, recycling of cofactors, reduction of aldehydes, ketones and C=C bonds.

## UNIT-V

### Biocatalysis in organic synthesis-II

Oxidation reactions, oxidation of alcohols and aldehydes, biocatalytic carbon-carbon bondformations, aldol reaction, Michael-type additions, thiamine-dependant benzoin condensation, cyanohydrin formation, amino transfer reactions, halogenations and dehalogenations, enzymes in organic solvents, ester synthesis, lactone synthesis, amide synthesis, peptide synthesis, artificial enzyme mimics, and catalytic antibodies.

#### Course outcome:

*Student understood the knowledge about:*

- 1. The asymmetric oxidation and reduction, stereo selective reactions*
- 2. The Lewis, Enamine and Bronsted catalysis*
- 3. The different types of NHC and their synthesis*
- 4. The hemoenolate type reactions*
- 5. The advantages and disadvantages of biocatalysts*
- 6. The mechanistic aspects of enzyme catalysis,*
- 7. The different types of biocatalytic reactions and it uses*
- 8. The amide synthesis, peptide synthesis and artificial enzyme mimics*

#### References:

1. R. Gawley and J. Aube, Principles of Asymmetric Synthesis, 2nd Ed., Elsevier, 2012.
2. K. Faber, Biotransformations in Organic Chemistry, 6th Ed., Springer, 2011.

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### Course Outcome Vs Programme Outcome

	PO1	PO2	PO3	PO4	PO5	PO6	PO7
CO1	9	6	9	6	9	9	6
CO2	9	6	9	6	9	9	6
CO3	9	6	9	6	9	9	6
CO4	6	6	9	6	9	9	6
CO5	6	6	9	6	9	9	6

**Level of correlation: 9 – High; 6 – Medium; 3 – Low; and 0- no correlation.**

**SUBJECT CODE: 18PCH3P**

**6 Hrs / 5 Credits**

## CP-III- INORGANIC CHEMISTRY PRACTICAL-I

### Course objectives:

1. *To learn the qualitative analysis by semimicro method*
2. *To know the usage of photoelectric colorimeter for quantitative estimation*
3. *To study the volumetric analysis by iodimetric titration method*
4. *To learn the gravimetric estimations by using sintered crucibles*
5. *To know about the complex preparations*

### 1. Semi micro qualitative analysis of a mixture containing two common and two Rare cations.

### 2. Colorimetric estimation of Copper, Ferric, Nickel, Chromium and Manganese using photoelectric colorimeter.

### 3. Titrimetry and Gravimetry

- (i) Cu(V), Ni(G); (ii)Cu(V), Zn(G); (iii)Fe(V), Zn(G); (iv)Fe(V), Ni(G);  
(v)Zn(G), Cu(V)

### 4. Preparation of the following complexes

1. Tetramminecopper(II) sulphate
2. Potassiumtrioxalatochromate(III)
3. Hexathiourealead(II)nitrate
4. Potassium trioxalaoaluminate(III)
5. Tristhioureacopper(II) sulphate
6. Tristhioureacopper(II) chloride

### Course outcome:

*Student understood the knowledge about:*

1. *The qualitative analysis by semimicro method*
2. *The usage of photoelectric colorimeter for quantitative estimation*
3. *The volumetric analysis by iodimetric titration method*
4. *The gravimetric estimations by using sintered crucibles*
5. *The complex preparations*

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### Course Outcome Vs Programme Outcome

	<b>PO1</b>	<b>PO2</b>	<b>PO3</b>	<b>PO4</b>	<b>PO5</b>	<b>PO6</b>	<b>PO7</b>
<b>CO1</b>	6	6	9	9	9	9	9
<b>CO2</b>	6	6	9	9	9	9	9
<b>CO3</b>	6	6	9	9	9	9	9
<b>CO4</b>	6	6	9	9	9	9	9
<b>CO5</b>	6	6	9	9	9	9	9

**Level of correlation: 9 – High; 6 – Medium; 3 – Low; and 0- no correlation.**

**CP-IV – ORGANIC CHEMISTRY PRACTICAL-II****Course objectives:**

1. To study the separation of organic compounds and qualitative analysis
2. To know the synthesis of organic compounds by single stage
3. To learn the estimation of organic compounds by quantitative analysis
4. To study the synthesis of organic compounds by two stage

**1. Qualitative analysis of organic mixture**

Pilot separation, bulk separation, Analysis, Derivative, determination of m.p/ b.p of the derivative.

**2. Preparation of organic compounds (single stage)**

1. methyl-m-nitrobenzene from methylbenzoate (nitration)
2. Glucose pentaacetate from glucose (Acetylation)
3. Resacetophenone from resorcinol (Acetylation)
4. o-Chlorobenzoic acid from anthranilic acid (Chlorination & Diazotisation)
5. Phenyl azo-2-naphthol from aniline (diazotization)

**3. Quantitative analysis of organic compounds**

Estimation of phenol, aniline, ketone, glucose, saponification value and iodine value of oil.

**4. Preparation of organic compounds (double stage)**

1. p-Bromoacetanilide from aniline (Acetylation + Bromination)
2. Acetyl salicylic acid from methyl salicylate (Hydrolysis + Acetylation)
3. 1, 3, 5 – tribromobenzene from aniline (Bromination + Diazotisation + Hydrolysis)
4. p-Nitroaniline from acetanilide (Nitration + Hydrolysis)
5. Benzilic acid from benzoin (Rearrangement)
6. Benzanilide from benzophenone
7. p-Aminobenzoic acid from paranitrotoluene (Oxidation + Reduction)
8. p-Bromo aniline from acetanilide (Bromination + Hydrolysis)
9. m-Nitroaniline from nitrobenzene (Nitration + Reduction)

**Course outcome:**

*Student understood the knowledge about:*

1. The separation of organic compounds and qualitative analysis
  2. The synthesis of organic compounds by single stage
  3. The estimation of organic compounds by quantitative analysis
  4. The synthesis of organic compounds by two stage
- .....

### Course Outcome Vs Programme Outcome

	<b>PO1</b>	<b>PO2</b>	<b>PO3</b>	<b>PO4</b>	<b>PO5</b>	<b>PO6</b>	<b>PO7</b>
<b>CO1</b>	6	6	9	9	9	9	9
<b>CO2</b>	6	6	9	9	9	9	9
<b>CO3</b>	6	6	9	9	9	9	9
<b>CO4</b>	6	6	9	9	9	9	9
<b>CO5</b>	6	6	9	9	9	9	9

**Level of correlation: 9 – High; 6 – Medium; 3 – Low; and 0- no correlation.**

# **SEMESTER – II**

**SUBJECT CODE: 18PCH5**

**6 Hrs / 5 Credits**

## **CC-V – PHYSICAL CHEMISTRY – I**

### **Course objectives:**

1. *To know the unimolecular and bimolecular processes*
2. *To learn thermal and photochemical reactions*
3. *To study the first, second and third law of thermodynamics and their applications*
4. *To understand the various partition functions*
5. *To know the thermodynamic quantities*

### **UNIT – I**

#### **Chemical Kinetics-I**

Kinetics of opposing, consecutive and parallel reactions. Theories of reaction rates – simple collision theory – absolute reaction rate theory – application of ARRT to simple unimolecular and bimolecular processes – potential energy surfaces – kinetic isotopic effect.

Theory of unimolecular reactions – Lindemann's theory – Hinshelwood theory – treatment of KRR and KRRM theory – Slaters treatment – principle of microscopic reversibility – steady state approximation.

### **UNIT – II**

#### **Chemical Kinetics-II**

Chain reactions – characteristics of chain reactions – branched and stationary chain reactions – Thermal and photochemical reactions between hydrogen and halogens. Comparison of hydrogen halogen reactions — explosion reaction and discussion of explosion limits – gas phase auto oxidations – hydrogen and oxygen reaction.

Factors influencing reaction rates in solution – application of ARRT to solution kinetics – effect of solvents – double sphere and single sphere model – effect of ionic strength – influence of pressure on rates in solution – significance of volume of activation – substituent effect – LFER – Hammett and Taft equations.

**Study of Fast reactions:** Flow methods, pulse methods, relaxation methods, Shock-tube method & nuclear magnetic resonance method.



## UNIT – III

### Classical Thermodynamics

First law of thermodynamics, concept of work and heat, enthalpy and heat capacities, second law of thermodynamics, physical significance of entropy, direction of spontaneous change and dispersal of energy, Carnot cycle, efficiency of heat engine, coefficient of performance of heat engine, Gibbs function, Gibbs–Helmholtz equation, Maxwell relations.

Thermodynamic equation of state, thermodynamics of systems of variable composition, partial molar quantities, partial molar volume, chemical potential, Gibbs-Duhem equation, experimental determination of fugacity of real gases, third law of thermodynamics, absolute entropies, determination, exceptions to third law, unattainability of absolute zero.

## UNIT – IV

### Statistical Thermodynamics I

Introduction: Macro and micro states, ensembles (microcanonical and canonical), Maxwell-Boltzmann statistics, Boltzmann-Planck equation, Fermi-Dirac and Bose-Einstein statistics, negative absolute temperatures, partition function, evaluation of the partition function translational partition function, rotational partition function, vibrational partition function, electronic partition and nuclear partition function. Thermodynamic functions in terms of the partition function, internal energy, entropy, Helmholtz function, Gibbs function, residual entropy, equilibrium constant, isotope effects, heat capacity of monoatomic gases, population inversion, negative Kelvin temperature, Einstein's and Debye's theories of heat capacities of solids, nuclear spin statistics, statistical basis of entropy of H<sub>2</sub> gas.

## UNIT – V

### Non-equilibrium thermodynamics

Introduction, near equilibrium process, general theory, conservation of mass and energy, entropy production in chemical reactions, entropy production and entropy flow in open systems, transformation properties of rates and affinities, Onsager's theory, irreversible thermodynamics and biological systems, oscillatory reactions.

### Course outcome:

*Student understood the knowledge about:*

1. *Applications of ARRT Theory to unimolecular and bimolecular reactions*
2. *Linear free energy relations, Hammett and Taft equations*

3. *The first, second and third law of thermodynamics and their applications*
4. *Experimental determination of fugacity of real gases*
5. *Maxwell-Boltzmann, Fermi-Dirac and Bose-Einstein statistics*
6. *Thermodynamic functions in terms of the partition function*
7. *conservation of mass and energy*
8. *Irreversible thermodynamics and biological systems*

## References

### Unit-I & II

1. P.W. Atkins, Physical chemistry, ELBS.
2. Chemical Kinetics – K.J. Laidler Third Edition, Tata McGraw Hill.
3. Chemical Kinetics – Principles and Selected topics – I Amdur and C.G Hammer – McGraw Hill – 1996.

### Unit- III, IV & V

4. Glasstone, S. Thermodynamics for Chemists New Delhi Affiliated East West Affiliated private Ltd (1964).Rakshid, Thermodynamics.
5. Rice, Statistical Thermodynamics.
6. Lee, Sears, Turcotte, Satisfical thermodynamics New York Addison Wasley Co., (1963).

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### Course Outcome Vs Programme Outcome

	PO1	PO2	PO3	PO4	PO5	PO6	PO7
CO1	9	9	6	6	6	6	6
CO2	9	9	6	6	6	6	6
CO3	9	9	6	6	6	6	6
CO4	9	9	6	6	6	6	6
CO5	9	9	6	6	6	6	6

**Level of correlation: 9 – High; 6 – Medium; 3 – Low; and 0- no correlation.**

**CC-VI- INORGANIC CHEMISTRY – II****Course objectives:**

1. *To understand the weak and strong fields*
2. *To study the labile and inert complexes*
3. *To learn the organometallic compounds*
4. *To understand the chemistry of metal carbonyls and clusters*
5. *To study the silicates, silicones and cage compounds*

**UNIT – I****Co-ordination Chemistry**

Nomenclature of mono and poly nuclear complexes – crystal field theory – shapes of d orbitals – splitting of d orbitals in octahedral symmetry- CFSE-strong field and weak field splitting-calculation of CFSE for  $d^n$  system- splitting in tetrahedral symmetry- only weak field splitting-reasons- tetragonal symmetry- differences between tetrahedral and tetragonal symmetry- Jahn Teller distortion- splitting pattern in trigonal, square planar, trigonalbipyramidal, square pyramidal, cubic symmetries. Factors affecting the magnitude of splitting ( $10Dq$ ) -oxidation state of the metal ion, nature of the metal ion, number and geometry of the ligands, nature of the ligands – Spectrochemical studies, Jorgenson relation, evidences for CFT. Magnetic properties, computation of lattice energies, enthalpies of hydration, stability of particular oxidation states.

**M.O. theory** -octahedral, tetrahedral and square planar complexes. Pi bonding and M.O theory- ligands having filled and empty pi bonds-effect on  $10 Dq$ .- evidences for Pi bonding

**UNIT – II****Stability and Kinetics of Coordination Compounds**

Stability of coordination compounds : Detection of compound formation in solution. Stability constants—stepwise and overall formation constants—ph metric, polarographic, photometric methods of determining formation constants. Factors affecting stabilities—statistical and chelate effects.

Kinetics and mechanisms of reactions in solutions Labile and inert complexes - ligand displacement reactions- hydrolysis , aquation in octahedral and square planar complexes – trans effect- electron transfer reactions – complementary and non complementary types – inner sphere and outer sphere processes – isomerisation and racemisation.- reactions of coordinated ligands template effect and synthesis of macrocyclic ligands

### UNIT – III

#### **Photochemistry of coordination compounds:**

Photochemical reactions of coordination and organometallic compounds—photo oxidation-photoreduction-photo substitution-photo isomerisation reactions-complexes of pi acceptor ligands- carbonyls-18 electron rule-application to the structure of carbonyls-(mono and polynuclear)-application of IR to identify the terminal and bridging CO- preparation and properties of carbonyls- Ni(CO)<sub>4</sub>, Fe(CO)<sub>9</sub>, Cr(CO)<sub>6</sub>, Re<sub>2</sub>(CO)<sub>10</sub>, -Carbonylate anions-carbonyl hydrides- isolobal fragments-nitrosyl complexes preparation-bridging and terminal nitrosyls-bent and linear nitrosyls,-dinitrogen complexes.

### UNIT – IV

#### **Chemistry of Metal carbonyls and clusters**

Metal carbonyls, structure and bonding, vibrational spectra of metal carbonyls for bonding and structural elucidation, important reactions of metal carbonyls, preparation, bonding, structure and important reactions of transition metal nitrosyl, dinitrogen and dioxygen complexes, tertiary phosphine as ligand. Polyhedral model of metal clusters, effect of electronic configuration and coordination number, Structures of metal carbonyl clusters of three atoms M<sub>3</sub>(CO)<sub>12</sub> (M=Fe, Ru & Os), Four metal atoms (tetrahedra) [M<sub>4</sub>(CO)<sub>12</sub> {M= Co, Rh & Ir}] and octahedron of type M<sub>6</sub>(CO)<sub>16</sub> [M= Co & Rh]

### UNIT – V

#### **Inorganic Chains and cages**

Silicates: Various silicate, structures – structure property correlation – Silicones. Poly acids: Classification isopoly acids like polymolybdate, polyvanadate and polytungstate their structures.

Cage compounds: Nomenclature of Boranes and carboranes – Wade's rule – Styx number – preparation and structures of B<sub>4</sub>H<sub>10</sub> and borazine

**Course outcome:**

*Student understood the knowledge about:*

1. *Crystal field splitting energy and molecular orbital theory*
2. *The stability and kinetics of coordination compounds*
3. *Electron transfer reactions, complementary and non complementary reactions*
4. *Photochemical reactions of coordination and organometallic compounds*
5. *Application of IR to identify the terminal and bridging carbonyls*
6. *Vibrational spectra of metal carbonyls for bonding and structural elucidation*
7. *Nomenclature of Boranes and carboranes*
8. *Structures of silicates, silicones and polyacids*

**References****Unit – I &II**

1. Keith F Purchell and John C Koltz, Inorganic Chemistry, Saunders Golden Sunburst Series
2. F A Cotton and Wilkinson, Advance Inorganic Chemistry, V Edition, John Wiley and Sons
3. A B P Lever, Inorganic Electronic Spectroscopy, Elsevier

**Unit – III, IV & V**

4. James E Huheey, Inorganic Chemistry principles of structure and reactivity, 4<sup>th</sup> Edition, Aldeson – Wesley, New
  5. H.J. Emeleus and A.G.Sharpe , Modern aspects of inorganic chemistry.
  6. F A Cotton and Wilkinson, Advance Inorganic Chemistry, V Edition, John Wiley and Sons
- .....

**Course Outcome Vs Programme Outcome**

	<b>PO1</b>	<b>PO2</b>	<b>PO3</b>	<b>PO4</b>	<b>PO5</b>	<b>PO6</b>	<b>PO7</b>
<b>CO1</b>	9	6	6	3	6	6	6
<b>CO2</b>	9	6	6	3	6	6	6
<b>CO3</b>	9	6	6	3	6	6	6
<b>CO4</b>	9	6	6	3	6	6	6
<b>CO5</b>	9	6	6	3	6	6	6

**Level of correlation: 9 – High; 6 – Medium; 3 – Low; and 0- no correlation.**

**CHOICE-I**

**EC-II –NANO MATERIALS AND GREEN CHEMISTRY**

**Course objectives:**

1. *To know about the Techniques for characterization of nanoscale materials*
2. *To learn the synthesis and applications of nanomaterials*
3. *To study the principles and basics of green chemistry*
4. *To understand the various methods of green synthesis*
5. *To know the different literature resources*

**UNIT I**

**Basics of nanochemistry**

Definition of nano dimensional materials, size effects, importance of nanomaterials, classification of nanomaterials, simple examples of unique properties of nano sized materials, some important recent discoveries in nanoscience and technology

Techniques for characterization of nanoscale materials (basic aspects): atomic force microscope (AFM), transmission electron microscope (TEM), resolution and scanning electron microscope (SEM), scanning tunneling microscope (STM), scanning near field optical microscope (SNOM), and surface Plasmon Resonance spectroscopy.

**UNIT II**

**Synthesis and applications of nanomaterials**

Chemical methods in preparation of nanomaterials: sol–gel technique, co-precipitation hydrolysis, sonochemical method, combustion technique, colloidal precipitation, template process. Inorganic nanoparticles and nanoporous materials: oxide nanoparticles, oxomolybdates, nano catalysis.

Nature of carbon bond, new carbon structures, carbon clusters: discovery of C<sub>60</sub>, alkali doped C<sub>60</sub>, superconductivity in C<sub>60</sub>, larger and smaller fullerenes, carbon nanotubes: synthesis, single walled carbon nanotubes, structure and characterization, mechanism of formation, chemically modified carbon nanotubes, doping, functionalizing nanotubes, application of carbon nanotubes, nanowires, synthetic strategies, gas phase and solution phase growth, growth control, properties.

## UNIT III

### Principle of Green Chemistry

Twelve principles of Green Chemistry with their explanations and examples; Designing a Green Synthesis using these principles; Prevention of Waste/byproducts; maximum incorporation of the materials used in the process into the final products (Atom Economy); prevention/minimization of hazardous/toxic products; designing safer chemicals different basic approaches to do so; selection of appropriate auxiliary substances (solvents, separation agents), green solvents, solventless processes, immobilized solvents and ionic liquids; energy requirements for reactions – use of microwaves, ultrasonic energy.

## UNIT IV

### Methods of Green Synthesis

Green Synthesis of the following compounds: adipic acid, catechol, BHT, methyl methacrylate, urethane, aromatic amines (4- aminodiphenylamine), benzyl bromide, acetaldehyde, ibuprofen, paracetamol, turtural. Microwave assisted reactions in water: Hofmann Elimination, Hydrolysis (of benzyl chloride, benzamide, n-phenyl benzamide, methylbenzoate to benzole acid), Microwave assisted reactions in organic solvents: Esterification, Diels Alder Reaction, Decarboxylation. Ultrasound assisted reactions: Esterification, saponification, Alkylations, Cannizaro reaction, Strecker synthesis, Reformatsky reaction.

## UNIT V

### Literature Search

Primary and secondary sources of Literature – Journals, Patents, current contents – Chemical Abstract – Subject index, Substance index, Author index, formula index and other indices – Use of these indices with examples – Science citation index – Monographs and treatise – Literature search using computer – browsing and downloading of paper, articles (through 30hem.. Webs), Chemistry programmes – Chemdraw – Chems sketch

### Course outcome:

*Student understood the knowledge about:*

1. various types of Electron Microscopes
2. some important recent discoveries in nanoscience and nanotechnology

3. *Chemical methods in preparation of nanomaterials*
4. *Structure, characterization, mechanism and formation of carbon nanotubes*
5. *Twelve principles of Green Chemistry with their explanations*
6. *Synthesis of different compounds by green method*
7. *Uses of Microwaves and Ultra sounds in green synthesis*
8. *Primary and secondary sources of Literature*

## References

### Unit – I, II & III

1. <http://www.inflibnet.ac.in>
2. <http://www.springerlink.com>
3. <http://www.rsc.org>
4. <http://www.pubs.acs.org>
5. Kenneth . Klabunde, *Nanoscale Materials in Chemistry*, John Wiley & Sons,
6. *Nanotechnology: basic science and emerging technologies* – Mick Wilson KamaliKannangara, Geoff Smith, Michelle Simmons, BurkhardRaguseas Overseas Press (2005).

### Unit – IV & V

7. Paul T. Anastas *Green Chemistry*
8. Sanghi A Shrivastav *Green Chemistry*
9. M.Kidwai&Ahlavalia V.K. *Green Chemistry*
10. V. Kumar, *An Introduction to Green Chemistry*, Vishal Publishing CO. Jalandhar, 2007.
11. J.March, “*Advanced Organic Chemistry; Reactions, Mechanisms and Structure*” 6<sup>th</sup> Ed., Wiley – Interscience, 2007

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### Course Outcome Vs Programme Outcome

	PO1	PO2	PO3	PO4	PO5	PO6	PO7
CO1	6	6	6	9	9	9	9
CO2	6	6	6	9	9	9	9
CO3	6	6	6	9	9	9	9
CO4	9	9	6	6	6	9	6
CO5	6	6	6	9	9	9	6

**Level of correlation: 9 – High; 6 – Medium; 3 – Low; and 0- no correlation.**



## CHOICE-II

### EC-II- MEDICINAL AND PHARMACEUTICAL CHEMISTRY

#### Course objectives:

1. *To study the fundamentals of Medicinal chemistry*
2. *To learn about Antibiotics and aaantibacterials*
3. *To know the chemotherapeutic agents*
4. *To study the synthesis and antihypertensive drugs*
5. *To learn the various pharmaceutical techniques*

#### Unit I

##### Fundamentals of Medicinal Chemistry

Introduction to the history of medicinal chemistry – Pharmacokinetics: Introduction to drug absorption, distribution, drug metabolism and elimination. Concept of prodrug and soft drug. Drug Design – Lead compounds, structure – activity relationship (SAR) and the development of Quantitative Structure Activity Relationship (QSAR).

#### Unit II

##### Antibiotics and Antibacterials

Structural features and SAR of the following antibiotics – penicillin G, cephalosporin and their semisynthetic analogs ( $\beta$  – lactam), streptomycin (amino glycoside), terramycin (tetracycline), erythromycin (macrolide) and chloramphenicol.

#### Unit III

##### Chemotherapeutic agents

**Antineoplastic agents:** Classification, synthesis, assay, e.g., cyclophosphamide, ifosfamide, clorambucil, busulfan, decarbazine, methotrexate, azathioprine, 6-mercaptopurine, 5-fluorouracil and cisplatin.

**Antitubercular drugs:** Classification, synthesis, assay, e.g., chloroquine, primaquine, amadodiaquine, mefloquine and progunailpyrimethamine.

#### Unit IV

##### Synthesis and Therapeutic action and SAR of Antihypertensive drugs

Nifedipine, Captopril, hydralazine, sodiumnitroprusside, clonidine, methyl dopa and guanethidine.

## Unit V

### Pharmaceutical Analysis

Principles, instrumentation and applications to the following: Absorption spectroscopy (UV, visible & IR). Principles and applications of NMR, Mass spectroscopy, Chromatographic methods – TLC, HPLC and GC.

#### Course outcome:

*Student understood the knowledge about:*

1. *The fundamentals of Medicinal chemistry*
2. *The Development of Quantitative Structure Activity Relationship*
3. *The Antibiotics and antibacterials*
4. *The chemotherapeutic agents*
5. *Antineoplastic agents and Antitubercular drugs*
6. *The synthesis and antihypertensive drugs*
7. *The therapeutic action of drugs*
8. *The instrumentation and spectroscopic methods and their applications*

### Reference Books

#### Unit - I

1. Introduction to Medicinal Chemistry, A Gringauze, Wiley-VCH.
2. Wilson and Gisvold's Text Book of Organic Medicinal and Pharmaceutical Chemistry, Ed Robert F. Dorge.
3. An Introduction to Drug Design, S.S. Pandey and J.R. Dimmock, New Age International.

#### Unit -II

4. Burger's Medicinal Chemistry and Drug Discovery, Sixth Edition, Ed.M.E.vWolff, John Wiley.
5. The Organic Chemistry of Drug Design and Drug Action, R.B. Silverman, Academic Press.
6. Finar, I. L. & Finar, A. L. Organic Chemistry Vol. 2, Addison-Wesley (1998)
7. Finar, I. L. Organic Chemistry Vol. 1, Longman (1998)

#### Unit - III

8. Gringauz, A. Introduction to Medicinal Chemistry: How Drugs Act and Why? John Wiley & Sons (1997).
9. Patrick, G. L. Introduction to Medicinal Chemistry Oxford University Press (2001).
10. Medicinal Chemistry – Sriram.D
11. Medicinal Chemistry – Kar. Ashuthosh

#### Unit – IV & V

12. Introductory Medicinal Chemistry, J.B.Taylor and P.D.Kennewell, Ellsworth publishers, 1985.
13. Medicinal Chemistry – Laxmi.C
14. Pharmaceutical Chemistry – B. Jeyasree Gosh
15. Text book of Pharmaceutical Organic Chemistry – Mohammed Ali.

16. Synthetic Drug – Gurdeep Chatwal.

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**Course Outcome Vs Programme Outcome**

	<b>PO1</b>	<b>PO2</b>	<b>PO3</b>	<b>PO4</b>	<b>PO5</b>	<b>PO6</b>	<b>PO7</b>
<b>CO1</b>	6	6	6	9	9	9	9
<b>CO2</b>	6	6	6	9	9	9	9
<b>CO3</b>	6	6	6	9	9	9	9
<b>CO4</b>	9	9	6	6	6	9	6
<b>CO5</b>	6	6	6	9	9	9	6

**Level of correlation: 9 – High; 6 – Medium; 3 – Low; and 0- no correlation.**

**EDC – I – SUPRAMOLECULAR CHEMISTRY****Course objectives:**

1. *To understand the Basic concepts of supramolecular chemistry*
2. *To know the synthesis and different structures*
3. *To study the crystal engineering*
4. *To learn the designs and various interactions*
5. *To study molecular electronic devices*

**Unit-I****Basic Concepts of Supra Molecular Chemistry**

Basic concepts Terminology and nomenclature in supramolecular chemistry, definition of supramolecular chemistry, chemical interactions leading to supramolecular assemblies, nature of binding interactions in supramolecular structures: ion-ion, ion-dipole, dipole-dipole, H-bonding, cationpi, anion-pi, pi-pi and Van der Waals interactions.

**Unit-II****Synthesis and Different Structures**

Host-Guest chemistry Synthesis and structure of crown ethers, lariat ethers, podands, cryptands, spherands, calixarenes, cyclodextrins, cyclophanes, cryptophanes, carcerands, and hemicarcerands, host-guest interactions, pre-organization and complementarity, lock and key analogy, binding of cationic, anionic, ion pair and neutral guest molecules.

**Unit-III****Crystal engineering**

Crystal engineering: role of H-bonding, halogen bonding and other weak interactions, cocrystals, salts, polymorphs and their physico-chemical properties, coordination polymers, metal organic frameworks and their properties.

**Unit-IV****Designs and Various Interactions**

Self-Assembly Self-assembly of molecules: Design, synthesis and properties of the molecules, self assembling by H-bonding, metal-ligand interactions and other weak interactions, metallomacrocycles, catenanes, rotaxanes, helicates and knots, examples of recent developments in supramolecular chemistry.

## Unit-V

### Molecular devices

Molecular devices: Molecular electronic devices, molecular wires, molecular rectifiers, molecular switches, molecular logic. Relevance of supramolecular chemistry to mimic biological systems: cyclodextrins as enzyme mimics, ion channel mimics, supramolecular catalysis.

### Course outcome:

*Student understood the knowledge about:*

1. *Binding interactions in supramolecular structure*
2. *Synthesis and structure of crown ethers*
3. *H-bonding, halogen bonding and other interactions*
4. *Metal organic frame works and their properties*
5. *Design, synthesis and properties of the molecules*
6. *Metal – ligand and other weak interactions*
7. *Molecular electronic devices*
8. *Supramolecular chemistry to mimic biological system*

### References:

#### Unit-I, II & III

1. J.M. Lehn, Supramolecular Chemistry-Concepts and Perspectives, Wiley-VCH, 1995.
2. P. D. Beer, P. A. Gale and D. K. Smith, Supramolecular Chemistry, Oxford University Press, 1999.
3. J. W. Steed and J. L. Atwood, Supramolecular Chemistry, 1st Ed., Wiley, 2000.
4. J.W. Steed, Core Concepts in Supramolecular Chemistry and Nanochemistry, 1st Ed., John Wiley & Sons, 2007.

#### Unit- IV & V

5. J.D. Seader, I. W. Hamley, Introduction to soft mater Synthetic and Biological selfassembly materials, Separation process principles, 2nd Ed., Wiley, 2010.
6. G. R. Desiraju, J. J. Vittal and A. Ramanan, Crystal Engineering: A Textbook, World Scientific, 2011.

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### Course Outcome Vs Programme Outcome

	PO1	PO2	PO3	PO4	PO5	PO6	PO7
CO1	6	6	9	9	9	9	9
CO2	6	6	9	9	9	9	9
CO3	6	6	9	9	9	9	9
CO4	9	9	9	6	6	9	6
CO5	6	6	9	9	9	9	6

**Level of correlation: 9 – High; 6 – Medium; 3 – Low; and 0- no correlation.**

# **SEMESTER – III**

**CC-VII – ORGANIC CHEMISTRY – II****Course objectives:**

1. *To learn about the chemistry of alkaloids and steroids*
2. *To study about the terpenes and flavonoids*
3. *To learn the chemistry of carbohydrates and proteins*
4. *To study about the chemistry of nucleic acid and antibiotics*
5. *To study the retrosynthesis and disconnection approach*

**UNIT – I****Alkaloids and Steroids**

General methods of determining structure. Classification of alkaloids – structural elucidation of (-) quinine, morphine, conine, atropine, reserpine, ephedrine. Biosynthesis of alkaloids.

Steroids – Occurrence, nomenclature, basic skeleton, diel's hydrocarbon and stereochemistry. Isolation, structure determination and synthesis of cholesterol, bile acids, androsterone, testosterone, estrone, progesterone, aldosterone, bio synthesis of steroids.

**UNIT – II****Terpenes and flavonoids**

Terpenes – Introduction structural elucidation of sentoxin, phytol, abietic acid and  $\beta$  carotene. Anthocyanins and flavones – Occurrence, nomenclature and general method of structure determination, isolation and synthesis of apigenin, luteolin, quercetin, myrcetin, aureusin, cyaniding – 7 – obinoside, cyaniding, Histidine. Biosynthesis of flavonoids : Acetate pathway and shikimic and pathway.

**UNIT – III****Carbohydrates**

Determination of the configuration of the saccharides, ring structure of mono saccharides Glycosides, Hudson's rule. Methods for determining the size of the sugar rings – Conformational analysis. Structure determination of starch, cellulose, peptides and proteins : synthesis of peptides – primary, secondary, tertiary and quaternary structure of proteins protection protection of N-terminal and C-terminal groups of proteins – biosynthesis of proteins.

**UNIT – IV**

## Nucleic acids

Chemistry of nucleic acids – Structure of DNA, properties, biological implications of DNA, Replication of DNA, structure of RNA – types of RNA and their functions. Antibiotics – introduction – structural elucidation of penicillin, streptomycin, cephalosporin, terramycin.

## UNIT-V

### Retrosynthesis

Concepts in organic synthesis: retrosynthesis, disconnection, synthons, linear and convergent synthesis, umpolung of reactivity, protecting functional groups, protection of NH and OH groups, acetals as protecting groups for diols, protection of carbonyl groups in aldehydes and ketones, protection of the carboxyl group, protection of double and triple bonds.

### Course outcome:

*Student understood the knowledge about:*

1. *Structural elucidation and biosynthesis of alkaloids and steroids*
2. *Structural elucidation of terpenes*
3. *Nomenclature and general method of structure determination of flavonoids*
4. *Determination of the configuration of carbohydrates*
5. *Synthesis of peptides and different structures of proteins*
6. *Properties and biological implications of nucleic acids*
7. *Structural elucidation of antibiotics*
8. *The retrosynthesis and disconnection approach*

### References

#### Unit – I & II

1. Organic chemistry volume II I.L. Finar., ELBS.
2. O.P. Agarwal, Chemistry of organic natural products Vol I and Vol II 1997. Goel publications.
3. Chatwal Anand, Natural Products, Vol I and Vol II.

#### Unit – III & IV

4. Gurdeep Chatwal, Natural products chemistry.
5. Advanced Organic chemistry, Bahul and Arun Bahul.

#### Unit – V

6. Organic chemistry VII edition, Morrison and Boyd. (Retro synthesis)
7. Strategies and tactics in organic synthesis, M. Harmata.
8. Organic synthesis – Disconnection approach, Stuart Warren.

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### Course Outcome Vs Programme Outcome

	PO1	PO2	PO3	PO4	PO5	PO6	PO7
CO1	6	9	6	6	9	6	6
CO2	6	6	6	6	9	6	6
CO3	6	6	6	6	9	6	6
CO4	6	6	6	6	9	6	6
CO5	6	6	6	6	9	6	6

**Level of correlation: 9 – High; 6 – Medium; 3 – Low; and 0- no correlation.**

**CC-VIII – PHYSICAL CHEMISTRY – II**

**Course objectives:**

- 1. To understand about the classical mechanics and wave mechanics*
- 2. To study the approximation methods*
- 3. To learn the fundamentals of Group theory*
- 4. To know the application of Group theory to Spectroscopy*
- 5. To study the Rotational, Vibrational, Raman and Electronic spectrum*

**UNIT – I**

**Quantum Chemistry I**

Classical mechanics – General principles and basic assumptions conservation laws – Lagrangian and Hamiltonian equations of motion inadequacy of classical mechanics

Wave particle dualism – uncertainty principles – functions-orthogonality and Normalisation-– operator algebra – operator. Linear and Hermitian--eigen function and eigen values. Postulates of quantum mechanics- Angular momentum operator--commutation relations.

Applications of wave mechanics to simple systems – particle in a box – one and three dimensional – quantum numbers. Zero point energy.

**UNIT – II**

**Quantum chemistry II**

Rigid rotator – Harmonic Oscillator – rotational and vibrational quantum number and selection rules– Bohr's correspondence principle – Hydrogen atom --shapes and nodal properties of orbital.

Approximation methods – many electron atoms – wave function – one electron orbitals – Pauli's principle and Slater determinants – variation method – application to hydrogen and helium atoms – perturbation method for nondegenerate systems – application of perturbation theory to helium atom. Hartree – Fock self consistent field method. L – S and J – J coupling.

Born – Oppenheimer approximation : Hydrogen molecule ion. LCAO method. MO and VB treatments of the hydrogen molecule. Hybridization and molecular orbitals of H<sub>2</sub>O, NH<sub>3</sub> and CH<sub>4</sub>. Huckel pi-electron method for butadiene and benzene.

## UNIT – III

### Fundamentals of Group Theory

Molecular symmetry elements and symmetry operations, point groups- low symmetry, higher symmetry and special symmetry point groups–Group-definition and properties of a group,group multiplication table for  $C_{2V}$  and  $C_{3V}$  point groups-- matrix representation of symmetry operations and transformation matrices — representation of a group-reducible and irreducible representations – Great orthogonality theorem –characters – construction of a character tables–  $C_{2V}$ ,  $C_{3V}$ ,  $C_{2h}$ .

## UNIT – IV

### Application of Group Theory to Spectroscopy

Symmetry of Normal modes of vibrations, application of Group theory to normal modes of vibrations and to normal mode analysis – symmetry properties of integrals – application for spectral selection rules of vibration spectra – IR and Raman active fundamentals symmetry of molecular orbitals and symmetry selection rule for electronic transitions in simple molecules like water, ammonia and ethylene.

## UNIT –V

### Fundamentals of molecular spectroscopy

Rotational spectrum : Diatomic molecules. Energy levels of a rigid rotor selection rules. Poly atomic molecules - Isotope effect. Vibrational spectrum : Infrared spectrum : vibrating diatomic molecules, diatomic vibrating rotator-. Raman spectrum : Rayleigh and Raman scattering stokes and antistokes lines, concept of polarizability, pure rotational Raman spectra- vibrational Raman spectra Electronic spectrum : Electronic spectra of diatomic molecules – Born-Oppenheimer approximation – Franck -Condon principle – Dissociation energy – Rotational fine structure—Fortrat diagram

### Course outcome:

*Student understood the knowledge about:*

1. *Classical mechanics and applications of wave mechanics*
2. *The Variation and Perturbation method*
3. *LCAO, MO and VB treatments of the Hydrogen molecule*
4. *Symmetry elements, operations and point groups*
5. *Symmetry of Normal modes of vibrations*

6. *Applications for spectral selection rules of vibration spectra*
7. *Rotational and Vibrational spectrum*
8. *Raman spectrum and electronic spectrum*

## References

### Unit – I & II

1. R.K. Prasad, Quantum Chemistry, third Reprint new age International limited.
2. Quantum Chemistry, Ira N. Levine Prentice Hall.
3. Introduction to Quantum Chemistry, A.K. Chandra Tata Megraw Hill.

### Unit – III & IV

4. P.W. Atkins, Physical chemistry, ELBS.
5. Chemical Applications of group theory, F.A. Cotton.

### Unit – V

6. C.N. Banwell, Fundamentals of molecular spectroscopy

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## Course Outcome Vs Programme Outcome

	PO1	PO2	PO3	PO4	PO5	PO6	PO7
CO1	9	9	6	3	9	6	6
CO2	6	9	6	3	9	6	6
CO3	6	9	6	3	9	6	6
CO4	6	9	6	3	9	6	6
CO5	6	9	6	3	9	6	6

**Level of correlation: 9 – High; 6 – Medium; 3 – Low; and 0- no correlation.**

**CC-XI – INORGANIC CHEMISTRY – III****Course objectives:**

1. *To study about the metal ions in biological system*
2. *To learn the transport and storage of oxygen*
3. *To know about the electron transfer in biological system*
4. *To study the Nitroegnase systems*
5. *To know the medicinal bioinorganic chemistry*

**UNIT – I****Metal ions in biological systems**

Macrocyclic ligands – synthesis – crown ethers, cryptands and spirans - Essential and trace metals – Na<sup>+</sup>/K<sup>+</sup> pump – Role of metal ions in biological processes. Bioenergetics and ATP cycle – DNA Polymerization, Glucose storage, metal complexes in transmission of energy. Chlorophylls, photo system I, photo system- II in the cleavage of water, model systems.

**UNIT – II****Transport and storage of oxygen**

Heme proteins and oxygen uptake, structure and function of haemoglobin, myoglobin, hemocyanins, and hemerythrin, model synthetic complexes of iron, cobalt and copper.

**UNIT – III****Electron transfer in biological systems**

Structure and function of metalloproteins in electron transport processes – cytochromes and iron-sulphur proteins, synthetic models.

**UNIT – IV****Nitrogenase systems**

Biological Nitrogen fixation, molybdenum nitrogenase, spectroscopic and other evidence, other nitrogenase model systems.

**UNIT – V****Medicinal Bioinorganic Chemistry**

Metal ion toxicity-Sources –general mechanism of metal ion toxicity – chemical speciation of metals in environment – Toxic effects of metals: Cadmium, Mercury, Aluminium, Iron and Copper. Detoxification – Basic requirements of chelating drug - Detoxification by metal chelates(representative chelating drugs) Chemotherapy – Cisplatin

in chemotherapy – Drug action and mechanism – Gold containing drugs as Anti-Rheumatic agents – Lithium in Psychopharmacological drugs.

**Course outcome:**

*Student understood the knowledge about:*

1. *Synthesis of macrocyclic ligands*
2. *Role of metal ions in biological processes*
3. *Structure and function of globins*
4. *Model synthetic complexes of iron, cobalt and copper*
5. *Structure and function of metalloproteins*
6. *Electron transport mechanisms*
7. *Biological Nitrogen fixation*
8. *Metal ion toxicity and toxic effect of metals*

**References**

**Unit – I, II, III, IV &V**

1. Principles of Bioinorganic chemistry, S.J.Lippard and J.M.Berg. University Science Book.
2. Bioorganic chemistry, I.Bertini, H.B.Gray, S.J.Lippard and J.S.Valentine, University Science Books.
3. Inorganic Biochemistry Vol.I&Vol.II L. Ed. G. Eichhorn, Elsevier.
4. Hussain Reddy, Bioinorganic chemistry.

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**Course Outcome Vs Programme Outcome**

	<b>PO1</b>	<b>PO2</b>	<b>PO3</b>	<b>PO4</b>	<b>PO5</b>	<b>PO6</b>	<b>PO7</b>
<b>CO1</b>	6	6	6	3	6	9	6
<b>CO2</b>	6	6	6	3	6	9	6
<b>CO3</b>	6	9	6	3	9	9	6
<b>CO4</b>	9	6	6	3	6	6	6
<b>CO5</b>	9	6	6	3	6	9	6

**Level of correlation: 9 – High; 6 – Medium; 3 – Low; and 0- no correlation.**

## CHOICE-I

SUBJECT CODE: 18PCHE3

6 Hrs / 5 Credits

### EC-III – PHYSICAL METHODS IN CHEMISTRY

#### Course objectives:

1. *To learn about the Electronic spectra of metal complexes*
2. *To study about the IR and Raman spectroscopy*
3. *To learn about the NMR spectroscopy*
4. *To understand the ESR and Mossbauer spectroscopy*
5. *To study about magnetic properties and Photoelectron Spectroscopy*

#### UNIT I

##### Electronic Spectra of Transition metal complexes

Spectroscopic ground states, spectral terms, R-S coupling and J-J couplings- term symbol – selection rules—microstates—Pigeon hole diagram for  $p^2$  and  $d^2$  configuration. Orgel and Tanabe – sugano diagrams for transition metal complexes ( $d^1$ - $d^9$  states) electronic spectra of transition metal complexes—calculation of  $Dq$  values -- Racah parameters and Beta parameters, Nephelauxetic effect, charge transfer spectra.

#### UNIT – II

##### IR and Raman Spectroscopy

Combined uses of IR and Raman spectroscopy in the structural elucidation of simple molecules like  $H_2O$ ,  $ClF_3$ ,  $NO_3^-$  ion,  $ClO_3^-$  ion, - effect of coordination on ligand vibrations- uses of group vibrations in the structural elucidation of metal complexes of urea, thiourea, cyanide, thiocyanate, nitrate, sulphate, and dimethyl sulphoxide - effect of isotopic substitution on the vibrational spectra of molecules- vib. Spectra of metal carbonyls with reference to the nature of bonding, geometry, and number of C-O stretching vibrations- group theoretical treatment.

#### UNIT – III

##### NMR spectroscopy

Nuclear spin, Nuclear resonance, saturation, Shielding of magnetic nuclei --chemical shift and its measurement, factors influencing chemical shift --deshielding, spin-spin interaction. factors influencing coupling constant, spin decoupling.  $^{13}C$  NMR,  $^{31}P$  NMR, P-NMR, FT-NMR. Spectrum of paramagnetic molecules – Isotropic shift—lanthanide shift reagents – fluxional behaviour of molecules.

#### UNIT – IV

## **ESR and Mossbauer spectroscopy**

ESR- Zeeman effect, hyperlinesplittings ( isotropic systems ) – coupling constants – Zero field splitting and Kramers degeneracy – esr of transition metal complexes. McConnell equation--g-value-factors affecting g-value.

Mossbauer spectroscopy—Dopler effect and isomer shift, quadrupole interactions (NQR) – MB spectrum of Iron and tin compounds.

## **UNIT –V**

### **Magnetic properties, Diffraction Methods, and PES**

Magnetic properties—Types of magnetism, quenching of orbital angular momentum (A,E and T term).determination of magnetic susceptibility by Guoy method. Magnetic properties of lanthanides and actinides.

Space groups- Difference between crystal symmetry and molecular symmetry- X ray diffraction– Neutron diffraction and electron diffraction – elementary treatment.

Photo electron spectroscopy (PES) – principle and applications.

### **Course outcome:**

*Student understood the knowledge about:*

- 1. Spectroscopic states and Term symbols*
- 2. Orgel and Tanabe- sugano diagrams*
- 3. Effect of coordination on ligand vibrations*
- 4. Group theoretical representations*
- 5. NMR spectrum of paramagnetic molecules*
- 6. Hyperfine, Zerofine splitting and ESR transitions of metal complexes*
- 7. Determination magnetic susceptibility and magnetic properties*
- 8. X-ray, Neutron and Electron diffraction methods*

### **References**

#### **UNIT: I, II, III, IV & V**

1. Modern spectroscopy, J. M. Hollas, John Wiley.
2. Physical methods in chemistry, R.S.Drago, SaundersCollege
3. Introduction to Molecular Spectroscopy, G.M.Barrow, Mc.Graw Hill.
4. Introduction to Magnetic Resonance, A.Carrington and A.D.Maclachalan.
5. Group theory and Application to Chemistry, K.V.Raman, New Delhi, Tata. Mc Graw Hill.

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### Course Outcome Vs Programme Outcome

	<b>PO1</b>	<b>PO2</b>	<b>PO3</b>	<b>PO4</b>	<b>PO5</b>	<b>PO6</b>	<b>PO7</b>
<b>CO1</b>	9	9	6	6	6	6	6
<b>CO2</b>	9	9	6	6	6	6	6
<b>CO3</b>	9	9	6	6	6	6	6
<b>CO4</b>	9	9	6	6	6	6	6
<b>CO5</b>	9	9	6	6	6	6	6

**Level of correlation: 9 – High; 6 – Medium; 3 – Low; and 0- no correlation.**

## CHOICE-II

### EC-III - CORROSION SCIENCE

#### Course objectives:

1. *To study basic concepts and forms of corrosion*
2. *To know about atmospheric and underground corrosion*
3. *To study phenomena of polarization, energy and power density*
4. *To study about primary cells*
5. *To know about fuel cells*

#### Unit I

##### Basic aspects of corrosion

Importance of corrosion studies – EMF and Galvanic series – Classification of corrosion – passivity – theories of passivity, criteria for selecting metals exhibiting passivity – oxidation of metals – high temperature corrosion. Forms of corrosion – definition, factors and control methods of various forms of corrosion such as pitting, inter-granular, dezincification, stress corrosion, crevice corrosion and corrosion fatigue, fretting corrosion, film form corrosion and erosion corrosion.

#### Unit II

##### Environmental aspects and electrolytic factors

Atmospheric corrosion – classification, factors influencing atmospheric corrosion – temporary atmospheric corrosion preventive methods. Corrosion in immersed condition – effect of dissolved gases, salts, pH, temperature on the rate of flow of corrosion. Underground corrosion – corrosion process in soil, factors influencing soil corrosion. Biological and marine corrosion – definition, mechanism and control methods.

#### Unit III

##### Energy Conversion

Electrochemical energy conversion – thermodynamic reversibility – characteristic and performance criteria – battery terminology Gibb's equation – EMF – phenomena of polarization, battery terminology – energy density – power density – basic principles and criteria for selection of anodes and cathodes – different types of primary cells and secondary cells – applications of primary and secondary cells – types of electrolytes – aqueous, non-aqueous, molten salt and solid electrolytes.

#### Unit IV

##### Energy storage devices

Basic electrochemical reactions and performance characteristics of the following primary systems (1) Laclancy dry cell (2) Metal air cells such as Zinc/air. Iron/air and

Aluminium/air. (3) Button cells – Zn – MnCO<sub>2</sub>. Mercuric oxide cells and Lithium cells. (4) Solid electrolyte cells (5) Activated battery – water activated battery such as Mg/AgCl and Mg/CuCl systems, Lead-Acid, Ni-Cd, Ni-Fe, Ni-Metal hydride and lithium – ion batteries – basic electrochemical reactions – charge/discharge characteristics – electrode design and separators– raw material characterizations – components and assembly of cells.

## Unit V

### Fuel cells

Introduction – types of fuel cells, advantages – thermodynamics and efficiencies – electro catalysis of hydrogen oxidation and oxygen reduction – porous electrodes. Types, current –voltage relationship – limiting current density, mercury porosimetry. Various fuel cell systems– alkaline, phosphoric acid, molten carbonate, solid oxide and solid polymer fuel cell systems.

### Course outcome:

*Student understood the knowledge about:*

1. *The basic concepts and forms of corrosion*
2. *The atmospheric and underground corrosion*
3. *Biological and marine corrosion*
4. *The phenomena of polarization, energy and power density*
5. *Different types of primary and secondary cells*
6. *Basic electrochemical reactions*
7. *Raw materials, components and assembly of system*
8. *Advantages and efficiency of fuel cells*

### References

#### UNIT- I, II, III, IV & V

1. D.Pletcher and F C Walsh, Industrial Electrochemistry, Vol. II, Blakrid Academic Professional, London, 1993.
2. D Jones, Principles and prevention of corrosion Macmillan Publications New York, 1992.
3. J J Meketta, Cathodic Protection Theory and practice, Marcel Dekker Publication, New York, 1993.
4. S N Banerjee, An introduction to corrosion and corrosion inhibition, Oxonian Press Ltd., New Delhi.
5. L L Shrier, Corrosion Vol I & II Goege Nouns Ltd., Southampton Street, London.
6. M G Fonlana& N D Greene, Corrosion Science and Engineering. McGraw Hill Book Co., New York.

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**Course Outcome Vs Programme Outcome**

	<b>PO1</b>	<b>PO2</b>	<b>PO3</b>	<b>PO4</b>	<b>PO5</b>	<b>PO6</b>	<b>PO7</b>
<b>CO1</b>	9	9	6	6	6	6	6
<b>CO2</b>	9	9	6	6	6	6	6
<b>CO3</b>	9	9	6	6	6	6	6
<b>CO4</b>	9	9	6	6	6	6	6
<b>CO5</b>	9	9	6	6	6	6	6

**Level of correlation: 9 – High; 6 – Medium; 3 – Low; and 0- no correlation.**

**CP-XIII -PHYSICAL CHEMISTRY PRACTICAL (Non Electrical)**

**Course objectives:**

1. *To know about the molecular weight determination methods*
2. *To study the determination of distribution coefficient and equilibrium constant*
3. *To learn comparison of acids by kinetic studies*
4. *To understand about Conductometric titrations*
5. *To study the Potentiometric titrations*

**Non Electrical**

1. Determination of molecular weight of given unknown substance by Rast Method (Determination of  $K_f$  value of given solvent)
2. Determination of molecular weight by transition temperature method. (Determination of  $K_f$  value of given substance)
3. CST of phenol – water system – Effect of impurities on CST.
4. Determination of eutectic temperature and eutectic composition of a primary mixture of compound A & B (phase diagram of compound formation)
5. i. Determination of partition or distribution coefficient of iodine between  $CCl_4$  and water.  
ii. Determination of equilibrium constant of the reaction between KI and  $I_2$  and to find out the concentration of the given KI solution.
6. Comparison of strength of acid by kinetics of hydrolysis of ester.
7. Determination of energy of activation ( $E_a$ ) and Arrhenius factor (A) for the acid catalysed hydrolysis of ester.
8. Effect of ionic strength on kinetics of reaction – primary salt effect (Determination of concentration of the given  $KNO_3$  solution)
9. Determination of concentration of the given oxalic acid by studying the adsorption of oxalic acid on charcoal (Adsorption Isotherm)
10. Determination of solubility and heat of solution of the given oxalic acid.

**PHYSICAL CHEMISTRY PRACTICAL (Electrical)**

**Conductometric titrations**

1. Determination of strength of strong and weak acid present in the given mixture of acids using 0.1N NaOH and crystalline  $NH_4Cl$ .
2. Determination of strength of NaOH and NaOAc present in the given mixture using 0.1N HCl and crystalline NaOAc.
3. Determination of strength of HCl and  $NH_4Cl$  in the given mixture using 0.1N NaOH and crystalline  $NH_4Cl$ .
4. Determination of strength of  $Cl^-$  and  $I^-$  present in the given mixture of halides using 0.1N  $AgNO_3$  and crystalline KCl (conductometric precipitation titration)
5. Determination of ionization constant of a weak acid (determination of cell constant of a conductivity cell)

- Determination of strength of  $K_2SO_4$  (conductometric precipitation titration) determination of solubility and solubility product of  $BaCl_2$ .

### Potentiometric Titrations

- Determination of strength of strong and weak acid potentiometrically using 0.1N NaOH and a standard solution of HCl.
- Determination of strength of given ferrous sulphate solution potentiometrically using ferrous sulphate (standard solution) and 0.1N  $K_2Cr_2O_7$  (link solution)
- Determination of strength of given KI solution using KI (standard solution) and  $KMnO_4$  (link solution) (potentiometric redox titration)
- Determination of strength of  $Cl^-$  and  $I^-$  ions present in the given solutions using 0.04N  $AgNO_3$  solution and 0.02 N KCl (standard solution).

### Course outcome:

*Student understood the knowledge about:*

- The molecular weight determination methods*
- Determination of partition coefficients*
- Eutectic temperature and eutectic composition of a primary mixture*
- Determination of energy of activation and Arrhenius factor*
- The adsorption method*
- Determination of acid – base strength by conductometric titrations*
- Determination of strength of halides by conductometric precipitation titration*
- Determination of strength of KI solution by potentiometric redox titration*

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### Course Outcome Vs Programme Outcome

	PO1	PO2	PO3	PO4	PO5	PO6	PO7
CO1	9	9	9	9	9	9	6
CO2	9	9	9	9	9	9	6
CO3	9	9	9	9	9	9	6
CO4	9	9	9	9	9	9	6
CO5	9	9	9	9	9	9	6

**Level of correlation: 9 – High; 6 – Medium; 3 – Low; and 0- no correlation.**

# **SEMESTER – IV**

**CC-X – ORGANIC CHEMISTRY – III****Course objectives:**

1. To study about the aliphatic substitution reactions
2. To learn about the aromatic substitution reactions
3. To know the elimination reactions and reagents in organic synthesis
4. To study about the addition reactions
5. To learn about the oxidation and reduction reagents and molecular rearrangements

**UNIT – I**

**Aliphatic nucleophilic substitution** : SN1, SN2, and SNi mechanisms-effect of substrate structure, leaving group, attacking nucleophile and solvent-neighboring group participation—substitution in allylic carbons and reactivity-ambident nucleophiles.

**Aliphatic electrophilic substitution** : SE1, SE2, and SEi mechanism-effect of substrate structure, leaving groups, attacking electrophiles and solvent-Stark-Enamine reaction-decarboxylation of aliphatic acids- halogenation of aldehydes and ketones.

**UNIT - II**

**Aromatic electrophilic substitution** : Aromatic ion mechanism-orientation and reactivity- nitration, halogenation, friedel Craft reaction-Gattermann, Kolbe-Schmidt , Reimer-Tiemann, Hauben-Hoesch reactions.

**Aromatic Nucleophilic substitution:** SNAr, SN1, benzyne, SRN1 mechanisms – effect of substrate structure, leaving groups, attacking nucleophiles and solvents – selected reactions – Zeigler alkylation, Chichibabin reaction- reactions involving diazonium group as leaving group – cine substitution – von Richter reaction.

**UNIT – III****Elimination Reactions**

E<sub>1</sub>, E<sub>2</sub>, E<sub>1</sub>CB and E<sub>i</sub> – Mechanism – Stereochemistry of Eliminations – Hoffman and Saytzeff rules, competition between elimination and substitution reactions – Chugaev reaction dehydration of alcohols, dehydrohalogenation – Hoffman degradation. Cope elimination – Bredt's rule.

**Reagents in Organic Syntheses:** Complex metal hydrides – LiAlH<sub>4</sub>, NaBH<sub>4</sub>, tri tert-butoxyaluminium hydride, Gilman's reagents, Lithium dimethylcuprate, lithium di-isopropyl amide, dicyclohexylcarbodiimides, 1,3-dithianestrimethyl silylodide, DDZ, SeO<sub>3</sub> – phase transfer catalyst, Crown ethers and Merrifield resins.



## UNIT – IV

### Addition Reactions

Addition to carbon – carbon multiple bonds – electrophilic addition, Nucleophile and free radical addition, orientation and reactivity – Birch reduction, hydroxylation, hydroboration, epoxydation, Diels – Alder reaction, Michael addition ozonolysis, carbenes and their addition to double bonds.

**Addition to carbonyl groups:** Mannich, Crossed Cannizzaro, Stobbe, Benzoin condensation, formation of ketenes. Oppenauer Oxidation, MPV reduction, Darzen'sglycidic ester condensation. Wittig reaction.

## UNIT –V

### Oxidation and Reduction

Oxidation with chromyl chloride, periodic acid, Selenium dioxide, lead tetra acetate. Osmium tetroxide and H<sub>2</sub>O<sub>2</sub>. **Reduction**-Catalytic hydrogenation and dehydroxylation selection in reduction. Clemmensen reduction, Wolf – Kishner reduction, reduction with LiALH<sub>4</sub>, NaBH<sub>4</sub>, Tri tertiary butoxyaluminium hydride, sodium cyanoborahydridetrialkyl tin hydride, hydrazines.

**Molecular Rearrangements:** Mechanism of the following- wagnerMeerwin-Dienone phenol- Wolf-Lozson-Schmidt-Bayer Villiger-Stevens-Wittig-Favoraski rearrangements.

### Course outcome:

*Student understood the knowledge about:*

1. Aliphatic nucleophilic substitution reactions
2. Aliphatic electrophilic substitution reactions
3. Aromatic electrophilic substitution reactions
4. Aromatic nucleophilic substitution reactions
5. Elimination reactions and reagents in organic syntheses
6. Addition Reactions and Addition to carbonyl groups
7. Applications of oxidation and reduction reagents
8. Molecular Rearrangements

### References

#### Unit-I & II

1. Advanced organic chemistry – F.A. Carey and R.J. Saundberg, Plenum
2. A guide book to mechanism in organic chemistry – Peter sykes, Longman
3. Structure and mechanism in organic chemistry – C.K. Ingold, Cornell University press.

#### Unit-III

4. Principles of organic synthesis – R.O.C.Norman and J.M.Coxcon, blackie academic and professional.
5. Reaction mechanism in organic chemistry – S.M. Mukherji and S.P.Singh Macmillan.

**Unit-IV**

6. Spectrometric identification of organic compounds – R.M.Silverstein, G.C.Bassler and T.C.Morrill, John wiley.
7. Application of spectroscopy of organic compounds – J.R. Dyer, Prentice Hall

**Unit-V**

8. Raj K Bansal, Organic reaction mechanisms 3<sup>rd</sup> edition.
  9. Jerry March, Advanced organic chemistry, Reaction Mechanism and structure, 4<sup>th</sup> Edition.
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**Course Outcome Vs Programme Outcome**

	<b>PO1</b>	<b>PO2</b>	<b>PO3</b>	<b>PO4</b>	<b>PO5</b>	<b>PO6</b>	<b>PO7</b>
<b>CO1</b>	9	6	6	6	9	6	6
<b>CO2</b>	9	6	6	6	9	6	6
<b>CO3</b>	9	6	6	6	9	6	6
<b>CO4</b>	9	6	6	6	9	6	6
<b>CO5</b>	9	6	6	6	9	6	6

**Level of correlation: 9 – High; 6 – Medium; 3 – Low; and 0- no correlation.**

**SUBJECT CODE: 18PCH11**

**6 Hrs / 5 Credits**

**CC-XI – PHYSICAL CHEMISTRY – III**

**Course objectives:**

1. *To study about the activity of ions*
2. *To know about the electro-kinetic phenomena*
3. *To study about the electro-analytical methods*
4. *To study about thermal methods of analysis*
5. *To learn the computer applications in chemistry*

**UNIT – I**

**Ionics**

**Transport of ions** in solution- Debye-Huckel theory- radius of ionic atmosphere and its calculation - Debye-Huckel-Onsager equation modification – asymmetry and electrophoretic effect – evidences for ionic atmosphere - Falkenhagen and Wien's effects- extension to Debye Huckel Onsager theory-

**Activity of ions** in solution- Experimental determination- Debye-Huckel limiting law (derivation, verification and modification) - activity coefficient at higher conc- Bjerrum model.

**Electrode- Electrolyte equilibrium**- Nernst equation- and its limitations- equilibrium electrode potentials- classification of electrodes- concentration cells- liquid junction potentials- thermodynamic quantities from EMF data.

**UNIT – II**

**Electrokinetic phenomena**

**Electrokinetic phenomena:** Theories of electrical double layer - Electrical double layer potential- theory of multiple layers at electrode electrolyte interface- double layer capacity- electrokinetic phenomena- zeta potential- electro osmosis- sedimentation potential

**Processes at the electrodes**- the rate of charge transfer- exchange current density- Butler-Volmer equation- Tafel equation-

**Electrocapillary phenomena:** Electrocapillary curves – ECM. Lippmann equation and Lippman potential –Capillary electrometer – contact angle method.

**Electrochemical energy**- Storage systems- primary and secondary batteries- fuel cells.

**UNIT – III**

**Electro Analytical Methods**

Polarography: Principle, experimental technique – dropping mercury electrode – Residual, migration and diffusion currents – Half-wave potential – Ilkovic equation –

Analytical applications of polarography – Differential pulse polarography, cyclic voltametry – principle, experimental setup – application – Amperometric titration – principle and types – Titration between  $Pb^{2+}$  and  $K_2Cr_2O_7$ . electrogravimetry – theory of electrolysis, experimental set up diagram- applications – ion selective electrodes: principle and applications – DSC: Principle and applications – TMA: Principle and applications

#### UNIT – IV

##### Thermal methods of Analysis

Thermal methods of analysis – Principle – instrumentation – methods of obtaining thermogram- TGA curves for  $AgNO_3$ ,  $CuSO_4$ ,  $CaC_2O_4 \cdot H_2O$  Differential thermal analysis – Principle – instrumentation – DTA curves for the above compounds. Factors influencing DTA- applications of DTA. Study of Organic reactions, Decomposition of complexes, Thermometric titration.

#### UNIT – V

##### Computer in chemistry

C programming – structure of a C program – Data types, variables, constants, keywords, operators, expressions. Control structure – if, if-else, nested if-else, while, while-do, for, nested for, go to, continue, break, switch case statements. Arrays – user defined functions (recursion, call by value and call by reference) – string functions – preprocessors – storage class – structure, union. Pointer expressions, arithmetic passing pointers through arrays and functions – file handling, introduction to loops. C programming – simple applications to chemistry.

##### Course outcome:

*Student understood the knowledge about:*

1. *Transport of ions in solution*
2. *Nernst equation and its limitations*
3. *Theories of electrical double layer and theory of multiple layers*
4. *Primary and secondary batteries and energy storage system*
5. *Analytical applications of polarography*
6. *Electro-gravimetric analysis and its applications*
7. *Applications of Thermo-gravimetric method*
8. *C programming applications to simple chemistry problems*

##### References

##### Unit-I & II

1. Bockris J O M and Reddy A K N, Modern electrochemistry Volumes I & II. New York, Plenum Press, 1970.
2. Glasstone S An introduction to electrochemistry, New Delhi, East – West Press Pvt. Ltd., 1956

##### Unit-III

3. Noel M and Vasu K I, Cyclic Voltametry and the frontiers of electrochemistry, Oxford & IBH, 1990
4. F.W. Fifield and D. Kealey, —Principles and practice of Analytical Chemistry, Blackwell Publishing, Fifth Edition, 2000.
5. 2. J.S. Fritz and G.H. Scheink, —Quantitative Analytical Chemistry, Allyn and Bacon, Inc., Boston, Fifth Edition, 1987.

**Unit-IV**

6. 3. G.D. Christian, Analytical Chemistry, John Wiley and Sons, Inc., Fifth Edition, 1994.
7. 4. D.A. Skoog, D.M. West, F.J. Holler and S.R. Crouch, —Fundamentals of Analytical Chemistry, Thomson-Brooks.Cole, Eighth Edition, 2004.
8. 5. H.H. Willard, L.L Merritt, J.A. Dean and F.A. Settle, Jr., CBS Publishers and Distributors, New Delhi, Sixth Edition, 1986

**Unit-V**

9. E.Balagurusamy, Programming in C, Tata McGraw Hill, New Delhi.

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**Course Outcome Vs Programme Outcome**

	<b>PO1</b>	<b>PO2</b>	<b>PO3</b>	<b>PO4</b>	<b>PO5</b>	<b>PO6</b>	<b>PO7</b>
<b>CO1</b>	9	6	6	3	9	9	6
<b>CO2</b>	9	6	6	3	9	9	6
<b>CO3</b>	9	6	6	3	9	9	6
<b>CO4</b>	9	9	6	3	9	6	6
<b>CO5</b>	9	6	6	3	9	3	6

**Level of correlation: 9 – High; 6 – Medium; 3 – Low; and 0- no correlation.**

**CC-XII –ORGANIC SPECTROSCOPY****Course objectives:**

1. To understand the UV-Visible spectroscopy and ORD-CD
2. To learn the Infra Red spectroscopy and Raman spectroscopy for organic molecules
3. To know about Proton NMR spectroscopy
4. To learn the difference between the  $^1\text{H}$  NMR and  $^{13}\text{C}$  NMR
5. To understand the mass fragmentation arrangements by mass spectrometry method

**UNIT – I****UV – VIS and ORD – CD**

**UV – VIS:** Laws of light absorption – chromophores and auxochromes – types of electronic transitions – bathochromic, hypsochromic, hypochromic and hyperchromic effects; Applications of UV – VIS spectroscopy – use of model compounds and additivity – dienes, polyenes and  $\alpha$ ,  $\beta$  – unsaturated carbonyl compounds – Woodward – Fieser rules – Calculation of  $\lambda_{\text{max}}$  for organic molecules; absorption spectra of polyenes, polyenyenes and aromatic compounds; stereochemical factors in electronic spectroscopy;

**ORD – CD:** Definition – circular birefringence and circular dichroism; plain dispersion curves and their applications; single and multiple cotton effect curves; structural and stereochemical applications – axial haloketone rule, octant rule for ketones; comparison of ORD and CD.

**UNIT – II****IR and Raman**

**IR :** Molecular vibrations – stretching and bending vibrations, Hooke's law – Overtone and combination band; Factors influencing vibrational frequencies – effect of substituents, conjugation, distortion, geometry, hydrogen bonding – Fermi resonance; Characteristic group frequencies of organic molecules; interpretation of IR spectra of organic molecules.

**Raman :** Theory, application of Raman spectra to organic, inorganic and biological species, quantitative applications, Resonance Raman spectroscopy.

**UNIT – III** **$^1\text{H}$  NMR**

Origin – relaxation and saturation; Chemical shift, factors influencing chemical shift; magnetic equivalence – homotopic, enantiotopic and diastereotopic protons; spin – spin

coupling – Criteria for first order and non – first order spectra – representation of non-equivalent hydrogens by alphabets; geminal, vicinal and long range couplings – Karplus equation – NMR of simple AX and AMX type organic molecules, identification of H in various chemical environments to assign structure to the organic molecules using chemical shift values and coupling. Simplification of spectra – high fields, deuterium exchange, shift reagents – satellite spectra – multiple resonance – spin decoupling, spin tickling and INDOR.

## UNIT – IV

### <sup>13</sup>C NMR

<sup>13</sup>C NMR : Distinction between <sup>1</sup>H and <sup>13</sup>C NMR – theory and experiment – factors affecting intensity of signals – nuclear Overhauser effect – chemical shift and its dependence on polar and steric effects (gamma gauche effect); additivity relationships - C-C and C-H couplings – off resonance, gated and single frequency decouplings – relationship between coupling constant and ‘s’ character; effect of shift reagents on <sup>13</sup>C chemical shifts; applications of <sup>13</sup>C NMR to find the different carbon functional groups. COSY,NOESY, ROSY,CIDNP and INDOR.

## UNIT – V

### Mass spectrometry

Introduction, ion production – EI, CI, FD and FAB, factors affecting fragmentation, Ion analysis, ion abundance. Mass spectral fragmentation of organic compounds. Common functional groups, molecular ion peak, meta stable peak, McLafferty rearrangement. Nitrogen rule. High resolution mass spectrometry. Examples of mass spectral fragmentation of organic compounds with respect to their structure determination.

### Course outcome:

*Student understood the knowledge about:*

- 1. Woodward – Fischer rules and calculation of  $\lambda_{max}$  for organic molecules*
- 2. Structural and stereo-chemical applications and comparison of ORD and CD*
- 3. Interpretation of IR spectra of organic molecules*
- 4. Application of Raman spectra to organic, inorganic molecules and biological species*
- 5. Identification of H in various chemical environments to assign structure to the organic molecules*
- 6. Applications of <sup>13</sup>C NMR to find the different carbon functional groups*
- 7. Applications of 2D and 3D NMR spectrum*

8. *Mass spectral fragmentation of organic compounds with respect to their structure determination*

**References**

**Unit-I & II**

1. William Kemp, Organic Spectroscopy, ELBS II Edition, Spectroscopy of organic compounds.
2. P.S. Kalsi, Organic Spectroscopy, Wiley Eastern Ltd, Madras.
3. C.Djerassi, Optical rotatory dispersion – application to organic chemistry, McGraw Hill, 1960.

**Unit-III & IV**

4. R.M. Silverstein, C.G. Bassler and Monsil, Spectrometric identification of organic compounds, John Wiley & Sons, New York.
5. J. Dyer, Application of absorption spectroscopy of organic compounds, Prentice Hall of India Pvt. Ltd., New Delhi.
6. W.Kemp, NMR in Chemistry, MacMillan Ltd, 1986.
7. J.B. Lambert, H.F. Shunnel, L. Verbit, R.G. Cooks and G.H. Stout, Organic structural analysis, MacMillan, 1976.
8. G.C. Levy and G.L. Nelson, Carbon – 13 Nuclear Magnetic Resonance for organic chemists, Wiley – Interscience, 1972.
9. R.J. Abraham and P. Loftus, Proton and carbon – 13 spectroscopy, Heydon & Sons., 1978.

**Unit-V**

10. R.A.W. Johnstone, Mass spectrometry for organic chemists, Cambridge, 1972.
11. M.C. Hamming and N.G. Foster, Interpretation of Mass spectra of organic compounds, Academic Press, 1972.
12. D.H. Williams and I.Fleming, Spectroscopic methods in organic chemistry, Tata McGraw Hill, 4th Edition, 1988.

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