

# **KARPAGAM ACADEMY OF HIGHER EDUCATION**

Deemed to be University

(Established Under Section 3 of UGC Act 1956)

EachanariPost, Pollachi Main Road,

Coimbatore -641021



## **COURSE OF STUDY & SCHEME OF EXAMINATION**

### **M.Phil. & Ph.D. COURSE IN CHEMISTRY**

**2017- 2018**

**Part-I Course Work Syllabus for M.Phil and Ph.D Chemistry**

<b>Subject Code</b>	<b>Title of the Course</b>	<b>Credit</b>	<b>Exam Hours</b>	<b>Marks</b>
<b>Paper-I(Compulsory)</b>				
17RCH101	Research Methodology and Pedogogy	4	3	100
<b>Paper-II(Compulsory)</b>				
17RCH201	Physical Methods in Chemistry	4	3	100
<b>Paper-III(Any One)</b>				
17RCH301 A	Organic Chemistry	4	3	100
17RCH301B	Physical Organic chemistry	4	3	100
17RCH301C	Electro Chemistry	4	3	100
17RCH301D	Environmental Chemistry	4	3	100
17RCH301E	Chemistry of Crystalline solids	4	3	100
17RCH301F	Organometallic Chemistry of Transition metals	4	3	100
17RCH301G	Chemistry of Biomolecules	4	3	100
17RCH301H	Polymer Chemistry	4	3	100

**Part I – M. Phil./ Ph.D.,**

**CHEMISTRY**

**Paper-I: Research Methodology and Pedagogy (Effective from the academic year 2017-2018 and onwards)**

**Course Objective:**

- To learn and practice the literature survey aspects of projects and prepare the scope and goals for the proposed project.
- To learn, practice and improve the research presentation skill and with latest tools
- To learn and understand the research publication ethics
- To learn the tools like LaTeX
- To understand the error analysis
- To learn the emission spectroscopy

**Course Outcome:**

1. Enable the student potential to organize, coordinate and focus research aptitude with confidence
2. Improve the awareness on indexing, quality evaluation, author index of publications
3. Improve the presentation skills through seminars
4. Expertise in LaTeX tool for report preparation
5. Understood the error analysis
6. Learnt the emission spectroscopy

**UNIT I**

Research Methodology - Objectives of Research - Types of Research - Criteria for good Research . Defining the Research Problem - Research Design. Dissertation writing- Guidelines for review of literature - Materials and methods, results and discussion. Interpretation of results, presentation of results, summary, presentation of references and appendix. Use of Computers in Research – Data base Operations like creation – updating – indexing/sorting and searching of data, data entries and analysis, graphical applications.

**UNIT II**

Data Analysis: Errors in chemical analysis - classification of errors – determination of accuracy of methods - improving accuracy of analysis - significant figures - mean, standard deviation-comparison of results : “t” test, “f” test, and “chi” square test – rejection of results-presentation of data.Sampling – introduction – definitions - theory of sampling-techniques of sampling - statistical criteria of good sampling and required size - stratified sampling vs random sampling – minimisation of variance in stratified sampling – transmission and storage of samples.

### **UNIT III**

Definition of problem: Necessity of defining problem, Technique involved in defining a problem. Surveying the available literature. Building up of own literature collection, citation techniques.

Research Design: Subject of study; Place of study; Reason of such study; Type of data required; Method of data collection; Periods of study; Style of data presentation.

Developing a research plan: Research objective; Information’s required for solving the problem; Different methods used to solve a problem.

Publication of Journal Articles: Concept, types of journals, components of a journal article, preparation of the manuscript, from manuscript to publication and online submission.

Submission of Research Proposals: Leading funding agencies in India, Submission of research project proposals with prescribed formats.

### **UNIT IV**

Flame emission and atomic absorption spectroscopy and Fluorometric Analysis: Types of atomic spectroscopy – emission methods - absorption methods - fluorescence methods - applications of atomic emission spectroscopy – flames and flamespectra. Fluorescence and phosphorescence – applicationoffluorometricanalysis.

HPLC and Gas Chromatography:Theory of chromatography - detectors - Application of gas/mass analysis. Principles of high performance liquid chromatography - gradient elution, isocratic elution, sampling detectors for liquid chromatography - quantitative analysis by HPLC.

### **UNIT V**

Pedagogical Methods in Higher Education Objectives and roll of higher education – Important characteristics of an effective Lecture – Quality teaching and learning – Lecture preparation – Characteristics of instructional design – Methods of teaching and learning : Large group – Technique – Lecture, Seminar, Symposium, Team Teaching, Project, Small group Technique – Simulation, role playing Demonstration, Brain storing, case discussion, and assignment, Methods

of evaluation – Self evaluation, student evaluation, Diagnostic testing and remedial teaching – Question banking – Electronic media in education: - ‘e’ learning researches – web based learning

### **References:**

1. J. D. Dick,(1973). Analytical chemistry. McGraw Hill, N.Y. also available in International students edition McGraw Hill, Mogakusha.
2. J.Dyer, (1965), Applications of absorption spectroscopy of organic compounds. Prentice- Hall, Englewood Cliffs,N.J
3. S.M Khopkar,(1998), Basic concepts of analytical chemistry, New Age International, New Delhi
4. B. K. Sharma.(2000),Instrumental methods of chemical analysis, Krishna Prakashan Media,2000
5. Skoog.D.A and M. West.(2006), Principles of instrumental analysis, Brookes Cole Publishers,Caleifornia
6. Willard.H, L. Merrit Jr and A. Dean.,Instrumental methods of analysis
7. Vedanayagam, E.G (1989) Teaching Technology for college teachers. NewDelhi: Sterling Publishers ( P)Ltd.,
8. Rajasekar.S (2005) Computer Education and educational computing.Hyderabad: NeelkamalPublications.
9. Kumar K.L. (1997) Educational Technologies, New Delhi: New age International.

**Part I – M. Phil./ Ph.D.,**

**CHEMISTRY**

**Paper-II: Physical Methods in Chemistry (Effective from the academic year 2017-2018 and onwards)**

**Course Objective:**

- To develop fundamental understanding of spectroscopic techniques - their origin from the interaction of radiation with matter.
- Principles and instrumentation of major spectroscopic techniques.
- Application of each spectroscopic technique for chemical structure characterization.
- Develop an ability to rationally exploit a variety of spectroscopic techniques for future research or industrial assignments.
- It is expected that at the end of this course students will be able to decipher the structure of reasonably complex molecules using spectroscopic techniques.
- To discuss about electron spectroscopy and thermal analysis

**Course Outcome:**

- Develop fundamental understanding of spectroscopic techniques - their origin from the interaction of radiation with matter.
- Principles and instrumentation of major spectroscopic techniques.
- Application of each spectroscopic technique for chemical structure characterization.
- Develop an ability to rationally exploit a variety of spectroscopic techniques for future research or industrial assignments.
- It is expected that at the end of this course students will be able to decipher the structure of reasonably complex molecules using spectroscopic techniques.
- Discussed about electron spectroscopy and thermal analysis

**UNIT I**

**U.V - Visible spectroscopy:**

Electronic excitation – origin of different bands - intensity of bands – selection rules – laws of photometry – correlation of electronic absorption with molecular structure – chromophoric groups – conjugated systems – systems of extended conjugation – aromatic systems – empirical rules – experimental methods – photometric methods – photometric titrations.

I.R. spectroscopy: Molecular vibrations – selection rules – force constant – band assignments – applications – organic structures – finger printing – identification of common functional groups – applications.

## UNIT II

<sup>1</sup>H and <sup>13</sup>C NMR spectroscopy: Proton chemical shifts – aromatic ring systems – anisotropic effects – <sup>13</sup>Carbon chemical shifts – mechanisms of spin - spin coupling – vicinal, geminal and long range proton – proton coupling.

Analysis of NMR spectra: Accumulation of spectra by the pulsed NMR technique – nuclear relaxation – Fourier transformation – the pulsed FT NMR spectrometer.

Double resonance technique and relaxation mechanisms: Homonuclear decoupling – heteronuclear decoupling – proton decoupling technique in <sup>13</sup>C spectrum – INDOR and Nuclear overhauser effect (NOE) – <sup>13</sup>C relaxation mechanisms – measurement of relaxation times – spin-lattice relaxation (T<sub>1</sub>) spin-spin relation (T<sub>2</sub>) measurements – assignment technique in <sup>13</sup>C spectra – chemical shift correlation quantitative measurement in <sup>13</sup>C – NMR – relaxation reagents – intensity standards.

## UNIT III

ESR Spectroscopy: Theory – instrumentation – derivative curves ‘g’ values – ‘g’ shift – origin of hyperfine splitting – isotropic systems – anisotropic systems – anisotropic effect zero field splitting – Kramers degeneracy – applications to organic and inorganic systems – identification of free radicals.

X-ray Photoelectron Spectroscopy: Introduction – Theory of XPS – Instrumentation – Applications of XPS to organic and inorganic systems.

## UNIT IV

Mass Spectrometry: Theory – instrumentation – various types of mass spectrometers – magnetic focusing instruments – sample handling – production and reactions of gaseous ions – isotopic abundance – determination of molecular weights and formulae – metastable peaks – nitrogen rule – ion fragmentation mechanisms – rearrangements – use of mass spectrometry in the structural elucidation of organic compounds – mass spectra of compounds containing different functional groups.

## UNIT V

Instrumental Methods Thermal Methods: Principle and applications of Differential Thermal analysis (DTA), Differential Scanning Calorimetry (DSC), Differential Thermal Gravimetry (DTG) and Thermo Gravimetry (TG). Effects of experimental conditions on the course of thermo analytical curves. Diffraction Methods: Fundamentals of X-Ray Diffraction- Powder and

Rotating crystal methods- use of X-ray powder diffraction data in identifying crystalline solids- details for cubic systems- Comparison of X- ray, neutron and electron diffractions. Nanoscale Characterization: Principle and applications of SEM and TEM.

#### References:

1. Becker .K.,(2000). High Resolution NMR. AcademicPress.
2. Cullity. B.D (1975). Introduction to X-Ray Diffraction. Addison-WesleyPublishers
3. Drago,R.S.(1965) Physical methods in Inorganic Chemistry. Reinhold Publishing Corporation.
4. Hamming and Foster (1972). Interpretation of Mass Spectra of Organic Compounds. AcademicPress.
5. McLafferty (1973). Interpretation of Mass Spectra. Published by BenjaminPress.
6. Raw.Johnstone (1975). Mass Spectrometry for Organic Chemistry. Published by The ChemicalSociety.
7. Scharz (1964).Physical methods in Organic Chemistry. Oliver & BoydPublishers.
8. Weilie Zhou., Zhong Lin Wang.(2006). Scanning Microscopy for Nanotechnology. SpringerPublishers.
9. West, A.R.(1985). Solid state Chemistry and its applications. Published by WileyDefault.



**Part I – M. Phil./ Ph.D.,  
CHEMISTRY  
Paper III: Special Paper I – Organic Chemistry (Effective from the academic year 2017-  
2018 onwards)**

**Course Objectives**

This course enables the students

- To understand theory of concerted reaction.
- To provide a versatile knowledge of different name reactions and their application in synthesis.
- To learn about familiar addition and elimination reactions.
- To gain knowledge about reaction intermediates.
- To understand the principles and reaction mechanisms involving various electrophilic and nucleophilic, addition and elimination reactions.
- To relate the different organic reaction mechanisms.

**Course outcomes (CO's)**

On the completion of this course, students should have to

1. Learned the concept theory of concerted reactions.
2. Familiarized the various types of electrophilic and nucleophilic substitution reactions and their Mechanism
3. Learned the familiar addition and elimination reactions
4. Learned the concept of reaction intermediates.
5. Understood about synthesize aromatic compounds using electrophilic and nucleophilic substitution, addition and elimination reactions.
6. Described the various organic reaction mechanisms.

**UNIT I**

Theory of Concerted Reactions: Definitions - molecular orbitals – frontier orbitals – frontier orbital approach – correlation diagrams – the aromatic transition state concept – general rule for pericyclic reactions.

Electrocyclic Reactions: Definition – thermal electrocyclic reactions – photochemical electrocyclic reactions – metal catalysed electrocyclic reactions.

Cycloadditions: Introduction – selection rules for thermal polyene cyclo additions – Diels – Alder reaction – The retro diels – alder reaction – 1,3 Dipolar cycloadditions – Retro 1,3 – dipolar additions.

**UNIT II**

Modern reagents in Organic synthesis: Sodium cyanoborohydride – osmium tetroxide – lithium dimethyl copper – thallium trifluoro acetate – sodium hydrogen telluride – silver hexa fluorantimonate – Thiobenzoyl chloride – trichloro silane- vanadium oxytrifluoro – phosphonitrile chloride – ruthenium tetroxide – barium manganate – benzene selenic acid – benzene selenyl

bromide/chloride, aluminium chloride/phosphoryl chloride.

### UNIT III

Stereochemistry, Conformational Analysis & Retrosynthetic analysis Stereoselective, stereospecific and regiospecific reactions – stereoselectivity in carbonyl addition- Cram's rule – configuration – conformation – torsional strain – Vander waals strain – gauche interaction – allylic strain – conformation analysis of acyclic molecules. Retrosynthetic Analysis of Simple Organic compounds: Retrosynthetic analysis of mono & difunctional open chain target molecules and monocyclic target molecules.

### UNIT IV

Chromatography: Theory, Instrumentation & application in the chemical analysis of column, paper, thinlayer, ion-exchange, Gas chromatography (GC) and High Pressure Liquid Chromatography (HPLC).

Natural products: Extraction, Isolation and structural elucidation (using spectroscopic methods) of terpenes, steroids, alkaloids and phenolic compounds.

### UNIT V

Problem solving: Solving the structure of simple organic molecules on the basis of UV, IR, NMR & Mass spectral data. (restricted to organic compound compounds having 12 carbon atoms).

### References:

1. Agarwal O.P, (2004). Natural Product Chemistry, Vol. I, Goel Publishing House, Meerut
2. Agarwal O.P, (2004). Natural Product Chemistry, Vol. II, Goel Publishing House, Meerut
3. Mackie R.K. and D.M.Smith, 1982. "Guide book to Organic Synthesis", ELBS,
4. Reagents for Organic synthesis – Feiser & Feiser Vols. I –XII.
5. Silverstein and Webster, 1998. "Spectrometric Identification of Organic Compounds", 6th Ed., Wiley
6. Skoog D.A. and D.M. West, (2004). Fundamentals of Analytical Chemistry, 8th Edition, Thomson book store, Singapore
7. Usharani S., (2002). Analytical Chemistry, Mac Millan India Ltd., Chennai

**Part I – M. Phil./ Ph.D.,**

**CHEMISTRY**

**Paper III: Special Paper II – Physical Organic Chemistry (Effective from the academic year 2017-2018 onwards)**

**Course Objectives**

On successful completion of the course the students should have

- To know about versatile knowledge of rearrangements
- To understand the different organic (radical and concerted) reactions and their applications in synthesis.
- To learn about unimolecular and bimolecular surface reactions and LFER
- To explain the concepts in organic photochemistry
- To describe the basic ideas about pericyclic reactions
- To implement this basic concept to design and produce the new organic molecules

**Course outcomes (CO's)**

1. Understood the versatile knowledge of rearrangements
2. Understood the different organic reactions (radical and concerted).
3. Learned about the unimolecular and bimolecular surface reactions and LFER
4. Explained about the molecular rearrangements, Pericyclic reactions and Cyclo addition and sigmatropic reactions
5. Described the basic ideas of pericyclic reactions.
6. Designed new form of organic compounds using these basic concepts.

**UNIT-I**

Theories of Reaction Rates:

Absolute reaction rate theory – thermodynamic treatment of ARRT – Significance of reaction co- ordinate – application of ARRT to simple unimolecular and bimolecular process –potential energy surfaces – partition functions and activated complexes. Eyring equation, estimation of free energy, enthalpy and entropy of activation and their significance – kinetic isotopic effect.

Homogeneous catalysis

Acid – Base catalysis – Hammett acidity function, Bronsted relationship – enzyme catalysis – mechanism of single substrate reactions – Michaelis – Menten law-influence of pH and temperature.

**UNIT II**

2.1 Reaction in solution

Introduction – Unimolecular & Bimolecular surface reaction (Langmuir & Freundlich adsorption isotherm only)- application of ARRT to solution kinetics – the influence of solvent- the ionization of neutral molecules - kinetics of ionization- primary and secondary salt effect.

## 2.2. Oxidation & Reduction

Oxidation with chromium and manganese compounds – Oxidation with per acids and other peroxides – oxidation with periodic, lead tetra acetate, mercuric acetate – selenium dioxide.

Catalytic hydrogenation and dehydrogenation metal hydride reductions and related reactions dissolving metal reductions and related reactions-reductions and the hydroactive and its derivatives.

## UNIT III

### Quantitative structure and Reactivity Relationships

The linear free energy principle – (LFER) linear relationship involving difference reaction - the cettler correlation. The Hammett equation – steric effects – resonance interaction – normal substituent constants  $-\sigma$  - ,  $\sigma$  + constants – inadequacy of dual hypothesis – regularities in through resonance effect – the Yukawa Tsuno equation – systematic deviation – steric inhabitation of resonance – Taft equation – correlation of aliphatic and aromatic relativities.

## UNIT IV

Photo Organic chemistry: Light absorption – unimolecular photo physical processes – Jablonski diagrams –radioactive transitions – internal conversion – intersystem crossing – energy pooling – excimers and exciplexes.

Photochemical reactions: Introduction –cis – trans Isomerisation – Norrish type I reaction – Norrish type II reaction – Thermal generation of excited states. Zimmerman rearrangement,photochemical rearrangement of enones. photorearrangement of cyclohex – 2 – enones – rearrangements of 2 – cyclopentenones and related compound.

## UNIT V

### Theory of Concerted Reactions:

Definitions – molecular orbital – frontier orbital – frontier orbital approach –correlation diagrams – the aromatic transition state concept – general rule for pericycle reactions.

### Electro cyclic Reactions:

Definition – thermal electro cyclic reactions – photochemical electro cyclic reactions – metal catalyzed electro cyclic reactions.

Cycloadditions:

Introduction – selection rules for thermal polyene cyclo additions – Diels – Alder reaction

– The retro diels – alder reaction – 1,3, - Dipolar cycloadditions – Retro – 1,3 – dipolar cyclo additions.

### References:

1. Gilchrist, P.L., and R.C. Storr (1972). Organic Reactions & Orbital Symmetry. CUP Archive Publishers.
2. Laidler, K.J., (1975). chemical kinetics, 2nd Ed. Tata Mc. Graw Hill.
3. Louis P. Hammett, Physical organic chemistry, Mc. Graw Hill Ltd., Tokyo.
4. Moore, W.J., (1982). Physical chemistry 5th Ed. Orient Longman.
5. Rastoghi K.K., Mukherjee, (1978). Fundamentals of photo chemistry, Wiley Eastern.
6. Thomas, H. Lowry, Kathleen S. Huettenlocher, Richard, Horper, and Rao (1986).
4. Mechanism and Theory in Organic Chemistry. Published by Macmillan.
5. Woodward, and Hofman (1971). The Conservation of Orbital Symmetry. Published by Verlag Chemie.

**Part I – M. Phil./ Ph.D.,**

**CHEMISTRY**

**Paper-III: Special Paper III-Electrochemistry**

**(Effective from the academic year 2017-2018 and onwards)**

**Course Objectives**

This course enables the students

- To provide knowledge on fundamental understanding of chemical kinetics and to establish a relationship between the rate of reaction and the concentration of the reactants (the rate law, or rate equation).
- To apply the chemical kinetics concept to study the enzyme mechanisms.
- To provide knowledge to the students about coulometric methods and its application.
- To investigate the adsorption, classification of adsorption and factors affecting of adsorption over corrosion application.
- To remember the basic polarography concepts.
- To understand the theories of catalysis and types of catalysis.

**Course outcomes**

On the completion of this course, students have to

1. Student understood theories of reaction rates, how reaction rates are measured and represented in rate laws.
2. Understood the applications of chemical kinetics in studying enzyme mechanisms
3. Provided the knowledge of coulometric methods and applications.
4. Evaluated the electrochemical principles involved in corrosion and energy storage.
5. Remembered the basic polarography techniques.
6. Understood the theories of catalysis and types of catalysis

**UNIT I**

Introduction and Principles:

Definition –Cost of corrosion-importance of corrosion studies-classification of corrosion–expressions for corrosion rate.Electrochemical principles of corrosion : Faraday’s laws –Types of electrochemical cells formed in corrosion process. thermodynamic principles of corrosion : Electrochemical series/ standard electrode potentials and thermodynamic corrosion theory- Galvanic series of metals and alloys and limitations. Forms of corrosion (Definition –cause and effects ) : Galvanic –Crevice –Pitting -Intergranular – Selective leaching –Erosion-Stress-Hydrogen damage.

**UNIT II**

Kinetics of Corrosion: Importance –Graphical presentation of kinetic data –exchange current density –different types of polarization of electrodes.Activation polarization and Tafel plots – Mixed potential theory – Application of electrode kinetics to experimental observations-Faradic impedance and corrosion.

### **UNIT III**

Kinetics of Passivity: Introduction-electrochemical behaviour of active/passive metals-Flade potentials-criteria for selecting a metal exhibiting passivity-effects of various factors on electrochemical behaviour and corrosion rate of metal exhibiting passivity-measured versus theoretical anodic polarization behaviour-Theories of passivity.

### **UNIT IV**

Monitoring of Corrosion: Determination of corrosion and corrosion inhibition parameters-Non-electrochemical methods:Coupon-Electrical resistance-Gasometric methods:Electrochemical methods: Polarisation-Galvanostatic-Potentiostatic –Potentiodynamic-AC impedance-Hydrogen permeation.

### **UNIT V**

Corrosion control: Metals and alloys-metal purification-non metallic-cathodic and anodic protection – comparison.Alteration of environment : Changing the medium –use of inhibitors-classification of inhibitors –mechanism of inhibition-Coating (Elementary ideas only).

### **References:**

1. Herbert H.Uhlig and Winston Review.R. (1984). Corrosion and Corrosion control(An introduction to corrosion science and engineering) ,Third Edition,A Wiley Interscience Publication, NewYork.
2. Mars Fontana G. (1984).Corrosion Engineering, Third Edition, Mc.Graw HillBook Company,Singapore.
3. Mercer A.D. (1985).Test methods for corrosion inhibitors , J.Corr.Science,85.
4. Raj Narayan.P. (1983).An introduction to metallic corrosion and its prevention,Oxford and IBH Publishing C., NewDelhi.
5. Schmitt G. (1984). Application of inhibitors for acid media ,Corros.J,73.

**Part I – M. Phil./ Ph.D.,**  
**CHEMISTRY**  
**Paper-III: Special Paper IV-Environmental Chemistry**

**(Effective from the academic year 2017-2018 and onwards)**

**Course Objectives**

The course enables the students to

- Understand the industrial gases and inorganic chemicals which have an impact on the environment.
- Study about the general principles of metallurgy.
- Learn the environment and its segments.
- Discuss about the water pollution and water treatment.
- Explain the application of bio-catalysis in energy saving techniques.
- Apply this technique to design energy saving devices with eco-friendly method.

**Course Outcomes**

The course enables the students to

1. Understood the industrial gases and inorganic chemicals which have an impact on the environment.
2. Studied about the general principles of metallurgy.
3. Learned the environment and its segments.
4. Discussed about the water pollution and water treatment.
5. Explained the application of bio-catalysis in energy saving techniques.
6. Applying this technique to design energy saving devices with eco-friendly method.

**UNIT-1**

Chemistry of Water and Waste water:

Basic principles and their significance with special reference to colour, turbidity, alkalinity, acidity, chemical coagulation, hardness, water softening, disinfection, residual chlorine and chlorine demand, dissolved oxygen, biochemical oxygen demand, chemical oxygen demand, nitrogen, phosphate, sulphate, gas analysis, enzymes, factors affecting enzyme activity, bio-chemistry of carbohydrates, proteins, fats and oils under aerobic and anaerobic conditions, detergents and their degradation, composition and characteristics of sewage.

**UNIT II**



## Chemistry of air pollutants-I

Introduction, definition, classification of air pollutants, effect of air pollutants on man, materials, animals and plants, ambient air quality standards, harmful concentrations, geographical and meteorological factors in air pollution control, measurement of gas flows, volume, quantity and velocity.

## UNIT III

### Chemistry of air pollutants-II

Methods of sampling, particulate collection by liquid scrubbing, centrifugal spray scrubbers, venturi scrubbers, foam scrubbers; field sampling techniques such as deposition, absorption, filtration, condensation, adsorption, adhesion, electrostatic precipitation, thermal precipitation, analysis of air pollutants such as particulates sulphur dioxide, carbon monoxide, oxides of nitrogen, hydrogen sulphide, etc., control measures.

## UNIT IV

Chemistry of solid wastes: Chemistry of composting: mechanism involved in the decomposition of organic materials like hemicellulose, proteins, carbohydrates, food materials, organic insecticides, farm wastes, etc., by aerobic and anaerobic processes.

## UNIT V

Chemistry of Incineration and Pyrolysis: Incineration; definition; Incineration of solid waste; combustion characteristics of various inorganic and organic materials; heating values-determination of heating values of combustible liquid and solid wastes; air requirement for combustion; fate of trace constituents such as sulphur during incineration; gaseous pollutants; definition of pyrolysis; chemical changes taking place in organic and inorganic materials during pyrolysis; importance of pyrolysis in the solid waste disposal; chemistry of recycling of solid waste; recycling and reuse of materials such as paper, plastic, glass, etc.

## References:

1. American Public Health Association Inc., New York, (1976). Standard methods for the examination of water and wastewater.
2. Hagerty, D.J., J.L. Pavoni and J.E. Heer, (1973). Jr., Solid waste management, Van Nostrand Reinhold Co., New York.
3. Jacobs, M.B., (1960). Chemical analysis of Air pollutants, Interscience, New York.
4. Leithe, W. (1971). Translated by R. Kenor, The analysis of air pollutants, Ann Arbor
5. Ross, R.D., (1972). Air pollution and Industry, Van Nostrand Reinhold Co., New York

6. Sawyer, C.N. and P.L. McCarty, (1978). Chemistry of Environmental Engineers, McGraw Hill Publishers.
7. Stern, A.C., Ed., (1968). Air pollution, Vol. 1, 2 and 3, Academic press, New York.
8. Strauss, W. Ed., (1978). Air pollution control, part 1, 2 and 3, Wiley Interscience, New York,
9. Stumm, W. and J.J. Morgan, (1972). Aquatic Chemistry, Wiley Interscience.
10. Wilson, D.G., (1977). Hand book of solid waste management, Van Nostrand Reinhold Co., New York.

**Part I – M. Phil./ Ph.D.,**  
**CHEMISTRY**  
**Paper-III: Special Paper V- Chemistry of Crystalline solids**  
**(Effective from the academic year 2017-2018 and onwards)**

**Course Objectives**

The course enables the students to

- To understand the crystal system
- To learn about X-ray diffraction studies
- To know about crystal phenomena
- To understand the various types of solids and its properties
- To learn about conductors and insulators
- To gain knowledge about phase transition and its classification and transformations.

**Course Outcomes**

The course enables the students to

1. Understood the crystal structure
2. Learnt about X-ray diffraction studies
3. Knowledge about crystal phenomena
4. Understand the various types of solids and its properties
5. Learnt about conductors and insulators
6. Gained knowledge about phase transition and its classification and transformations

**UNIT I**

The crystal systems – lattices and crystal structures – symmetry properties – crystal classes – space groups – experimental methods of X-ray diffraction for powder and singlecrystal samples – structural analysis and refinement – electron and neutron diffraction in the determination of structures.

**UNIT II**

Crystal growth phenomena – introduction – nucleation – theories of nucleation – classical theories of nucleation – Gibbs Thomson equation for vapour – modified Thomson's equation for melt – Gibbs Thomson's equation for solution – energy of formation of a nucleus – spherical nucleus – cylindrical nucleus – heterogeneous nucleation – cap shaped nucleus, disc shaped nucleus.

**UNIT III**

Types of solids – close packing of spheres – binding in crystals – the bond model – non-stoichiometry – defects in solids – imperfection and physical properties – electrical, optical, magnetic and mechanical properties – magnetic materials – mixed oxides – spinels, insulators – semiconductors and superconductors.

#### UNIT IV

Low temperature solution growth- solution, solubility and super solubility – expression of super saturation – methods of crystallization – by slow cooling of solutions – by solvent evaporation – temperature gradient method. crystal growth system – constant temperature bath – crystallizer – filtration assembly – seed, seed mount platform and crystal revolution – unit – gel growth – introduction – principle of gel growth – various types of gel – structure of gel – growth of crystals in gels – importance of gel technique – experimental procedure – single diffusion method – double diffusion method – chemical reduction method – solubility reduction method – growth from the melt – Bridgman technique – Czochralski technique – zone refining.

#### UNIT V

Phase transitions – definition – Burger's classification – thermodynamic classification – Landau theory of phase transition – first order and second order transitions – structural changes with increasing temperature and pressure – martensitic transformations – order – disorder transitions. Thermal analysis – basic Principles – instrumentation – applications of thermogravimetry – differential thermal analysis and differential scanning calorimetry.

#### REFERENCES:

1. Anthony R. West (1987), Solid State Chemistry and its applications — John Wiley and Sons.
2. Azarov, L. V, (1960), Introduction to solids.
3. Chakrabarty, D. K, (1966) Solid State Chemistry — New Age international publishers
4. Charles Kittel, Principles of solid state Physics.
5. Cheetham A. K. and Peter Day (1991). Solid State Chemistry Techniques – Edited by – Oxford Science Publications.
6. Dent Glasser, L. S (1982) Crystallography and its applications — ELBS.
7. John Enemark, (1988) Introducing Chemists to X-ray Structure Determination, Journal of Chemical education, June.
8. Moore, W. J, (1962), Physical Chemistry.
9. Dr. Santhana Raghavan, P and Dr. P. Ramasamy, Crystal Growth Process and Methods – K. R. V. Publication

**Part I – M. Phil./ Ph.D.,**

**CHEMISTRY**

**Paper-III: Special Paper VI- Organometallic Chemistry of Transition metals**

**(Effective from the academic year 2017-2018 and onwards)**

**Course objectives**

This course enables the students

- To learn about nature of the bonding between organic ligands and metals.
- To understand about the metal alkyl complexes.
- To learn about the alkene and cyclopentadienyl complexes.
- To understand about the usage of organometallic compounds as catalysts
- To learn about the organometallic compound used as the catalyst in hydrogenation and hydroxylation of olefins.
- To study the concept of oxidation and polymerization of olefins.

**Course Outcomes**

On the completion of the course

1. Learned about the Alkyls and Arene complexes
2. Understood the bonding in olefin, acetylene and allyl systems
3. Known about the concepts of synthesis, structure and bonding in metallocenes
4. Understood the Organometallic reaction mechanisms and its applications
5. Learned about the Catalysis, hydrogenation of olefins and oxoprocess
6. Studied the concept of oxidation of olefins and polymerization

**UNIT I**

Definition of organometallic compound – 18 electron rule – effective atomic number rule – classification of organometallic compounds – the metal carbon bond types – ionic bond – sigma covalent bond – electron deficient bond – delocalised bond – dative bond – metal carbonyl complexes – synthesis, structure and reactions of metalcarbonyls – the nature of M-CO bonding – binding mode of CO and IR spectra of metal carbonyls – metal carbonyls – metal carbonyl anions– metal carbonyl hydrides– metal carbonyl halides – metal carbonyl clusters – Wades rule and isolobalrelationship – metal nitrosyls – dinitrogen complexes – dioxygen complexes.

**UNIT II**

Metal alkyl complexes – stability and structure – synthesis by alkylation of metal halides, by oxidative addition, by nucleophilic attack on coordinated ligands – metal alkyl and 18 electron rule – reactivity of metal alkyls – M-C bond cleavage reactions – insertion of CO to M-C bonds – double carbonylation – insertions of alkenes and alkynes – insertions of metals with C-H bonds – alkylidene and alkylidyne complexes – synthesis of alkylidene complexes in low oxidation states and in high oxidation states – bonding in alkylidene complexes – synthesis and bonding in alkylidyne complexes – reactivity of alkylidene and alkylidyne complexes.

Alkene complexes – synthesis of alkene complexes by ligand substitution, by reduction and by metal atom synthesis – bonding of alkenes to transition metals – bonding in diene complexes – reactivity of alkene complexes – ligand substitution – reactions with nucleophiles – olefin hydrogenation – hydrosilation – Wacker process – C-H activation of alkenes – alkyne complexes – bonding in alkyne complexes – reactivity of alkynes – alkyne complexes in synthesis – cobalt catalysed alkyne cycloaddition.

### UNIT III

Cyclopentadienyl complexes – metallocenes – synthesis of metallocenes – bonding in metallocenes – reactions of metallocenes – CpFe/Cp<sub>2</sub>Fe<sup>+</sup> couples in biosensors – bent sandwich complexes – bonding in bent sandwich complexes – metallocene halides and hydrides – metallocene and stereospecific polymerization of 1-alkenes – cyclopentadiene as a non-spectator ligand – monocyclopentadienyl (half-sandwich) complexes – synthesis and structures of allyl complexes – arene complexes – synthesis, structure and reactivity of arene complexes – multidecker complexes.

### UNIT IV

Role of organometallic chemistry in catalysis: Coordinative unsaturation – oxidative addition – addition reactions of specific molecules – hydrogen addition – HX addition – addition of X<sub>2</sub> – addition of RX – addition reactions of Si-H, C-C, C-Si and Si-Si bonds – elimination reactions – eliminations – alkane activation – intramolecular and intermolecular C-H activation – activation of sulphur heterocycles – insertion of carbon monoxide – isocyanide insertion – alkene insertion – alkyne insertion.

### UNIT V

Homogeneous catalysis by transition metal complexes: Hydrogenation reactions – reversible cis-dihydro catalysts – monohydride catalysts – hydrogenation of alk-1-ene – asymmetric hydrogenation – role of ruthenium complexes in 2001 Nobel Prize for chemistry – transfer hydrogenations – hydrosilation and hydroboration reactions – water gas shift reaction – reduction of carbon monoxide by hydrogen – hydroformylation of alkenes – alcohol carbonylation – decarbonylation reactions – C-C cross coupling and related reactions – alkene oligomerisations and polymerizations – Zeigler-Natta polymerization – alkene dimerisation and oligomerisations

– valence isomerisation of strained hydrocarbons – alkene and alkyne metathesis – oxidations of alkanes and alkenes – oxygen transfer reactions – supported homogeneous and phase transfer catalysis.

## References

1. Bockmann.M,(1996),Organometallics 1, complexes with transition metal-carbon bonds, Oxford science publications, Oxford.
2. Bockmann.M,(1996),Organometallics 2, complexes with transition metal-carbon bonds, Oxford science publications, Oxford.
3. Cotton.F.A, G. Wilkinson, C. A.Murillo and M. Bochmann, (1999).Advanced Inorganic Chemistry, Sixth Edition, John Wiley and sons, Inc, NewYork.
4. Haiduc.I and J. J. Zuckerman, Walter de Gruyter,Berlin, (1985).Basicorganometallic chemistry.
5. Huheey.E, Harpe(1978). Inorganic chemistry – Principles of structure and reactivity, JInternational Edition, Harper and Rone, NewYork.
6. Huheey J.E, E.A.Keiterand R.L. Keiter, (2000). Inorganic chemistry – Principles of structure and reactivity, Addison-Wesley Publishing Company,NewYork.

**Part I – M. Phil./ Ph.D.,**

**CHEMISTRY**

**Paper- III: Special Paper VII: Chemistry of Biomolecules**

**(Effective from the academic year 2017-2018 and onwards)**

**Course Objectives**

The students enable to

- Identify their chemical elements and the difference between simple sugars and complex carbohydrates.
- Compare and contrast the structure and function of the following carbohydrates and where they are found: glucose, glycogen, starch, cellulose, chitin.
- Determine presence of biomolecules like carbohydrates, proteins, lipids, etc. in known• and unknown samples.
- Determine the extent of adulteration in samples containing biomolecules.
- Identify their chemical elements and functional groups .Recognize the structure of an amino acid and the peptide bond that connects di-, tri, and polypeptides. Recognize the presence of 20 amino acids and that not all are essential amino acids.
- Identify their chemical elements and learn their property of insolubility in water.

**Course Outcomes**

The students have knowledge that

1. Identify their chemical elements and the difference between simple sugars and complex carbohydrates.
2. Compare and contrast the structure and function of the following carbohydrates and where they are found: glucose, glycogen, starch, cellulose, chitin.
3. Determine presence of biomolecules like carbohydrates, proteins, lipids, etc. in known• and unknown samples.
4. Determine the extent of adulteration in samples containing biomolecules.
5. Identify their chemical elements and functional groups .Recognize the structure of an amino acid and the peptide bond that connects di-, tri, and polypeptides. Recognize the presence of 20 amino acids and that not all are essential amino acids.
6. Identify their chemical elements and learn their property of insolubility in water.

**UNIT-I**

SUGARS:Introduction, classification of sugars. Sugars in edible nuts-cashew Synthetic sugars.



## **UNIT II**

**NON SUGARS:** Classification-characterisation-reactions-structural elucidation of starch and cellulose. Starch in edible nuts-cashew-analysis of starch: anthrone, phenol-sulphuric acid, O-toluidine methods.

## **UNIT III**

**PROTEINS:** Classification-characterisation, reactions of proteins. 1o, 2o, 3o, 4o-structure studies of proteins by X-ray crystallography. Proteins in edible nuts-albumin-biological importance. Analysis of proteins: Biuret method, Folin-lowry, Kjeldhal method, Bradford's method.

## **UNIT IV**

**ALLERGENS:** Introduction-tree nut allergens-analysis of tree nut allergens by ELISA method, hyper sensitivity- types of hyper-sensitivity.

## **UNIT V**

**TECHNIQUES OF FOOD PRESERVATION:** Preservatives: introduction, classification: class I, class II preservatives. Processing and packaging of food items with specific cases of edible nuts-cashew. Application of preservatives in packaging and value added products of edible nuts-cashew.

### **References:**

1. Organic chemistry of natural products: Gurdeep.R-Chatwal.
2. Text book of Biochemistry: Edward Staunton, John T. van Bruggel, Wibert Stodd.
3. Immunology: Kuby.
4. Text book of Biochemistry with clinical correlation: Devlin.
5. Proteins in Chemistry: Henry O. Daley J.R., Robert F. O'Malley.

**Part I – M. Phil.,/ Ph.D.,**

**CHEMISTRY**

**Paper- III: Special Paper VIII: Polymer Chemistry**

**(Effective from the academic year 2017-2018 and onwards)**

### **Course Objectives**

The course enables the student

- To study about the basic concepts of polymerization.
- To explain the coordination polymerization and apply the Ziegler-natta catalyst in polymer synthesis.
- To understand the molecular weight determination methods of the polymer and apply it identifies the polymer properties.
- To discuss about the polymer processing and properties of commercial polymers
- To apply the polymer processing technique to prepare the polymer products
- To list out the commercial polymers and its application

### **Course outcomes**

The students have

1. Studied about the basic concepts of polymerization.
2. Explained the coordination polymerization and apply the Ziegler-natta catalyst in polymer synthesis.
3. Understood the molecular weight determination methods of the polymer and apply it identifies the polymer properties.
4. Discussed about the polymer processing and properties of commercial polymers
5. Applied the polymer processing technique to prepare the polymer products
6. Remembered the commercial polymers and its application

## **UNIT-I**

Chemistry of Polymerization

Addition polymerization – Free radical polymerization – Initiation, Propagation and termination – inhibitors and retarders. Ionic polymerization – cationic and anionic-Living polymers. Coordination polymerization – Ziegler – Natta catalysts. Condensation polymerization – Extent of reaction and DP – Carother's equation and its significance. Three dimensional polymerization – cross linking – gel point – Ring scission polymerization.

## **UNIT II**

Kinetics of Polymerization

Kinetics of free-radical polymerization- Kinetic chain length and DP. Derivation for rate expression and expression for kinetic chain length and hence degree of polymerization. Kinetics of polycondensation with polyester as example. Simple kinetic expression – catalyzed and uncatalyzed polycondensation.

## **UNIT III**

Techniques of Polymerization

Bulk polymerization – solution polymerization – Suspension polymerization – Emulsion polymerization – Advantages and disadvantages of these techniques – comparison of the above.

#### **UNIT IV**

Characterization of Polymers

Molecular weight determination – Method based on colligative property measurements – cryoscopy – ebullioscopy – osmometry – membrane osmometry- vapour –pressure osmometry – Methods based on viscosity. Measurements – viscometry –Light scattering method – ultracentrifuge technique- End group analysis – GPC method. Thermal methods of analysis in polymers – TGA, DTA,DSC.

#### **UNIT V**

Polymer structure and Physical Properties

Crystalline melting point, Glass transition temperature – Properties involving deformations.

#### **References:**

1. Billmeyer, F.W. (1984) A Text Book of Polymer Science, Wiley – IntersciencePublication
2. Gowariker V.R Viswanathan. N.V Sreedhar. J (1986) Polymer Science, New Age International (P) LtdPublishers
3. Odian G. (2004) Principles of Polymerization, Wiley IntersciencePublications
4. Cowie J.M.G. (1991) Polymers: Chemistry & Physics of Modern Materials, 2nded. Chapman &Hall
5. Arora. M.G Singh M., Yadav M.S (1994) Polymer Chemistry, Anmol Publishers Pvt.Ltd.,