DEPARTMENT OF CHEMISTRY

BHARATHIAR UNIVERSITY: COIMBATORE - 641 046.

M.Sc. Chemistry – 2018-2019 onwards

Under choice based credit system (CBCS)

| S1. | Credit/M | Paper Code | General Title | Specific Title of the paper |
|------|----------|------------|-----------------------|-------------------------------------|
| No | arks | | | |
| 110. | | | | |
| | | | Semester I | |
| | | | | |
| | | | | |
| 1. | 4/100 | CHMA13A | Organic Chemistry-I | Reaction Mechanisms |
| | | | | |
| | 4/100 | | | |
| 2. | 4/100 | CHMA13B | Inorganic Chemistry-I | Coordination Chemistry |
| | | | | |
| 3 | 4/100 | CHMA13C | Physical Chemistry-I | Electro Chemistry & Photo Chemistry |
| 5. | 4/100 | CINVITISE | Thysical Chemistry-1 | Electro chemistry & Thoto chemistry |
| | | | | |
| 4. | 4/100 | CHMA1EA | Elective – I | Physical methods in chemistry |
| 5 | 4/100 | CUMA 1ED | Elective II | Water treatment and Polymers |
| 5 | 4/100 | CHWAIED | Elective - II | water treatment and Porymers |
| 6 | 4/100 | CHMA13P | Practicals-I | Organic Practicals |
| | | | | |
| | | | | |
| 7 | 2/50 | GS06 | Supportive-I | Chemistry in Context |
| | | | | |
| | | | | |

M.Sc Chemistry-2018-19 onwards-obe-UD Page 2 of 67

Annexure No:50A SCAA Dated:11.06.2018

| | | | Semester II | |
|----|-------|---------|------------------------|---|
| 8 | 4/100 | CHMA23A | Organic Chemistry –II | Natural Products, Proteins, and Stereochemistry |
| 9 | 4/100 | CHMA23B | Inorganic Chemistry-II | Bio Inorganic chemistry |
| 10 | 4/100 | CHMA23C | Physical Chemistry II | Quantum Chemistry and Electrochemistry |
| 11 | 4/100 | CHMA2EA | Elective-III | Inorganic spectroscopy Energy Diary and Drug chemistry |
| 12 | 4/100 | CHMA2EB | Elective - IV | Energy, Diary and Drug enermony |
| 13 | 4/100 | CHMA23P | Practicals-II | Inorganic Practicals |
| 14 | 2/50 | GS73 | Supportive-II | Chemistry in Day- to-day Life |
| | | | | |

| | | | Semester III | |
|----|-------|---------|--------------------------|--|
| 15 | 4/100 | CHMA33A | Organic Chemistry-III | Organic Photochemistry & Spectroscopy |
| 16 | 4/100 | CHMA33B | Inorganic Chemistry- III | Solid state and Nuclear chemistry |
| 17 | 4/100 | CHMA33C | Physical Chemistry-III | Chemical kinetics surface chemistry |
| 18 | 4/100 | CHMA3EA | Elective-V | Bio Organic Chemistry |
| 19 | 4/100 | CHMA3EB | Elective-VI | Industrial Organic Chemistry |
| 20 | 4/100 | CHMA33P | Practicals -III | Physical Chemistry Practicals |
| 21 | 2/50 | GS | Supportive III | Chemistry of Environment |

| | | | Semester IV | |
|----|-------|---------|----------------------------|---|
| 22 | 4/100 | CHMA43A | Organic Chemistry-IV | Aromaticity, Alkaloids, Steroids and Organic structure |
| 23 | 4/100 | CHMA43B | Inorganic Chemistry- IV | Organometallic Chemistry |
| 24 | 4/100 | CHMA43C | Physical Chemistry- IV | Thermodynamics (Classical and statistical) |
| 25 | 4/100 | CHMA43D | Analytical Chemistry | Analytical methods and Techniques |
| 26 | 8/200 | CHMA4LV | Project work | |

As per the CBCS, each PG student is allowed to choose 3 supportive courses offered by the other departments of the university.

OBE FORMAT

NAME OF THE DEPARTMENT:

CHEMISTRY

Programme Objectives

PO1:

Students learn the essentials of major fields in Chemistry namely Analytical, Organic, Inorganic and Physical Chemistry which would make them to understand the pivotal role played in the field of plant and animal biology, energy, materials, health sector and environment.

PO2:

Students will be encouraged to exchange their knowledge and skills for developing independent writing in their field of study.

PO3:

Students will be allowed to design their own research project based on their firm theoretical understanding.

Programme Specific Outcome

| PSO1 | • | To build the firm foundation in the fundamentals and correlate the application with the current developments in chemistry. |
|------|---|--|
| PSO2 | • | To get sufficient expertise in the operational knowledge and laboratory skills in all major fields of chemistry |
| PSO3 | • | To emphasize on integrating various disciplines of Science and encourage for interdisciplinary approach. |
| PSO4 | • | To acquire problem solving capacity, interpretation of results with the use of sophisticated instruments and devises new preparation techniques. |
| PSO5 | • | To motivate the students to prepare for competitive examinations, job carriers and get trained for industrial entrepreneurship. |
| PSO6 | • | To make current awareness on social, economic, and environmental problems facing globally |

Title of the Subject: **Organic Chemistry –I** (Reaction Mechanisms)

Code No.: CHMA13A

No. of Teaching hours: 65

Number of Credits: 4

Course Objectives:

- To understand the reaction mechanisms of the aliphatic and aromatic electrophilic and nucleophilic substitution reactions.
- To know about the principles of molecular rearrangements and it is essentially involving in the name reactions.
- To acquire basic knowledge about the addition and elimination reaction.
- To understand the basic principles of oxidation and reduction reactions

Contents

Unit – I

Aliphatic and aromatic nucleophilic substitution reactions:

Bonding - structure and reactivity - acids and bases (hard and soft acid base theory) - methods of determination and the study of reaction mechanisms.

 S_N^{-1} , S_N^{-2} , S_N^{-i} and neighbouring group mechanisms - kinetics - effects of structure - solvent and leaving and entering group - stereochemistry - hydrolysis of esters - Wurtz reaction - Claisen and Dieckmann condensation - Williamson reactions.

Different mechanisms of aromatic nucleophilic substitution - Ziegler alkylation - Chichibabin reaction - cine substitution - diazonium group as leaving group.

Unit - II

Aliphatic and aromatic electrophilic substitution reactions:

 S_E^1 and S_E^2 reactions - mechanisms and reactivity - typical reactions involving migration of double bond - keto-enol tautomerism - halogenation of carbonyl compounds - Stork enamine reactions - decarboxylation of aliphatic acids - Friedel Crafts acylation of olefinic carbon.

Aromatic electrophilic substitution - reactivity - orientation and mechanisms nitration - halogenation and sulphonation - Friedel Crafts alkylation - Friedel Crafts arylation (Scholl reaction) and acylation - Jacobsen reaction - formylation with (i) disubstituted formamides(Vilsmeyer- Haack reaction) (ii) zinc cyanide and HCl (Gattermann reaction) (iii) chloroform (Reimer - Tiemann reaction) - carboxylation with (i) carbonyl halides (ii) carbon dioxide (Kolbe Schmidt reaction) - amidation with isocyanates - hydroxyalkylation (hydroxyalkyl - dehydrogenation)- cyanodehydration of aldehydes and ketones (Bradsher reaction and Bischler - Napieralski rection) - haloalkylation - aminoalkylation and amido alkylation - thioalkylation -acylation with nitriles (Hoesch reaction) - cyanation hydroxylation.

Unit - III Molecular Rearrangements:

Molecular rearrangements - intramolecular rearrangements - 1,2- shifts in carbonium ions - Wagner-Meerwein and related rearrangements - Demjanov rearrangement - migration to carbonyl carbon - Neber rearrangement –Benzilic acid- Baeyer-Villiger rearrangement rearrangements to electron deficient nitrogen and oxygen - dienone-phenone - Favorski -Wolf - benzidine - Claisen - Cope rearrangement, Ylides: Stevens-Wittig-Sommelet-Gruvenstein-Zimmermann rearrangements- non-cyclic rearrangements - Chapman - Wallach rearrangement.

Unit - IV

Addition and elimination reactions:

Addition to C-C and C-O multiple bonds - electrophilic, nucleophilic and free-radical additions - additions to conjucated systems - orientation - Birch reduction - hydroboration - Michael condensation - 1,3 dipolar additions - Diels-Alder reactions - carbene addition to double bonds - hydration of olefines.

Mannich reaction - Meerwein-Pondorf reduction - Grignard reactions - Aldol -Claisen - Stobbe - Darsen - Wittig - Thorpe and benzoin condensations - Cannizarro reaction.Elimination reactions - E1 and E2 mechanisms - orientations - Hofmann and Saytzeff rules - elimination versus substitution - Chugaev reaction - Hofmann degradation and Cope elimination - dehydration of alcohols - dehydrohalogenation - mechanisms and orientation in pyrolytic elimination.

Unit - V

Oxidation and Reduction:

Formation of C=C, C-C bonds by dehydrogenation - dehydrogenation by quinones, SeO₂, Hg(OAc)₂, and Pb(OAc) _ formation of C-C bond in phenol coupling - acetylene coupling - allylic oxidation - oxidation of alcohols, glycols, halides and amines to aldehydes and ketones - ozonolysis - oxidation of olefinic double bonds and unsaturated carbonyl compounds - oxidative cleavage of the C-C bond - Sommelet reaction and selectivity in reduction - metal hydride reduction- metal alkoxide reduction - reduction by dissolving metals - Clemmensen reduction - Wolf Kishner reduction - metal ammonia reduction (Birch reduction) - reduction of nitro compounds - acyloin condensation - catenanes.

Carbenes and nitrenes - structure and generation - addition reaction with alkenes - insertion reactions.

References

- 1. Jerry March, Advanced organic chemistry Reactions, mechanism and structure, Mc Graw Hill Kogakusha Ltd., 1977.
- 2. Lowry and Richardson, Mechanism and theory in organic chemistry, Harper & Row Publishers, New York 1981.

- 3. Muk herji and S. P. Singh, Reactions mechanisms in organic chemistry, Mc Millan 1976.
- 4. Raj K.Bansal Organic Chemistry Reaction mechanisms,Mc.Graw-Hill Publishing Company Ltd,2006

Course Outcomes

On successful completion of the course, the students will be able to

| CO1 | To remember the basic principles of reaction mechanisms involving the | | |
|-----|---|--|--|
| | various electrophilic, nucleophilic, addition, elimination, oxidation, | | |
| | reduction reactions & molecular rearrangements | | |
| CO2 | To understand the basics of electrophilic, nucleophilic, addition, elimination, | | |
| | oxidation, reduction reactions & molecular rearrangements through the name | | |
| | reactions. | | |
| CO3 | To apply the mechanism in chemical reactions to solve the reaction pathway. | | |
| CO4 | To assessment different types of reaction mechanism involving in chemical | | |
| | synthesis during their project work. | | |

Course prepared by : Dr. A. Kannan

Title of the Subject: Inorganic Chemistry –I (Coordination Chemistry) Code No: CHMA13B

No of Credits: 4

No of Teaching hours:60

Course Objectives

- Learn about the various theories of complexes, basics of electronic spectroscopy of transition metal complexes, mode of coordination with various geometry
- > Learn about the important inorganic polymers and their applications

Contents

Unit - I

18 electron rule - EAN rule - theories of coordination compounds - valence bond theory - crystal field theory - splitting of d orbitals in different symmetries - crystal field stabilization energy - factors affecting the magnitude of 10 Dq - evidence for crystal field stabilization - spectrochemical series - site selection in spinels - tetragonal distortion from octahedral symmetry - Jahn-Teller distortion - molecular orbital theory - octahedral complexes - tetrahedral and square planar complexes - pi bonding and molecular orbital theory - experimental evidence for pi bonding.

Unit - II

Term states of dn ions - electronic spectra of coordination compounds - selection rules - band intensities and band widths - energy level diagrams of Orgel and Tanabe - Sugano - spectra of Ti3+, V3+, Ni2+, Cr3+, Co2+, Cr2+ and Fe2+ - calculation of 10Dq and B for V3+ (oct) and Ni2+ (oct) complexes. Magnetic properties of coordination compounds - change in magnetic properties of complexes in terms of spin orbit coupling - temperature independent paramagnetism - spin cross over phenomena.

Unit - III

Substitution reactions in square planar complexes - the rate law for nucleophilic substitution in a square planar complex - the trans effect - theories of trans effect - mechanism of nucleophilic substitution in square planar complexes - kinetics of octahedral substitution ligand field effects and reaction rates - mechanism of substitution in octahedral complexes reaction rates influenced by acid and bases - racemisation and isomerisation - mechanisms of redox reactions - outer sphere mechanisms - excited state outer sphere electron transfer reactions - inner sphere mechanisms - mixed valent complexes.

Unit - IV

Structure of coordination compounds with reference to the existence of various coordination numbers - complexes with coordination number two - complexes with coordination number four - tetrahedral and square planar complexes - complexes with coordination number five - regular trigonal bipyramidal and square pyramidal - site preference in trigonal bipyramidal complexes - site preference in square planar complexes - isomerism in five coordinate complexes - coordination number six - distortion from perfect octahedral symmetry - trigonal prism - geometrical isomerism in octahedral complexes - coordination number seven and eight.

Unit - V

Inorganic chains - rings - cages and clusters - catenation - heterocatenation - intercalation chemistry - one dimensional conductor - isopolyanions - heteropolyanions - borazines - phosphazenes - phosphazene polymers - ring compounds of sulphur and nitrogen - homocyclic inorganic systems - cages - boron cage compounds - metal clusters - dinuclear clusters - trinuclear clusters - tetranuclear clusters - hexanuclear clusters - structural prediction of organometallic clusters.

Power point Presentations, Group discussions, Seminar ,Quiz, Assignment, Experience Discussion, Brain storming, Activity, Case study

Assignment: Theories of coordination complexes and isomerism in various coordination geometries

Power point presentation: Term symbols, Orgel diagram and Tanabe - Sugano diagram **Seminar**: Various types of electron transfer mechanisms and inorganic polymers.

Books for Study:

- 1. Gurdeep Raj. (2014). *Advanced Inorganic Chemistry*. 12th Edition. Geol Publishing House.
- 2. R.D. Madan. (2011). *Advanced Inorganic Chemistry*. 3rd Edition. S. Chand & company, New Delhi.
- 3. U.K.Malik, G.D.Tuli, and R.D. Madan, (2010). *Selected Topics in Inorganic Chemistry*, S. Chand Publication.
- R. Gopalan. V. Ramalingam, (2001) Concise Coordination Chemistry, 3rd edition, Vikas Publishing house pvt. Ltd

Books for Reference:

- 1. Inorganic Chemistry *Principles of structure and reactivity*, Fourth Edition J. E. Huheey, E. A. Keiter and R. L. Keiter Addition Wesley Publishing Co, NY, 1993.
- 2. Advanced Inorganic Chemistry F. A. Cotton and G. Wilkinson
- 3. Mechanism of Inorganic reactions F. Basolo and R. G. Pearson
- 4. *Inorganic Chemistry* R. B. Heslop and P. L. Robinson 5. Introduction to Ligand Fields B. N. Figgis Wiley Eastern Ltd, New Delhi, 1976.

Course Outcomes (CO)

| K1 | CO1 | Understand the various concepts of coordination chemistry and realize the importance of electronic spectroscopy and magnetic properties of | | |
|----|-----|--|--|--|
| | | coordination compounds. | | |
| K2 | CO2 | Gaining the knowledge on various types of inorganic reaction mechanism | | |
| | | in different geometries. | | |
| K3 | CO3 | Acquiring knowledge on various types of electron transfer mechanism of | | |
| | | metal complexes and their importance. | | |
| K4 | CO4 | Inferring various symmetries/geometries of coordination complexes and | | |
| | | their isomerism and important applications of some inorganic polymers. | | |

prepared by : Dr. R. Prabhakaran

Title of the Subject: PHYSICAL CHEMISTRY – INumber of credits: 4Code No.: CHMA13CNumber of Teaching hours: 60

Course Objectives :

- To give a thorough introduction to the study of electrochemistry, photochemistry and nanoscience.
- To learn the theories and basics of electrochemistry, photochemistry and various applications of electrochemical/photochemical and nanotechnological approaches.
- To study the concepts and fundamentals of electrochemical and photochemical reactions.

Unit – I ELECTROCHEMISTRY - I

Ions in Solutions: Conductivity of solutions and their measurement - the Arrhenius ionisation theory - transport numbers and mobilities of ions - measurement of transport numbers - Hittorff method and moving boundary method - ionic activities and activity coefficients and their determination by various methods - Debye-Huckel-Onsager theory - ionic atmosphere - Debye-Huckel limiting law - Electrolytic conductance – Kohlrausch's law and its applications; ionic equilibria; conductometric and potentiometric titrations.

Unit – II ELECTROCHEMISTRY - II

Metal/Electrolyte Interface: Outer Helmholtz plane (OHP) and Inner Helmholtz plane (IHP) - potential profile across double layer region - potential difference across electrified interface - Structure of the double layer - Helmholtz-Perrin, Gouy-Chapman, and Stern models – Electrode kinetics - Butler-Volmer equation-one step one electron transfer kinetics - exchange current density - Tafel equation and plots - Polarizable and non-polarizable interfaces - Hydrogen overpotential – Theories of hydrogen overvoltage - Mechanism of hydrogen evolution reactions - Passivity – electrochemical corrosion and its protection.

Unit – III ELECTROCHEMISTRY - III

Electrochemical Cells: Electromotive force - measurement of EMF - the potentiometer - the electrochemical potential - the cell EMF and the cell reaction - reversible cells - types of half cells - classification of cells - the standard EMF of a cell - standard electrode potentials - calculation of the EMF of a cell - Nernst equation and its limitations - calculation of solubility products - standard free energies and entropies of aqueous ions - electrode concentration cells - electrolyte concentration cells - cells with liquid junctions - oxidation - reduction reactions, measurement of pH, concentration cells with transference – Electrochemical energy systems - Li-ion batteries-Methanol Fuel cells.

Unit – IV PHOTOCHEMISTRY

Absorption and emission of radiation – Theories – Spontaneous and induced emission –Laser – Franck Condon principle - Type 1 & 2 – Physical properties of electronic excited state – Jablonski diagrams – Emission – Resonance emission – Selection rule – Fluorescence – Phosphorescence – Delayed fluorescence: E-Type and P-Type – Excimer and Exciplex complex formation – Stern-Volmer equation – Photosensitization and Chemiluminescence – Experimental techniques – Actinometry – Chemical actinometry – Biochemiluminescence – Photochromism – Photostabilization – Photosynthesis – PS I and PS II – Photochemical energy-storage reactions.

Unit – V COLLOIDS AND CHEMISTRY IN NANOSCIENCE & NANOTACHNOLOGY

Types of solutions – Types of colloidal solutions – Preparation of colloidal solutions – Condensation methods – Disintegraton methods – Purification of colloidal solutions – Dialysis – Ultrafiltration – Characteristics of colloidal solutions – Emulsions – Micelles.

Nanomaterials – Preparation: Plasma arcing - Chemical vapor deposition – Sol-gel method – silica gels – Zirconia and ytrrium gels – Aluminosilicate gels – Electrodeposition – Ball milling –Applications of nanomaterials – Machine tools – Batteries – High power magnets – Motor vehicles and aircraft – Medical applications.

References

- 1. Samuel Glasstone, "An Introduction to Electrochemistry", Maurice Press, 2007.
- 2. Gordon M.Barrow-Physical Chemistry, Mc Graw Hill Publishing Company Ltd, 2007.
- John O'M. Bockris, Amulya K. N. Reddy, "Modern Electrochemistry", Vol. I and II, Plenum Publishing, 2008.
- Rohatgi Mukherjee K.K., "Fundamentals of photochemistry", New Age International Pvt. Ltd., New Delhi, 2009.
- 5. Charles Kutal, Journal of Chemical Education 60 (1983) 882-887.
- 6. Atkins P.W., "Physical Chemistry", Oxford University Press, 8th Ed., 2006.
- Michael Wilson, Kamali Kannangara, Geoff Smith, Michelle Simmons and Burkhard Raguse, "Nanotechnology – Basic Science and Emergin Technologies", Chapman & Hall (CRC), 2004.

Course Outcomes:

On successful completion of the course, the students will be able to

- CO 1 Recollect the fundamentals of electrochemistry, photochemistry, nanoscience and nanotechnology.
- CO 2 Understand the principles and applications of electrochemical cell models, batteries and photochemical reactions. To comprehend the mechanism of energy drive systems.
- CO 3 Apply the various instrumental techniques related to electrochemical, photochemical and nanotechnology.
- CO 4 Apply the fundamentals of electrochemistry, photochemistry in device fabrication.

Course prepared by :Dr.T.Selvaraju

Title of the Subject: Physical Methods in Chemistry (Molecular spectroscopy and Surface morphological studies)

Code No.: CHMA1EA

Number of Credits: 4 (Four)

No. of Teaching hours: 60

Course Objectives:

- To study the principle and mechanism of different types of molecular spectroscopy.
- To acquire basic knowledge about the activity of molecules using various spectroscopic techniques.
- To study the basic principles of radiation chemistry and basic knowledge about various surface morphology analysis techniques.
- To understand the working principle of the different instruments and analysis the surface morphologies of the various material.

Unit – I ROTATIONAL SPECTROSCOPY

General introduction to electromagnetic spectrum – The rotation of molecules – Classification of rotors – Rigid rotors, Non-rigid rotors – Effect of isotopic substitution on the transition frequencies – diatomic and polyatomic molecules – Relative intensities of spectral lines – stark effect – Nuclear and electron spin interaction – Instrumentation – Chemical analysis by microwave spectroscopy.

Unit – II VIBRATIONAL SPECTROSCOPY

Simple harmonic oscillator – Vibrational motion of a diatomic molecule – Selection rule – Zero point energy – Force constant and bond strengths - Anharmonic oscillator - Vibrations of polyatomic molecules – Fundamental vibrations and overtones – Hot bands – Vibrational-rotational spectra of a diatomic molecule – Vibrations of polyatomic molecules - Instrumentation –Sampling techniques - Factors influencing vibrational frequencies - Application to organic and inorganic compounds - Finger print region - Identification of functional groups - Simple problems in functional group identification using IR spectrum.

Unit – III RAMAN SPECTROSCOPY AND ELECTRONICS SPECTROSCOPY OF ATOMS:

Pure rotational Raman spectra – Vibrational Raman spectra – selection rule - Polarization of light and the Raman effect – Structural determination from Raman spectroscopy – Techniques and Instrumentation.

Structure of atoms – Electronic angular momentum – many-electron atoms – photoelectron spectroscopy and X-ray fluorescence spectroscopy – Zeeman effect – Influence of nuclear spin – problems.

Unit – IV ULTRAVIOLET AND VISIBLE SPECTROSCOPY

Electronic spectroscopy of molecules - Electronic spectra of diatomic molecules - Physical principles – Chromophores and auxochromes - Laws of absorption – Absorption transitions - Instrumentation - Solvent effects - Applications of UV spectroscopy - Effects of conjugation -Woodward-Fieser rules - α , β -Unsaturated carbonyl compounds, dienes trienes and polyenes - Aromatic systems with extended conjugation – Heteroaromatic compounds - Simple problems – Absorption spectra of charge transfer complexes.

Unit – V RADIATION CHEMISTRY AND MORPHOLOGICAL STUDIES:

Radiation chemistry: Source of high energy – interaction of high energy radiation with matter – primary and secondary process –G-value –radiolysis of water – reactions of hydrated electrons OH and H radicals – experimental techniques (Dosimetry).

Introduction to Surface characterization methods – AFM, SEM, FE-SEM, HR-TEM, STEM - Sample preparation of characterization only.

References:

- 1. Banwell C. N., "Fundamentals of Molecular Spectroscopy", Tata McGraw-Hill Publishing Company Limited, New Delhi, 4th Edition, 2004.
- 2. Chang Basic principles of spectroscopy.
- 3. Donald L. Pavia, Gary M. Lampman and George S. Kriz, Jr Introduction to Spectroscopy: A Guide for students of organic chemistry.
- 4. D.H.Williams-Ian Fleming, Spectroscopic Methods in Organic Chemistry, Mc Graw Hill Publishing Company Ltd, 2006.
- 5. G. Friedlander, J.W. Kennedy and J.M. Miller, Nuclear and Radiochemistry, Wiley, 1964.
- 6. Zhou W, Wang Z. L, "Scanning Microscopy for Nanotechnology: Techniques and Applications", Springer, New York, USA, 2006.

Course Outcomes:

On successful completion of the course, the students will be able to

- CO1 To know the fundamental concepts and application of various analytical techniques.
- CO2 To acquire intense knowledge about the basic principles, instrumentation and applications of UV-Visible, Raman, Rotational, Vibrational and Electronic spectroscopy.
- CO3 To gain the in-depth knowledge of concepts in radiation chemistry and to learn about the surface morphology (particle shape and size) characterization of materials using various advanced instrumentation techniques.
- CO4 To learn how to interpret the data for well-known compounds, which is helpful to predict the unknown molecules.

Course prepared by : Dr. S.N.Karthick

| Title of the Subject : | Water Treatment, Fuels and Polymers | No. of Credits: | 4 |
|------------------------|--|--------------------------|----|
| Code No | CHMA1EB | No. of Teaching Hours | 60 |

Course Objectives:

- To teach the students the essential role of water in industries
- To teach the importance of various types of fuels and their applications
- To create awareness on environmental pollution
- To impart the knowledge on the chemistry of polymers and its applications

Contents

Unit I: Water Treatment

Sources of water – Molecular structure and physical properties – Hydrogen Bonding – Water as a solvent – Quality characteristics of water: total acidity and alkalinity, hardness of water – methods of determination of hardness, total solids, disadvantages of using hard water - Comparative account on physical and chemical properties of H_2O and D_2O .

Unit II: Water conditioning

Softening of water: Desalination, Clark's process, lime-soda process, ion-exchange process; demineralization of water - Treatment of water: sterilization, flocculation, Industrial treatment – Treatment of wastes or effluents with organic and inorganic impurities, sewage and sewage treatment; Biochemical oxygen demand (BOD), chemical oxygen demand (COD)

Unit III: Fuels

Introduction – definition, calorific value, determination of calorific value- Classification of fuels – solid, liquid and gaseous fuels, Fossil fuels, Rocket fuels and nuclear fuels - advantages and disadvantages of solid fuels over liquid and gaseous fuels. Energy – unit of energy, sources of energy, renewable and non-renewable, conventional and non-conventional energies. Solar energy – solar photovoltaic cells and applications. Energy storage: Batteries and fuel cells – dry cell (primary cell), lead –acid battery (secondary cell), hydrogen-oxygen fuel cell, advantages of fuel cell. Future options for energy – Bio conversion & advantages

Unit IV: Environmental Pollution

Components of environment – Factors affecting environment - Environmental pollution – Definition, pollutants, classification of pollutants - Types of pollution: air, water soil, thermal, radioactive and noise pollutions - Prevention and control of pollutions

Unit V: Plastics (High Polymers)

Introduction, classification, difference between thermosetting and thermoplastics- Effect of polymer structure on properties - Formation of plastics : copolymerization, difference between addition and condensation polymerization – Properties and uses of plastics – Moulding of plastics - Commercial resins and plastics: bakelite, urea-formaldehyde, melamine-formaldehyde, epoxy, acrylic and silicon resins, polythene, PVA, PVC, cellulose, cellulose nitrate and acetate- Disposing of plastics : incineration, biodegradation, recycling and source reduction.

Books recommended

- 1. *Industrial Chemistry* (Including Chemical Engineering) -- B.K.Sharma (10th Edition, 1999)
- Outlines of Chemical Technology For the 21st Century M.Gopala Rao & Marshall Sittig (3rd Edition, 1997)

Course Outcomes (CO)

On successful completion of the course, the student will able to gain

| CO1 | Understood the properties of water and quality measurements |
|------------|--|
| CO2 | Learnt about the various water treatment techniques to get drinkable |
| | water |
| CO3 | To evolve strategy for conservation of energy and alternative energy resources |
| CO4 | To understand the toxicity and factors responsible for the air pollution |
| CO5 | Understood the importance of polymers and ways to minimize the usage of |
| | plastics and wastage disposal |

| PSO CO | ~ PSO1 | PSO2 | PSO3 | PSO4 | PSO5 |
|-----------|--------|------|------|------|------|
| CO1 | S | Н | S | S | М |
| CO2 | S | S | S | S | Н |
| CO3 | S | S | S | Н | М |
| CO4 | S | S | S | М | М |
| CO5 | S | S | S | Н | М |

Mapping

S-Strong; H-High; M-Medium; L-Low

Prepared by : Dr. M.V.Kaveri

| Title of the Subject | ORGANIC PRACTICALS | No. of Credits: | 4 |
|----------------------|-----------------------|-----------------------|----|
| Code No | CHMA13P | No. of Teaching Hours | 60 |

Course Objectives:

- To carry out the separation of organic components from the binary mixture.
- To quantify the organic compound by using substitution reaction.
- To learn to prepare simple organic compound in single stage
- To know the purification and recrystallisation techniques for the synthesized compounds.

Contents

1. Qualitative analysis: Analysis of two component mixtures - separation and characterisation of the components.

2. Quantitative analysis:

Estimation of phenol, aniline and reducing sugars

3. Single stage preparation:

Preparation of about eight organic compounds by single stage.

- (i) Benzoic acid from ethyl benzoate
- (ii) Acetanilide from aniline
- (iii) Acetylsalicyclic acid from salicyclic acid
- (iv) 2,4,6-Tribromoaniline from aniline
- (v) p-Bromoacetanilide from acetanilide
- (vi) m-Dinitro benzene from nirobenzene
- (vii) Picric acid from phenol
- (viii) Benzanilide from aniline

Reference Books

- 1. Vogel's Text book of practical organic chemistry, 5th edition, Prentice Hall, 2008
- 2. N.S.Gnana Prakasam, G.Ramamurthy, Organic chemistry Manual, S.Viswanathan Co., Ltd

Course Outcomes (CO)

On successful completion of the course, the student will be

| CO1 | Able to determine the presence of functional groups in a given unknown |
|-----|--|
| | organic compound |
| CO2 | To design the protocol for the preparation of an organic compound by |
| | single stage which meets the industrial standards |
| CO3 | Understood the basic conditions such as solubility, hydrolysis, acetylation, |
| | bromination, nitration to prepare suitable derivative |
| CO4 | Imbibing professional ethics in the synthesis of new compounds |

Mapping

| PSO CO | PSO1 | PSO2 | PSO3 | PSO4 |
|-----------|------|------|------|------|
| CO1 | S | Н | S | S |
| CO2 | S | S | S | S |
| CO3 | S | Н | S | Н |
| CO4 | S | S | S | Н |

S-Strong; H-High

Prepared by : Dr. M.V.Kaveri

| Title of the Subject | CHEMISTRY IN | No. of Credits: | 2 |
|----------------------|--------------|-----------------|----|
| : | CONTEXT | | |
| Code No | GS06 | No. of Teaching | 25 |
| | | Hours | |

Course Objectives:

- To learn the principles of Green chemistry
- To recall the factors involved in the air pollution which affects the environment
- To Enable the students to know about the various energy resources
- To understand the principles of preparation properties and applications of plastic

Contents

Unit - I

Air- Introduction- Definition- Composition of air- Air pollution-Definition-Air pollutants-Types of Air pollution - Causes of Air pollution on human health-Prevention of Air pollution.

Unit - II

Water-Introduction-Definition-Sources of water-Types of water-Water quality parameters-Water pollution- Definition-Types of Water pollution- Causes of Water pollution on human health-Prevention of Water pollution.

Unit – III

Energy - Introduction- Definition-Sources of energy- Types of energy- Renewable energy sources- Non-renewable energy sources- Nuclear energy-Applications.

Unit - IV

Polymers –Introduction-Definition- Types of polymers based on physical property-Characteristics of polymers- polyethylene – PVC- Synthetic fibres –Definition, Nylon 66, and Terylene.

1. versatile knowledge of aromaticity,

References

- 1. Fundamental concepts of applied Chemistry, Jayashree Ghosh, 1st edition, S.Chand and company
- 2. Environmental Chemistry, A.K.De, 8th edition, New age international publishers
- Chemistry in context applying chemistry to society-, Lucy Pryde Eubanks, Catherine H. Middlecamp, Norbert J. Pienta, Carl E. Heltzel, Gabriela C. Weaver, 5th edition, McGraw Hill

Course Outcomes (CO)

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

| CO1 | To understand the toxicity and factors responsible for the air pollution |
|------------|--|
| CO2 | To realize the impact of man made pollution on ecosystem |
| CO3 | To evolve strategy for conservation of energy and alternative energy resources |
| CO4 | To understood the toxicity of plastics and minimize the usage of plastics |
| CO5 | To interpret the hazards due to man made pollution, radio activity and proper |
| | disposal of plastics to save the environment |

Mapping

| PSO CO | PSO1 | PSO2 | PSO3 | PSO4 |
|-----------|------|------|------|------|
| CO1 | М | Н | S | S |
| CO2 | S | S | S | S |
| CO3 | М | S | S | Н |
| CO4 | S | S | S | Н |

S-Strong; H-High; M-Medium; L-Low

Prepared by : Dr. M.V.Kaveri

Title of the Subject: **Organic Chemistry –II** (Natural Products, Proteins, Stereochemistry and Heterocyclic Compounds) Code No.: **CHMA23A** Number of Credits: 4

No. of Teaching hours: 65

Course Objectives:

- To understand the versatile knowledge about the isolation, synthesis, bio- synthesis and elucidation of various natural products.
- To understand the basic concept of conformational analysis and stereochemistry.
- To acquire basic knowledge about the heterocyclic chemistry involving in natural products.

Unit – I

Terpenoids:

Isolation and classification - general methods to elucidate the structure of terpenoids - methods of structure elucidation and synthesis as applied to zingiberine - eudesmol - caryophyllene - abietic acid - santonin - biosynthesis of terpenes.

Unit – II

Amino acids, proteins and nucleic acids:

Synthesis of amino acids and polypeptides - primary and secondary structure of a protein - the N-terminal and C- terminal residue analysis - oxytocin - enzymes and coenzymes - biosynthesis of protein .

Unit - III

Conformational analysis and stereochemistry:

Geometrical and optical isomers : R, S, E, Z configurational notations - different types of optical isomerism including dissymmetric over crowded molecules - stereochemistry of sulphur and nitrogen compounds - configurations - geometrical isomerism and configurations in mono and bicyclic ring systems - conformational analysis of acyclic system - cyclohexanes - perhydrophenantharene - decalins - carbohydrates - spiranes- allenes and biphenyls.Asymmetric Synthesis-Introduction-methods of asymmetric synthesis-auxiliary controlled methods-reagent controlled methods-catalyst controlled methods.

Unit - IV

Vitamins:

Structure and synthesis of vitamin B complex : vitamin B_1 (aneurin) - vitamin B_2 (riboflavin) - pantothenic acid - folic acid - vitamin H (biotin) - vitamin B_6 (pyridoxine) - vitamin B_{12} (cyanocobalamin) structure only - vitamin E (\Box - tocopherol) - vitamin K_1 (phylloquinone) and vitamin K_2 .

Unit - V

Heterocyclic compounds:

Structure - synthesis and reactions of the following systems

a) Small ring Heterocycles - Three membered and four membered Heterocycles- aziridines, oxiranes, thiranes, azetidines, oxitanes and thietanes.

b) Benzo fused Heterocycles – benzofurans, benzothiophenes, carbazole - chromone - flavanones - flavones - flavones - flavones.

References

- 1. I. L. Finar, Organic chemistry, vol. I and vol. II.
- 2. Nakanishi et. al., Natural product chemistry, vol. I, Academis press, 1974.
- 3. Newman, Terpenes and Terpenoids.
- 4. E. L. Eliel, Stereochemistry of carbon compounds, Mc Graw Hill, 1962
- 5. P.Ramesh, Basic principles of Organic Stereochemistry, Meenu publication, 2005.
- 6. Heterocyclic Chemistry, J. A. Joule, K. Mills and G. F. Smith, Chapman and Hall
- 7. Heterocyclic Chemistry, T. L. Gilchrist, Longman Scientific Technical
- 8. R. K. Bansal, Heterocyclic Chemistry; 3rd Ed., Wiley Eastern Ltd, New Delhi, 1999.

Course Outcomes

On successful completion of the course, the students will be able to

| CO1 | To remember the basic values of natural products such as terphenoids, |
|-----|---|
| | vitamins, amino acids, proteins and nucleic acids. To keep in mind the basic |
| | knowledge about conformational analysis as well as stereochemistry. |
| CO2 | To understand the concept of conformational analysis and also the |
| | stereochemistry of the organic molecules. To get an idea about heterocyclic |
| | chemistry in various natural products. |
| CO3 | To apply the concept of stereochemistry in optically active organic |
| | molecules. To gain the interest on uses of natural products such as vitamins, |
| | amino acids, proteins and nucleic acids in the human day to day life. |
| CO4 | To analyze the geometry of the molecules as well as the stereochemistry of |
| | the organic molecules. To analyze the functions of the natural products such |
| | as proteins, amino acids, nucleic acid and vitamins. |

Prepared by: Dr. A. Kannan

Number of Credits: 4 (Four)

Title of the Subject: Inorganic Chemistry- II (Bioinorganic Chemistry)

Code No.: CHMA23B

No. of Teaching hours:

Course Objectives:

- To understand the key role of various elements in the living systems.
- To acquire basic knowledge about the structure and functions of certain metalloenzymes.
- To gain insight into the small molecules binding and transport mechanism involving metallo enzymes
- To know about the mechanism of binding interactions of metal complexes with biomolecules and metal based drug action.

Unit-I: Metals in Biology

Metals and Non-metals in biological systems - Essential and trace elements - Role of different metal ions in biological systems - Sodium-Potassium pump - Ferritin - Transferrin-Blue copper proteins - Catecholase - Photosynthesis: Chlorophyll - Photosystem-I (PS-I) & II (PS-II) - Structure-function relationship.

Unit – II: Structure and Function of Various Metalloenzymes

Metalloenzymes - Definition - Examples - Active site structure and mechanism of action of - Carboxy peptidase-A and Carbonic anhydrase - Structure and function of Superoxide dismutase (SOD) (Fe-SOD, Mn-SOD, Cu-Zn couple SOD and Ni-SOD) and catalase enzymes - Xanthine oxidase - Nitrogenase

Unit - III: Heme and Non-heme Metalloenzymes

Phorphyrin system - Structure and functions of Hemoglobin and Myoglobin - Dioxygen binding, transport and utilization - Hemocyanin - Hemerythrin - Synthetic oxygen carriers - Vitamin B_{12} co-enzyme - Non-heme iron-sulphur proteins - Ferridoxins - Rubredoxins - Cytochromes.

Unit - IV: Metals in Medicine

Binding of metal ions and complexes to biomolecules, Types of binding - Nucleic acid structures - Fundamental interactions with nucleic acids - Binding interactions of tris-phenanthroline metal complexes with DNA - Techniques to monitor binding (Electronic absorption, Fluorescence and Circular dichroic spectral techniques, electrochemical behaviour, viscosity measurement and ploarimetry).

Chemotherapy - Radio diagnostic agents - MRI scanning - Chelating Agents (with special reference to EDTA) and therapy based on in vivo chelation of radio nucleotides - Dosage and toxicity.

Unit - V: Drug Discovery and Design

Drug discovery and design - Therapeutic index and chemotherapeutic index - Structure -activity relationship - Factors governing drug design - Computer aided drug design - Bleomycin – Doxorubicin - Cancer chemotherapy - Bioinorganic chemistry of platinum and ruthenium anticancer drugs - Mechanism of action of cisplatin - Clinical trials and their significance - Applications of Coordination complexes in medicine.

References:

- 1. I. Bertini, H. B. Gray, S. J. Lippard and J. S. Valentine, Bioinorganic Chemistry; University Science Books.
- 2. Dr Asim K Dass, Bioinorganic Chemistry 2007, Books and Allied (P) Limited.
- 3. J. E. Huheey, E. A. Kieter, and R. L. Keiter, Inorganic Chemistry, 4th Edition, Addision Wesely Publishing Company.
- 4. Keith F. Purcell and John C. Kotz, Inorganic Chemistry, 3rd Edition.
- 5. S. J. Lippard and J. M. Berg, 1994, Principles of Bioinorganic Chemistry, University Science Books

Course Outcomes:

On successful completion of the course, the students will be able to

- CO1 understand the key function of metal ions such as manganese, iron, cobalt, nickel, copper, zinc, molybdenum etc. in biological system, in particular in metalloenzymes.
- CO2 acquire intense knowledge about various biological roles such as metal ion transport and storage, electron- and proton transfer, O_2 transport, hydrolysis, etc. taking place at the active site of metalloproteins.
- CO3 gain knowledge about the medically-important topics such as i) metal in medicine, ii) interaction of metal ions with biomolecules, iii) the toxicity of metal ions, and use of iv) Ru and Pt complexes in cancer therapy. This would motivate the students to purse their research in the field of medicinal chemistry.
- CO4 Equip the student to answer the bioinorganic chemistry related questions which are frequently aroused in competitive examinations.

Prepared by: Dr. K.Sundaravel

: CHMA23C

Title of the Subject : PHYSICAL CHEMISTRY – II Number of credits :4

Code No.

Number of Teaching hours : 60

Course Objectives :

- To present the basic principles of quantum chemistry and group theory.
- To learn the theories and basics of quantum mechanical treatment and group theoretical approach.
- To motivate the student to visualize the atomic and molecular patterns.

Unit – I QUANTUM CHEMISTRY-I

Failure of classical mechanics and the success of quantum theory in explaining black body radiation - photoelectric effect and the H-atom spectrum - DeBroglie's matter waves - Heisenberg's uncertainty principle - Schrodinger equation - Born's interpretation of the wave function - requirements of the acceptable wave function.

Algebra of operators - sums and products of operators - commutator - linear operators - eigen functions and eigen values - correspondence between physical quantities in classical mechanics and operators in quantum mechanics - Hamiltonian operator - quantisation of angular momentum and its spatial orientation - average (expectation) values - postulates of quantum mechanics.

Unit – II QUANTUM CHEMISTRY-II

Particle in a one dimensional box - quantisation of energy - normalisation of wave function - orthogonality of the particle in a one-dimensional box wave functions - average position and average momentum of a particle in a one-dimensional box - illustration of the uncertainty principle and correspondence principle with reference to the particle in a one-dimensional box - particle in a three-dimensional box - separation of variables – degeneracy.

Schrodinger equation for simple harmonic oscillator of a diatomic molecule - illustration of the uncertainty principle and correspondence principle with reference to harmonic oscillator. Schrodinger equation for a rigid rotor of a diatomic molecule. Schrodinger equation for the H-atom (or H - like species) - separation of variables - energy levels - radial factors of the H-atom wave functions.

APPLICATIONS OF OUANTUM CHEMISTRY Unit – III

Need for approximation methods - the perturbation theory (first order only) application of the perturbation method to He- atom - the variation method - applications of variation method to He-atom.

Electron spin and the Pauli principles - symmetric and antisymmetric nature of the wave functions - Slater determinants - approximate wave function of many electron atoms - Born Oppenheiner approximation - Elementary concepts of MO and VB theories - Hybridization -Huckel theory of linear conjugated systems - Cyclic systems - Wood-ward Hoffman rules.

GROUP THEORY Unit – IV

Symmetry elements and symmetry operations - identity - centre of symmetry - axis of symmetry - plane of symmetry and improper rotation axis of symmetry. Groups and their properties - molecular point groups and classification - matrices-matrix representation of symmetry operations

Classes - representations - reducible and irreducible representations - properties of irreducible representations - Statement and proof of Great Orthoganality theorem and its consequences -Construction of character table for C_{2v} and C_{3v} point groups.

Unit – V **APPLICATIONS OF GROUP THEORY**

Standard reduction formula relating reducible and irreducible representations - Symmetries of normal modes of vibration in non-linear molecules (H₂O, NH₃, BF₃) - Selection rules for vibrational spectra - IR and Raman active fundamentals - Mutual exclusion rule -Symmetries of M.O and symmetry selection rule for electronic transition in ethylene and formaldehyde - Hybridization schemes for atoms in ethylene and butadiene.

References

- I. N. Levine Quantum Chemistry, 7th Ed., Pearson India, 2016.
 R. K. Prasad Quantum Chemistry, 4th revised Ed., New Age International Pvt. Ltd, 2014.
- 3. W. J. Moore Physical Chemistry, 5th Ed., 1998.
- 4. G.W. Castellan Physical Chemistry, 1983.
- 5. A. K. Chandra Introductory Quantum Chemistry, 4th Ed., 2017.
- 6. P. Atkins Physical Chemistry, Oxford University Press, 8th Ed., 2006.
- 7. Swarnalakshmi S. A Simple Approach to Group Theory in Chemistry, Universities Press,
 - 2009.
- 8. Raman, K.V. Group theory and its applications to chemistry", Tata Mac Graw Hill, 2004.
- 9. F. A. Cotton Chemical applications of group theory, Wiley India Pvt Ltd 3rd Ed., 2008.

Course Outcomes:

On successful completion of the course, the students will be able to

CO 1 – Understand the concepts of classical and quantum mechanics, to picture out the failure

of classical mechanics. To comprehend the approximate methods in quantum mechanics.

- CO 2 Recollect the dual character of electrons and apply the Schrödinger wave equation to particles in a system.
- CO 3 Apply group theory and categorize the molecules based on the structure and bonding interactions.
- CO 4 Analyze the solution in terms of energy and wave function for H, H like atoms and multielectron systems and to review the group theoretical approach towards Spectroscopy.

Course prepared by : Dr.T.Selvaraju

Title of the Subject: Inorganic Spectroscopy

Code No: CHMA2EA

Annexure No:50A SCAA Dated:11.06.2018

No of Credits: 3

No of Teaching hours:

Course objectives:

- To understand the role of spectroscopic methods in inorganic chemistry.
- To acquire basic knowledge about the application of spectral methods in structural elucidation of inorganic compounds.
- To get an insight on the use of several spectroscopic and analytical techniques for structural investigation of few metalloproteins.

Contents

Unit- I - IR, Raman, ORD & CD Spectroscopy

Infrared and (Resonance) Raman and spectra of metal complexes. - Molecular vibrations of di and triatomic molecules - Metal-ligand vibration - Band assignment - Resonance enhancement - Mechanisms - Excitation profiles, Multimode effect - Application to 2Fe-2S, 4Fe-4S and 3Fe-4S proteins and elucidation of binding mode of dioxygen in enzymes.

Circular Dichroism spectroscopy - Basic principle - Origin of optical activity -Chirality and nomenclature of chiral complexes - Cotton effect- optical isomerism in octahedral complexes - absolute configuration of complexes - stereoselectivity and conformation of chelate rings - Optical Rotatory Dispersion and linear dichroism -Examples - Magnetic circular dichroism theory - Determination of electronic ground state properties: saturation curves, temperature dependence in the linear limit. Application of CD in conformation analysis of biomolecule(s) (DNA).

Unit –II- Electron Paramagnetic Resonance Spectroscopy

ESR introduction - Zeeman Equation, g-value, nuclear hyperfine splitting interpretations of the spectrum, simple carbon centered free radicals. Anisotropy-gvalue and hyperfine splitting constant - McConnel's equation - Krammer's theorem – spin-orbit coupling – dipolar contribution – dipole-dipole interaction - ESR of transition metal complexes (copper, manganese and Vanadyl ions) – isotropic, axial and rhombic spectra of copper(II) systems – Application of EPR: Structural elucidation of coordination complexes: Determination of electron delocalization, bonding mechanism of dioxygen adducts of dinuclear cobalt complexes, determination of nuclear spin state – EPR of low-spin Hemes, blue copper proteins.

Unit –III- Inorganic NMR, NQR Spectroscopy

 31 P , 19 F NMR spectrum of HPX₂, P₄S₃, TiF₄, BrF₅, SF₄, SF₆, XeF₄O, C SIF₆^{2-,} B₃H₈⁻, NF₃, P₃N₃Cl₄F₂, ClF₅, ClF₃ Phosphorous and Hypophosphorous acid systems, HP(O)F₂, HOP(O)FH - use of lanthanide compounds as shift reagents. Applications to metalloproteins - paramagnetic complexes.

NQR - Principles – Introduction - Nuclear Quadrupole Energy Levels - Energy Levels and transition frequencies – Effect of a magnetic field - The Zeeman effect - Factors affecting the line width - Solid State Effects. Applications of NQR: Bonding in Boron trichloride and its adducts – Calculation of percentage of ionic character of a bond.

Unit IV - Mossbauer Spectroscopy

Introduction - Principle of the Mössbauer Effect and Basic Concepts of Mössbauer Spectroscopy - Doppler shift - Experimental Resonance Conditions - Sharpness of resonance - Recoil Effect - Cross-section for Resonant Absorption - Comparison Between Electronic and Nuclear Transitions - Mössbauer-Experiment (Mössbauer spectrometer black diagram only) - Hyperfine Interactions and Mössbauer parameters: Isomer Shift, Electric Quadrupole Splitting, Magnetic Dipole Splitting, Applications: Mossbauer spectra of high- and low-spin iron compounds and tin halides systems: Prussian blue-Turn bulls blue, iron-carbonyl compounds, Sodium nitroprusside, FeX₂, SnX₄, SnX₆, SnX₅Y (X & Y = F, Cl, Br, I) Tin halides - Spin Crossover, Molecular magnetism - Bioinorganic Compounds.

Unit V – Photoelectron Spectroscopy & X-ray Absorption Spectroscopy

Photoelectron spectroscopy (UV and X-ray) – Physical principle – Experimental details -Koopman's theorem - chemical shift and correlation with electronic charges – Applications of PES.

X-ray absorption spectroscopy (XAS) and Extended X-ray absorption fine structure (EXAFS) – Applications of X-ray absorption spectroscopy. X-ray Absorption Edges - X-ray Fluorescence - Measurement of X-ray Absorption Spectra -Theoretical Description of EXAFS Spectra - Single scattering, Multiple scattering – Data

reduction and analysis - Applications: structure determination, Resolution of crystallographic disorder, Oxidation state, prediction of molecular symmetry, determinations of atoms present in the first coordination sphere (Edge & EXAFS analysis) – Structure of Metal clusters.

Reference Book:

- 1. Lawrence Que, Jr.- Physical Methods in Bioinorganic Chemistry
- 2. R. S. Drago Physical methods in Inorganic Chemistry
- 3. A. K Das Bioinorganic Chemistry.
- 4. E. A.V Ebsworth, D. W. H. Rankin and S. Cardock- Structural Methods in Inorganic Chemistry.

Course outcomes:

On successful completion of this course students will be able to

CO1: Student will know complete knowledge about the basics of Inorganic spectroscopy and its application to the structure determination of inorganic compounds.

CO2: Student can able to solve the problems related to inorganic spectroscopy.

CO3: Particularly students will learn about the basics and application of IR, Raman, ORD, CD, EPR, NMR, NQR, Mossbauer spectroscopy, Photoelectron spectroscopy and X-ray absorption spectroscopy.

Prepared by: Dr. B.Murugesapandian

| Title of the Subject : | Energy, Diary and | No. of Credits: | 4 |
|------------------------|-------------------|-----------------|----|
| | Drug Chemistry | | |
| Code No | CHMA2EB | No. of Teaching | 60 |
| | | Hours | |

Course Objectives:

- To teach the students about the various factors responsible for the air pollution
- To learn about the energy conservation mechanism
- To study the types of drugs and their action on various diseases
- To learn the principle, properties and production of diary related products
- To acquire the knowledge on different types of soil, effective utilization of fertilizers and insecticides

UNIT-1

POLLUTION-ENVIRONMENTAL ISSUE: The air we breathe-composition of airburning of hydrocarbons- air quality-ozone-oxygen/ozone screen-biological effect of UV radiation-ozone formation and distribution in the atmosphere-paths of ozone destructionchlorofluorocarbons and their interactions with ozone.

Chemistry of global warming-green house effect-earth's energy balance-vibrating molecules and the green house effect-molecular response to radiation-methane and other green house gases-climate modeling-Neutralizing the threat of acid rain.

UNIT-II

NEW ENERGY SOURCES FOR THE NEW CENTURY: Renewable energy sources-Introduction to Solar energy-Waste Bio-Mass energy-Sea wave energy-Tidal energy-Ocean thermal conversion energy-Geothermal energy-Wind energy-Nuclear fusion energy.

Solar Energy-Fuel from sunlight-splitting of water-hydrogen from sunlight-hydrogen economy-fuel cells-batteries-photovolataics-stealing the sun.

Nuclear energy- nuclear fission and fusion-production of electricity by nuclear reactor-radioactivity and the hazards of radioactivity-living with nuclear power.

UNIT –III

DRUGS CHEMISTRY: Antibacterial Drugs-Sulpha drugs, (ii) Antibiotics-Sulphanilides-Properties of Sulphanilamides, Mechanism of Action of Sulpha drugs, Sulphanilamide, Sulphadiazine, Cibazole, Sulphafurazole, Prontosil; Antibiotics; Classification of Antibiotics; Chloramphenical; Penicillin; Streptomycin; Tetracycline; Macrolides.

Anticonvulsant Agents-Barbiturates-Synthetic uses; Mydantoin; Oxazolinediones; Acetyl Urea derivatives; Succinimides; Miscellaneous.

Acquired Immuno Deficiency Syndrome (AIDS)-Introduction; Prevention; Treatment-Heterocyclic compounds as (eg., Quinoline, Carbazole, Coumarin and Naphthyridines)-HIV Integrase Inhibitors – Anti-HIV natural products - Synthesis.

Awareness through chickun-guinea-Chikungunya, Causes; Virus; mosquito; Emergent in drug discovery- Comparative studies with malaria.

UNIT-IV

DAIRY CHEMISTRY: Milk and Milk products-Composition of Milk; Flavour and aroma of Milk; Physical properties of Milk; Effect of heat on Milk; pasteurization; Homogenisation; milk products; Cream; butter; ice cream; milk powder

UNIT-V

AGRICULTURAL CHEMISTRY: Soil Chemistry-Introduction; Soil classification & survey; Properties of Soil; Soil Texture; Soil Water; Soil Temperature; Soil Colloids; Soil Minerals; Soil pH acidity and alkalinity; Buffering Soil; Soil Fertility; Soil formation.

Insecticides, Fungicides and Herbicides- Introduction; Methods of Pest Controls; Methods of using Pest Controls; insecticides; the arsenic compounds; Fluorine compounds; Boron compounds; Mercury compounds; Copper compounds; Sulphur compounds; Modern Insecticides; Some Important Herbicides; Rodenticides; Benefits of Pesticides; Adverse Environmental effects of pesticides.

Fertilizers- Classification of Fertilizers; Important example for Fertilizers; Nitrogeneous fertilizers, Phosphate fertilizers, Potash fertilizers; Effects of fertilizers.

Manures, compost and saw dust- Farm yard Manure; Compost; Reinforcing Manure; Green Manure Crops; Saw dust; Night soil, sewage and sludge; Bio gas production and Manure.

REFERENCES

1) Chemistry in Context: Applying Chemistry to Society, Conard L. Stanitski. Luey Pyrde Eubenks. Catherine H. Middle Camp and Wilmer J. Stratton, third edition, **2000**, Mc Graw Hill.

2) Chemistry of the environment, Bailey, Clark, Ferris, Isrause, Strong, second edition, **2001**, Elsevier publications.

3) Energy resources and the environment, V. K. Prabhakar, 2001.

4). Fundamental Concepts of Applied Chemistry, Jayashree Ghosh, S.Chand, 2005

5). I. P. Singh, S. B. Bharate and K.K.Bhutani, Current Science, Vol. 89, NO. 2, 25, July-2005

Course Outcomes (CO)

On successful completion of the course, the student will able to gain

| CO1 | Understood the Quality of air, pollutants and its lethal effects |
|------------|---|
| CO2 | Acquired knowledge on sustainable energy |
| CO3 | Studied the usage of drugs for different diseases |
| CO4 | To understand the process of making different dairy products |
| CO5 | Impart their knowledge on soil fertility, residue and proper usage of fertilizers |

Mapping

| PSO CO | - PSO1 | PSO2 | PSO3 | PSO4 | PSO5 |
|-----------|--------|------|------|------|------|
| CO1 | S | Н | S | S | М |
| CO2 | S | S | S | S | Н |
| CO3 | S | S | S | Н | Н |
| CO4 | S | S | S | Н | М |
| CO5 | S | S | S | Н | М |

S-Strong; H-High; M-Medium; L-Low

Course Prepared by

Dr. M.V.Kaveri / Dr.T.Suresh

Course Approved by

Professor and Head

| Title of the Subject | INORGANIC | No. of Credits: | 4 |
|----------------------|------------|-----------------|----|
| : | PRACTICALS | | |
| Code No | CHMA23P | No. of Teaching | 60 |
| | | Hours | |

Course Objectives:

- To equip the students with analytical skills by analyzing the given inorganic salt mixture containing two common cations and two rare cations
- To perform systematic qualitative analysis with the strong theoretical back ground
- To impart knowledge on the quantitative analysis of different metal ions
- To enable the students to prepare simple complexes by using published reactions

Contents

1. Qualitative analysis:

Qualitative analysis employing semi-micro methods and spot tests of mixtures of common cations and ions of the following less familiar elements.

Tungsten, selenium, molybdenum, cerium, thorium, zirconium, vanadium, uranium and lithium.(minimum 5)

2. Colorimetry:

Colorimetric estimations of copper, nickel, iron and chromium using photoelectric colorimeter.

3. Titrimetry:

Complexometric titrations involving estimations of calcium, magnesium, nickel, zinc and hardness of water.

4. Preparation of inorganic complexes:

About six preparations involving different techniques selected from the following.

- (i) Nickel ammonium sulphate
- (ii) Tris(thiourea)copper(I) chloride
- (iii) Potassium tris(oxalato)ferrate
- (iv) Hexamminecobalt(III) chloride
- (v) Ammonium hexachloro stannate(IV)
- (vi) Tetrammine copper(II) sulphate
- (vii) Chloropentamminechromium(III)nitrate
- (viii) Hydroxyl amine hydrochloride

(ix) a versaurapentampingechromium (UL) chloride

Reference Books

- 3. V.V.Ramanujam, Inorganic Semimicro qualitative analysis, 3rd edition, National Publishing company,1974
- 4. R.Mukhopadhyay & P.Chatlerjee, Advanced Practical Chemistry, Book & Allied (p) ltd 2007. C
- 5. J.Men dham, R.C. Denney, M.J.K.Thomas Darid &J.Bares, Vogels quantitative chemical analysis, 6h edition prentice hall 2000.

Course Outcomes (CO)

On successful completion of the course, the student will be

| CO1 | Able to identify the nature of any unknown metal ions |
|------------|--|
| CO2 | To identify the presence of microlevel compounds occurring in crude |
| | form in the nature |
| CO3 | To determine the water quality in terms of metal content |
| CO4 | Able to design and prepare the starting material leading to the synthesis of |
| | therapeutic compounds |

Mapping

| PSO CO | PSO1 | PSO2 | PSO3 | PSO4 |
|-----------|------|------|------|------|
| CO1 | S | Н | S | S |
| CO2 | S | S | S | S |
| CO3 | S | S | S | Н |
| CO4 | S | S | S | М |

S-Strong; H-High;

Prepared by : Dr. M.V.Kaveri

Title of the Subject:SUPPORTIVE -IINumber of Credits: 2 (Four)(CHEMISTRY IN DAY TO DAY LIFE)

Code No.: GS73

No. of Teaching hours: 25

Course Objectives

- To acquire the fundamental concepts related to the chemistry in daily life
- To understand the importance of different types of commercial products for the environment
- To apply the basic concepts of chemistry in the manufacture of commercial products for the society
- To find the efficiency and the utility of the byproducts derived from the basic and applied concepts of chemistry
- To have knowledge about the basic concepts of various micronutrients, fertility, dyes, disfectants and detergents.
- To introduce the properties, structural elucidation, applications and the demerits of the products of the applied chemistry.

Contents

Unit – I Essential Micronutrients

Carbohydrates - Proteins - Lipids - Nucleic acids and Vitamins – Definition, Sources, Classification, Applications and Diseases due to deficiency.

Unit – II Soil Nutrients and Food Additives

Fertilizers – Pesticides - Insecticides – Definition, Classification, Characteristics and Uses. Additives –Definition, Characteristics, Uses and Abuse of additives in foods and beverages.

Unit – III Dyes, Paints and Pigments

Dyes – Definition, Classification based on mode of application and structure, Applications. Paints – Definition, Ingredients, Characteristics, uses and drying process. Pigments - Varnishes - Definition, Characteristics, Types and Uses.

Unit – IV Soaps, Detergents and Disinfectants

Soaps and Detergents - Definition, Ingredients, Classification, Characteristics and Uses. Disinfectants – Definition, Characteristics and Uses. Perfumes - Definition, Characteristics, Raw materials and perfumes used in soaps - Cosmetics.

Power Point Presentation: Micronutrients

Seminar: Fertilizers, Pesticides and Insecticides

Assignment: Dyes and Paints

Books for Reference:

- 1. K.Bagavathi Sundari (2006), Applied Chemistry, MJP Publishers.
- 2. Des W.Connell (2016). Basic Concepts of Environmental Chemistry, Second edition, Taylor & Francis Group.
- 3. Ley E.Manahan (2009), Fundamentals of Environmental Chemistry, Third Edition, CRC Press, Taylor & Francis Group.

Course Outcomes (CO)

| K1 | CO1 | To introduce the concepts, definition and importance of the chemistry in the |
|----|-----|--|
| | | form of various products. |
| K2 | CO2 | To understand the occurrence, source, types, uses and demerits of the |
| | | industrial products |
| K3 | CO3 | To gain the knowledge of the implementation of fundamental chemistry |
| | | concepts in the manufacture of commercial products for the society |
| K4 | CO4 | To analyze the structural relationship of the commercial materials with the |
| | | effect of applications and the biological implications of micronutrients |

| PSO CO | PSO1 | PSO2 | PSO3 | PSO4 | PSO5 |
|-----------|------|------|------|------|------|
| CO1 | Н | Н | М | Н | Н |
| CO2 | S | М | Н | Н | S |
| CO3 | М | S | S | S | М |
| CO4 | М | Н | Н | М | Н |

S-Strong; H-High; M-Medium; L-Low

Prepared by : Dr. I.Prabha

Number of Credits: 4

Title of the Subject: **Organic Chemistry –III** (Spectroscopy & Organic Photochemistry)

Code No.: CHMA33A

No. of Teaching hours: 65

Course Objectives:

- To understand the basic principles of Mass and NMR spectroscopy and their application in organic molecules
- To gain the basic principles of photochemistry of alkane and ketone in aromatic systems
- To acquire the knowledge about pericyclic reactions and dealt with stereochemistry of the organic molecules involved in pericyclic reactions.

Contents

Unit – I

Mass Spectroscopy:

Presentation and analysis of spectra - determination of molecular formula - nitrogen rule - isotopic abundance analysis - metastable ions and peaks - the molecular ion peak. Fragmentation process - symbolism (scission only) - even and odd electron ions - scission with rearrangement - Retro Diels-Alder rearrangement - McLafferty rearrangement - double band and (or) ring equivalents implied from a formula.

Fragmentation associated with functional groups - aliphatic compounds - aldehydes - ketones - carboxylic compounds - esters - amides - alcohols - thiols - amines - ethers - sulphides and halides - aromatic compounds - eliminations due to ortho group.

Unit – II

Nuclear Magnetic Resonance Spectroscopy:

Magnetic properties of nuclei - theory of nuclear resonance - chemical shifts - spinspin coupling - shielding and deshielding mechanisms - chemical exchange - applications of NMR to organic compounds - nuclear magnetic double resonance - resonance with other nuclei - 13C NMR (elementary idea only). Applications of organic spectroscopy: Structure determination of organic compounds by using UV-Vis, IR, 1H & 13C-NMR and Mass spectroscopic techniques (simple molecules only – restricted to 12 carbon systems with/without one hetero atom).

Unit - III

Photochemical Excitation and Ketone Photochemistry:

Light absorption – Experimental techniques – Electronic transitions – Franck – Condon principle – Jablonski diagrams – Intersystem crossing – Energy transfer – Molecular orbital view of excitation – The geometry of excited states – Reactivity of electronically excited ketones –alpha - cleavage - gamma - hydrogen transfer Norrish Type I, Type II, Type III reactions – Photoreduction – Oxetane formation – Reactivity of Pi, Pi* excited ketones – Photochemistry of alpha, beta - unsaturated ketones – Optical pumping – Dienone phenol rearrangement.

Unit - IV

Photochemistry of Alkenes and Aromatic Compounds:

Olefin photochemistry – conjugated olefins – Isomerisation and rearrangements – Cis trans isomerisation – valence isomerisation – rearrangement of 1,4 and 1,5 dienes – dipimethane rearrangement - Cope and Claisen rearrangement – cycloaddition reactions – Photochemistry of Aromatic compounds – Arene photoisomerisation – Photodimerisation – Cycloaddition reactions – 1,2 cycloadditions – Photooxygenation – ene reaction.

Unit - V

Pericyclic Reactions and their Stereochemistry:

The stereochemistry of electrocyclic reactions – Symmetry properties of molecular orbitals – Symmetry control of electrocyclic reactions – perturbation theory in pericyclic reactions – Woodward Hoffmann rules – orbital correlation diagrams – The Frontier orbital theory – Electrocyclic conversion of 1,3 – dienes and 1,3,5 – trienes.

Sigmatropic reaction – Stereochemistry of sigmatropic reactions – cycloaddition – classification of cycloaddition reaction – orbital symmetry and cycloaddition – concerted Vs non-concerted cycloaddition - 2+2 and Diel's Alder reaction – Reactivity of dienophile and diene components – orientation – stereochemistry of Diel's Alder reaction.

References

- 1. I. L. Finar, Organic chemistry, vol. I and vol. II.
- 2. Nakanishi et. al., Natural product chemistry, vol. I, Academis press, 1974.
- 3. Newman, Terpenes and Terpenoids.
- 4. E. L. Eliel, Stereochemistry of carbon compounds, Mc Graw Hill, 1962
- 5. P.Ramesh, Basic principles of Organic Stereochemistry, Meenu publication, 2005.
- 6. Heterocyclic Chemistry, J. A. Joule, K. Mills and G. F. Smith, Chapman and Hall
- 7. Heterocyclic Chemistry, T. L. Gilchrist, Longman Scientific Technical
- 8. R. K. Bansal, Heterocyclic Chemistry; 3rd Ed., Wiley Eastern Ltd, New Delhi, 1999.

Course Outcomes:

On successful completion of the course, the students will be able to

| CO1 | To remember the basic principles of Mass and NMR spectroscopy. To keep |
|-----|--|
| | in mind the principles involved in photochemistry and pericyclic reactions |
| CO2 | To understand the concept of Mass and NMR spectroscopies involved in |
| | organic molecules and then knows about the photochemistry and |
| | pericycliclic reactions mainly play in organic molecules. |
| CO3 | To apply the concept of Mass and NMR spectroscopy to find out the known |
| | and unknown organic molecules. To apply the basic knowledge of |
| | photochemistry and pericyclic reactions into the organic molecules to find |
| | out the exact stereochemistry involved in the reaction systems. |
| CO4 | To analyze the organic reaction problems by using the following |
| | spectroscopy such as Mass and NMR such is frequently asking in |
| | competitive examinations. To investigate the organic chemistry problems by |
| | using photochemistry and pericyclic reactions in the competitive |
| | examinations like CSIR-UGC-NET and GATE. |

Course prepared by : Dr. A. Kannan

Title of the Subject: Inorganic Chemistry –III

No of Credits: 4

(Solid State and Nuclear Chemistry)

Code No: CHMA33B

No of Teaching hours: 60

Course Objectives:

- To gain the basics in solid state chemistry.
- To emphasize the significance of crystallographic properties and description of crystal structures.
- To acquire awareness about the defects in crystal structure and its effect in electrical properties.
- To understand the working principle and application particle accelerator and counters.
- To get knowledge about the application of nuclear chemistry.

Contents

Unit – I : Solid State Chemistry -I

The growth and form of crystals - the crystal systems and Bravais lattices - Miller indices and labelling of planes - symmetry properties - crystallographic point groups and space groups - fundamentals of X-ray diffraction - powder and rotating crystal methods - systematic absences and determination of lattice types - analysis of X-ray data for cubic system - structure factor and Fourier synthesis - electron and neutron diffraction and structure determination.

Unit - II: Solid State Chemistry -II

Types of solids - close packing of atoms and ions - bcc , fcc and hcp voids - radius ratio - derivation - its influence on structures - structures of rock salt - cesium chloride - wurtzite - zinc blende - rutile - fluorite - antifluorite - diamond and graphite - spinel - normal and inverse spinels and perovskite - lattice energy of ionic crystals - Madelung constant - Born-Haber cycle and its applications.

Unit - III: Solid State Chemistry -III

Metallic state - free electron and band theories - non - stoichiometry - point defects in solids - Schottky and Frenkel defects - linear defects - dislocations - effects due to dislocations - electrical properties of solids - insulators - intrinsic semiconductors - impurity semiconductors (n and p- type) and superconductors - elementary study of liquid crystals.

Unit – IV: Nuclear Chemistry - I

Nucleus: nuclear structure - stability of nuclei - packing fraction - even - odd nature of nucleons - n/p ratio - nuclear potential - binding energy and exchange forces - shell model and liquid drop model.

Decay of radionuclei: rate of decay - determination of half-life period - secular equilibrium and decay series.

Modes of decay: alpha, beta, gamma and orbital electron capture - nuclear isomerism - internal conversions - Q value - nuclear cross section - threshold energy and excitation functions.

Particle acceleration and counting techniques: linear accelerator - cyclotron and synchrotron - betatron - G. M. counter - proportional and scintillation counters.

Unit – V: Nuclear Chemistry - II

Different type of nuclear reactions with natural and accelerated particles - transmutation - stripping and pick-up - spallation - fragmentation, etc. - fission - characteristics of fission reaction - product distribution and theories of fission - fissile and fertile isotopes - U235, U238, Th232 and Pu239 - atom bomb - nuclear fusion - stellar energy - synthesis of new elements - principles underlying the usage of radioisotopes in analysis - agriculture - industry and medicine - mechanism of chemical reactions - uses of radioisotopes in analytical chemistry - isotopic dilution analysis - neutron activation analysis and dating methods.

Reference Book:

- 1. W.J. Moore Physical Chemistry, 4th edition
- 2. L.V. Azaroff- Introduction of Solids
- 3. W. E. Addision-Structural Principles in Inorganic Chemistry
- 4. N. B. Hannay Solid State Chemistry
- 5. R. A. Alberty Physical Chemistry
- 6. A. K. Das Fundamental Concepts of Inorganic Chemistry
- 7. P. Atkins & J. d. Paula Physical Chemistry
- 8. S. Glasstone Sourcebook of Atomic Energy
- 9. H. J. Arnikar Essentials of Nuclear Chemistry
- G. Friedlander, J. W. Kennedy, E. S. Macias, J. M. Miller- Nuclear and Radiochemistry 3rd Edition

Course outcomes:

On successful completion of this course students will be able to

CO1: Student will know through knowledge about the basics of solid state chemistry, X-ray crystal structure of the compounds, close packing of solids, important feature of spinels, lattice energy, various defects in crystals and electrical properties of solids.

CO2: Student will learn how to solve the problems in solid state chemistry.

CO3: Students will get clear idea about the basics of nuclear chemistry and its application in various fields.

Course prepared by : Dr. B.Murugesapandian Dr.K.Sundaravel

Title of the Subject : PHYSICAL CHEMISTRY – III Number of credits :4

Code No.

Number of Teaching hours : 60

Course Objectives :

• To learn the rate and order of different reaction kinetics.

: CHMA33C

- To give a thorough introduction about slow and fast reaction kinetics and macromolecules.
- To provide knowledge in homogenous and heterogeneous catalysis.

Unit - I CHEMICAL KINETICS

Rates of chemical reaction – kinetics of first, second and third order reactions – complex methods of determining rate laws, order and molecularity concepts –Theories of reaction rates –Arrhenius theory, hard-sphere collision theory of gas phase reactions – Potential energy surfaces – Activated complex theory for ideal gas reactions (formation in terms of partition functions) – Relation between activated complex theory and hard sphere collision theory – Thermodynamic formulation-activated complex theory (Enthalpies and entropies of activation) – Kinetic isotopic effect.

Unit - II KINETICS OF REACTION IN SOLUTION

Comparison between gas phase and solution reactions – Cage effect – The influence of the solvent on the reactions between ions and reaction between ions and neutral molecules – Influence of ionic strength on rates of reactions in solution – Significance of volume and entropy of activation – Secondary salt effect - Kinetic treatment of complex ion.

Parallel reactions of the same order (first or second order) – Reversible reaction of the same order (first or second order) – First order forward and second order backward – Consecutive first order reactions, steady state and rate determining step (or equilibrium) approximation of complex reactions – Chain reactions and explosions.

Unit - III FAST REACTIONS

Study by stop-flow techniques, relaxation methods – Flash photolysis, magnetic resonance methods - Kinetic theory of gases and its Postulates – Maxwell distribution of Molecular velocities - Expressions for most probable velocity, average velocity, root mean square velocity – Collision diameter, Collision frequency, Mean free path. Transport properties of gases – Thermal conductivity, Viscosity, Diffusion - principle of equipartition of energy.

Unit - IV HOMOGENEOUS CATALYSTS

Specific and general acid-base catalysis – Bronsted catalysis law – Acidity functions. Enzyme catalysis (single substrate reactions only) – Michaelis-Menton kinetics – Influence of pH and temperature on enzyme catalysis.

Surface Phenomenon and Heterogeneous catalysts - Adsorption and free energy relation at interfaces – Gibbs adsorption isotherm – Physisorption and chemisorptions – Adsorption isotherms (Langmuir and BET) – Measurement of surface area – Kinetics of heterogeneous catalysis (Langmuir Hinshelwood mechanism and Eley-Rideal mechanism) – Semiconductor catalysis.

Unit - V MACROMOLECULES

Addition and condensation polymers, number average and weight average molecular weights of macromolecules – Determination of molecular weights – Kinetics of polymerization, molecular and free radical mechanism – Polymerisation in solution – Stereochemistry.

References

- 1. K.J. Laidler, Chemical Kinetics, Pearson, 3rd Ed., 2003.
- 2. Gurdeep Raj, Chemical Kinetics, Krishna Prakashan Media Pvt. Ltd., 2016.
- 3. P. Atkins Physical Chemistry, Oxford University Press, 8th Ed., 2006.
- 4. W. J. Moore Physical Chemistry, 5th Ed., 1998.
- 5. A.A.Frost and R.G. Pearson, Kinetics and Mechanism, 1961.
- 6. F.W. Billmeyer, Text book of Polymer science, Wiley- Interscience, 3rd Ed., 2007.

Course Outcomes:

On successful completion of the course, the students will be able to

CO 1 – Get detailed knowledge about the rate of any reaction and various parameters which

affects the rate.

- CO 2 Understand the theories of catalytic activity and polymerization techniques.
- CO 3 Apply the catalytic principles in large scale industries.
- CO 4 Impart knowledge in solid and liquid phase kinetics.

Course prepared by: Dr.M.Illanchelian

| Title of the Subject | BIO-ORGANIC | No. of Credits: | 3 |
|----------------------|--------------------|-----------------|----|
| : | CHEMISTRY | | |
| Code No | CHMA3EA | No. of Teaching | 60 |
| | | Hours | |

Course Objectives:

- To teach the students the organic chemistry essential role in biology
- To teach the biosynthetic organic methodologies.
- To teach the mode of energy source in biological system
- To teach novel reagents involved in bioorganic reactions
- To teach the medicinal chemistry

Unit I:

Retrosynthetic analysis, Protection and Deprotection: An introduction to reterosynthesis - synthen – synthetic equivalent – target molecule, functional group interconversion. Retro synthetic analysis and Synthesis of simple organic molecules such as 1,2, 1,3, 1,4 and 1,5 dicarbonyl compounds both acylic and cyclic. Formation of 3, 4, 5 and 6 membered cyclic compounds. Use of standard reactions, like Grignard reactions, Robinson annulations. Protection and deprotection of functional groups (R-OH, RCHO, R-CO-R, R-NH₂ and R-COOH). Use of PTC (Phase-transfer catalyst) and Crown ethers in organic synthesis.

Unit II:

Bio-Organic Chemistry: Pyrimidines (cytocine and uracil) and purines (adenine and guanine only).

Nucleic acids - structure and synthesis of nucleosides - structure and synthesis of nucleotides -Structure of RNA and DNA and their biological importance.

UNIT III:

Bio-Energetics: Concept of energy – thermodynamic principles – first law, second law, combining the two laws – relationship between standard free energy change and equilibrium constant. Standard free energy values of chemical reactions – Adenosine triphosphate (ATP) as universal currency of free energy in biological systems – ATP hydrolysis and equilibria of coupled reactions – inter conversion of adenine nucleotides.

Unit IV:

Novel Reagents in Organic Synthesis: Synthesis and applications of Organolithium, Organomagnesium, Organozinc and Organo Copper reagents. Modern synthetic methods: Metal mediated C-C coupling reactions: Mechanism and synthetic applications of Heck, Stille, Suznki, Negishi, Sonogashina, McMurray, Metathesis, Carbonylation reactions.

UNIT V:

Medicinal Chemistry: Design, development and mechanism of action of drugs: Antimicrobial, anticancer, antidiabetic, antiinflammatory and antitubercular drugs and their mechanism of action. Cardiovascular drugs: Cardiotonic, Antihypertensive, Antirhythmic and Lipotropic drugs.

Metals in Drug design: Historical development and advantages-Immunopharmacology and drug development.

References

- 1. Organic Synthesis, 2nd Edition by Michael B Smith, McGraw-Hill, New York.
- R.K. Mackie and D.M. Smith. 1998, Guide book to organic synthesis, ELBS Publication.
- 3. I. L. Finar, 1986, Organic Chemistry, 5th Edition, Vol .II, ELBS Publication.
- L. Smith, Robert L. Hill .1. Robert Lehman, Robert J .Iet Rowitz, Philp Handler and abrahim white principles of Biochemistry General aspects, 7th Edition, McGraw Hill Int.
- 5. L. Stryer, Biochemistry, W.H.Freeman and Co., New York.
- http://www.cuchd.in/e-library/resource_library/university%20institutes %20of%20sciences/Fundamentals%20of%20Biochemistry/Chap-20.pdf.
- 7. B.l. Smith, 1980, Organic synthesis, Chapman and Hall, NY.
- 8. Francis.A. Carey, Richard J. Sundbreg, 2001, Advanced Organic Chemistry, 4th Edition, Plenum Press, New York.
- 9. Medicinal Chemistry for the 21st Century. Ed. C. G. Wermuth, Blackwell, Oxford, 1992, ISBN 0632034084.
- Drug Metabolism: Databases and High Throughput Testing During Drug Design and Development. Ed. P. W. Erhardt, Blackwell, Oxford, 1999. ISBN 0632054329.

11. Heterocyclic Chemistry, J. A. Joule, K. Mills and G. F. Smith, Chapman and Hall.

12. Heterocyclic Chemistry, T. L. Gilchrist, Longman Scientific Technical.

3. a versatile knowledge of aromaticity,

Course Outcomes (CO)

On successful completion of the course, the student will able to gain

| CO1 | Understood role and application of organic chemistry role in biology |
|------------|--|
| CO2 | Clinical skills in biology by using organic knowledge |
| CO3 | Learnt the knowledge of organic reagents in biology |
| CO4 | Gained Knowledge about medicinal chemistry |

Mapping

| PSO CO | PSO1 | PSO2 | PSO3 | PSO4 | PSO5 |
|-----------|------|------|------|------|------|
| CO1 | Н | S | М | Н | S |
| CO2 | Н | М | Н | S | Н |
| CO3 | М | S | S | М | М |
| CO4 | М | Н | Н | М | Н |

S-Strong; H-High; M-Medium; L-Low

Prepared by : Dr. T.Suresh

| Title of the Subject : | INDUSTRIAL ORGANIC CHEMISTRY | No. of Credits: | 3 |
|---------------------------|------------------------------------|--------------------------|----|
| Code No | СНМАЗЕВ | No. of Teaching Hours | 50 |

Course Objectives:

- To teach the students the essential role of industrial process of petrochemicals
- To teach methodologies involved in dyeing in industries.
- To teach preparation of soaps,oils and waxes
- To teach the chemistry of natural and synthetic polymers.

Unit –I

Industrial Organic Syntheses-Petrochemicals: Introduction-Raw material and basic processes-chemical processes used in industrial organic synthesis-petrochemicals-methanol-ethanol-rectified spirit from beer-methylated spirit-proof spirit-preparation of absolute ethanol from rectified spirit-acetaldehyde-acetic acid-isopropanol-ethylene glycol-glycerine-acetone-phenol-ethylacetate.

Unit –II

Hydrocarbons from Petroleum: Introduction-raw materials-saturated hydrocarbons from natural gas-uses of saturated hydrocarbons-unsatutated hydrocarbons acetylene,ethylene,propylene,butylenes.

Aromatic hydrocarbons-benzene,toluene,xylenes-chemical processing of paraffin hydrocarbons,-acetylene and aromatic hydrocarbons.

Unit-III

Dyes: Introduction-sensation of colour-colour and constitution-nomenclature-basic operations in dyeing-classification of dyes according to the mode of application.-synthesis, reaction and applications of diphenylmethane dyes-triphenylmethane dyes-phthalein dyes-xanthene dyes-acridine dyes-sulphur dyes-cyanine dyes.

Unit-IV

Oils , Fats, Waxes and Soaps: Introduction-Distinction between oils and fats-properties and its classifications-animal fats and oils-difference between, animal, vegetable and mineral oils-isolation of essential oils and their uses-saponification value-ester value-acid value-iodine value-wijs method-Reichert meissl value-Henher value-elaiden test-hydrogenation of oils – Soap and its manufacture-general consideration in soap making –manufacture of toilet and transparent soaps-oil to be used for soap-cleansing action of soap.

Unit –V

Natural and Synthetic Polymer: Introduction-types of polymerization and their utility, mechanism involved in preparation-thermoplastic and thermosetting polymers-phenolic resins, poyure than es, epoxyresins, alkyl resins. natural and synthetic rubber-types and their utility-polymer properties and structure.

References:

1. Industrial Chemistry (Including Chemical Engineering) -- B.K.Sharma (10th Edition)

2. *Outlines of Chemical Technology* – For the 21st Century – M.Gopala Rao & Marshall, Sittig (3rd Edition).

4. a versatile knowledge of aromaticity, Course Outcomes (CO)

On successful completion of the course, the student will able to gain

| CO1 | Understood role of industrial process and application of petrochemicals |
|-----|---|
| CO2 | Preparative skills in manufacturing soaps, dyes and waxes |
| CO3 | Learnt the knowledge of natural polymers as their behaviour |
| | |

Mapping

| PSO CO | PSO1 | PSO2 | PSO3 | PSO4 | PSO5 |
|-----------|------|------|------|------|------|
| CO1 | Н | S | М | Н | S |
| CO2 | Н | М | Н | S | Н |
| CO3 | М | S | S | М | М |

S-Strong; H-High; M-Medium; L-Low

Prepared by : Dr. T.Suresh

Title of the Subject: Physical Chemistry Practicals

Number of Credits: 4 (Four)

Code No.: CHMA33P

No. of Teaching hours: 60

Course Objectives:

- To learn the practical knowledge about the chemical kinetics, conductivity and potentiometric titrations using lab scale experimental methods.
- To motivate the students to understand the basic principles of chemical kinetics, potentiometric and conductometric titrations.
- To learn proper maintenance of record observations and data interpretation.

Contents

1. Chemical kinetics (I and II order) - 5 Nos.

(Determination of rate constant of acid catalysed hydrolysis of an ester, Determination of Arrhenius parameters, kinetics of persulphate - iodine reaction, study of primary salt effect, kinetics of iodination of acetone)

- 2. Molecular weight determination 1 No. (Rast method)
- 3. Phase study simple eutectic system 1 No.
- 4. **Distribution coefficient 2 Nos.** (partition coefficient of I₂, the study of equilibrium of the reaction between KI and iodine)

5. Conductivity experiments - 6 Nos.

(acid - base titration, mixture of acids vs NaOH, precipitation titrations, mixture of halides, Determination of dissociation constant, verification of Debye - Huckel Onsagar equation and Kohlraush law)

6. Potentiometry - 5 Nos

- (i) redox titrations
- (ii) acid base titrations
- (iii) precipitation reactions
- 7. Validation of **Freundlich adsorption isotherm.**
- 8. Determination of unknown concentration of the given solution using **photoelectric** colorimeter.

References:

- 7. P.S. Sindhu "Practical in Physical Chemistry", Macmillan, 2005.
- 8. H.R. Crockford, J.W. Nowell, "Laboratory manual of Physical Chemistry", John Wiley and Sons, Inc.

Course Outcomes:

On successful completion of the course, the students will be able to

 $\mathrm{CO1}$ – To validate the theory of electrochemistry and the measurement of electrical conductance

through the practical seasons.

CO2 – To understand the basic concepts of conductometric and potentiometric titrations and the

quantitative analysis of unknown solutions using the corresponding instruments.

CO3 – To know about the practical applications of chemical kinetics as well as to understand about

the adsorption studies.

CO4 -To learn the measurement of cell potential, conductivity, pH etc., using various electrochemical instruments.

Course prepared by: Dr. S.N.Karthick

Title of the Subject: SUPPORTIVE -III Number of Credits: 2 (Four) (CHEMISTRY OF ENVIRONMENT)

Code No.: GS

No. of Teaching hours: 25

Course Objectives

- To acquire the basic concepts related to the chemistry for the effect of environment and the role of inorganic materials in biological applications
- To understand the importance of different types, unique properties of the commercial products to the benefit of environment
- To apply the basic concepts of chemistry in the manufacture of commercial products for the society
- To find the efficiency and the utility of the byproducts derived from the basic concepts of chemistry To have knowledge about the basic concepts of soil nutrients and effects, inorganic compounds, milk and oil.
- To introduce the properties, structural elucidation, applications and the demerits of the products of the applied chemistry.

Contents

Unit – I Impact of Soil

Soil-Introduction-Definition-Classification of Soil- Environmental properties of Soil-Soil minerals-Soil contamination- Ecological and health effects of Soil contamination.

Unit – II Role of Medicinal Inorganic Compounds

Medicinal inorganic compounds-Alum, Phosphoric acid, Ferric ammonium citrate: Preparation, Properties and uses. Biological role of inorganic compounds-Sodium, Potassium, Calcium and Iodine: Sources, biological role and deficiency.

Unit – III Milk

Milk- Composition of milk-Properties of milk- Effect of heat on milk- Pasteurisation: Definition, process and its effects- Homogenisation- Milk products- Ice cream.

Unit – IV Introduction to Oil

Introduction- Oils- Definition, Classifications, Properties, and uses- Animal, Vegetable and Mineral oils- Fat-Definition- Functional properties- Types of Fat- Uses- Effect of fat on health.

Power Point Presentation: Environmental properties and contamination of soil

Seminar: Medicinal Inorganic Compounds

Assignment: Milk and its importance

Books for Reference:

- 1. K.Bagavathi Sundari (2006), Applied Chemistry, MJP Publishers.
- 2. Des W.Connell (2016). Basic Concepts of Environmental Chemistry, Second edition, Taylor & Francis Group.
- 3. Ley E.Manahan (2009), Fundamentals of Environmental Chemistry, Third Edition, CRC Press, Taylor & Francis Group.

Course Outcomes (CO)

| K1 | CO1 | To introduce the concepts, definition and importance of the environmental |
|----|-----|---|
| | | chemistry in the form of various products. |
| K2 | CO2 | To understand the occurrence, source, types, uses and demerits of the |
| | | industrial products and the inorganic compounds |
| K3 | CO3 | To gain the knowledge of the implementation of fundamental chemistry |
| | | concepts in the manufacture of commercial products and its impact to the |
| | | environment |
| K4 | CO4 | To analyze the structural relationship of the commercial materials with the |
| | | effect of applications and the biological implications of inorganic |
| | | compounds |

| PSO CO | PSO1 | PSO2 | PSO3 | PSO4 | PSO5 |
|-----------|------|------|------|------|------|
| CO1 | Н | Н | S | М | М |
| CO2 | М | S | М | М | Н |
| CO3 | М | М | S | S | S |
| CO4 | S | М | М | Н | Н |

S-Strong; H-High; M-Medium; L-Low

Prepared by : Dr. I.Prabha

| Title of the Subject : | Organic Chemistry | No. of Credits: | 4 |
|------------------------|-------------------|-----------------|----|
| | -IV | | |
| Code No | CHMA43A | No. of Teaching | 60 |
| | | Hours | |

Course Objectives:

- To motivate the students to comprehend a knowledge on Aromaticity and Green Chemistry approach for to save environment
- To learn about retero synthesis and biosynthesis of Alkaloids and Steroids
- To learn about naming reactions and their application in Organic Synthesis
- To learn about the basic ideas about organic reaction mechanism and their intermediates

Unit - I

Aromaticity: Aromaticity- Concept of aromaticity – aromaticity of benzenoid and non benzenoid compounds – effect of aromaticity on bond lengths – resonance – resonance energies – electronic absorption spectra and induced ring currents – Huckel"s rule – structure and synthesis of azulenes – ferrocenes – sydnones – tropolones – fulvenes – annulenes.

Green Chemistry: Designing a green synthesis, basic principles of green chemistry-Elementary idea of Microwave and Sono chemistry

Unit – II

Alkaloids: Structural elucidation and biosynthesis of dictamnine – chinconine – morphine – reserpine – aeronycine – cocaine – lysergic acid and nicotine.

Unit - III

Steroids: Structural elucidation and spectrum of cholesterol – erogosterol - vitamin-D – equilenin – estrone - progesterone, Stigmasterol, Steriod harmones, androsterone, testosterone, Oesterol, Oestradiol, biosynthesis of steroids – Structure - synthesis of bile acids.

Unit – IV

Named reactions: Baylis-Hillman reaction, Mannich, Simmons – Smith, Reformatsky, Ullmann, Wittig– Horner, Peterson, Acyloin condensation, Robinson annulations, Oppenauer oxidation, m-ClC₆H₄COOOH.

Functional group transformations: Carbonyls (aldehyde and ketone)- Preparation from alcohols, alkenes, alkynes, arenes and carboxlic acid derivatives. Reactions: Nucleophilic additions-cyanide, bisulfate, ammonia, amines, oximes, hydrazines,

semicarbazide, hydride, hydrogen, organometallicreagents, Cannizaro and

Benzoin condensation reactions. Reaction of enones-1,2- and 1,4-additions. Oxidation of carbonyl compounds and Wittig reaction. Amines (both aliphatic and aromatic)-Methods of preparation of amines by reduction of nitro compounds, imine, amides and cyanides, Hofmann degradation of amides and ammonolysis of halides.Reactions-basicity and different amines, alkylation, acylation, Hofmann acidity of salt formation, elimination and diazonium formation and its reactions. Reactions of aromatic amines

Unit – V

Reagents in Organic Synthesis: Use of the following reagents in Organic synthesis and functional group transformation. Diborane, $LiAlH_4$, Ozone, OsO_4 , DCC, 1,3-Dithiane, LTA, Peracetic acid, Raney Nickel, PPA, CH_2N_2 , Tri-n-butyl tin hydride, *n*-Butyl lithium, NBS, DDQ, DBU (Diaza bicyclo-undecane), SeO₂, Tri methyl silyl iodide, Gilman''s reagent, Lithium dipropyl amide.

References

- 1. L.G.Wade Jr., Organic Chemistry.
- 2. I.L.Finar, Organic Chemistry, Vol.I and Vol.II.
- 3. L.F.Fieser and M.Fieser, Steriods, Reinbold, 1959.
- 4. P.J.Garrat, Aromaticity, Mc Graw Hill, 1971.
- 5. Jerry March Advanced Organic Chemistry.
- 6. R. T. Morrison, R. N. Boyd and S. K. Bhattacharjee, Organic Chemistry, 7th Edition, Pearson Education.
- 7. P. Y. Bruice, Organic Chemistry, 4th Edition, Pearson Education.
- 8. T. W. Graham Solomons and C. B. Fryhle, Organic Chemistry, 10th edition, Wiley.
- 9. Fieser & Fieser Reagents in Organic Synthesis.
- 5. a versatile knowledge of aromaticity,

Course Outcomes (CO)

On successful completion of the course, the student will able to gain

| CO1 | To make the students understand about the concept of aromaticity, |
|------------|---|
| | stability of organic molecules and green chemistry approach for human |
| | wealth environment. |
| CO2 | To understand the Biosynthetic idea of Alkaloids and Steroids |
| CO3 | To apply the mechanisms in solving chemical reactions. |
| CO4 | To review different types of reagents involved in chemical synthesis. |

Mapping

| PSO CO | PSO1 | PSO2 | PSO3 | PSO4 | PSO5 |
|-----------|------|------|------|------|------|
| CO1 | S | Н | S | S | М |
| CO2 | S | S | S | S | Н |
| CO3 | S | S | S | Н | L |
| CO4 | S | S | S | М | М |

S-Strong; H-High; M-Medium; L-Low

Prepared by : Dr. T.Suresh

Title of the Subject: Inorganic Chemistry –IV (Organometallic Chemistry) Code No: CHMA43B No of Credits: 4

No of Teaching hours:60

Course Objectives

- Learn about the development of organometallic chemistry and types of bonds in organometallic complexes
- Learn about the important organometallic complexes and their applications in various organic transformations as homogeneous/ heterogeneous catalysts
- Recognition of organometallic chemistry in Noble Prize for chemistry in 2001, 2005 and 2010

Contents

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 metal carbonyls - 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 – Wade's rule and isolobal relationship - 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 and alkylidyne complexes - synthesis and bonding in alkylidyne complexes - reactivity of alkylidene and alkylidyne complexes - synthesis and bonding in alkylidyne complexes - reactivity of alkylidene and alkylidyne complexes.

Unit - III

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 - IV

Cyclopentadienyl complexes - metallocenes - synthesis of metallocenes - bonding in metallocenes - reactions of metallocenes - Cp_2Fe/Cp_2Fe^+ couples in biosensors - bent sandwich complexes - bonding in bent sandwich complexes - metallocene halides and hydrides - metallocene and stereospecific polymerisation 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 - V

Organometallic compounds in homogeneous catalytic reactions - coordinative unsaturation - acid-base behaviour reaction - migration of atoms or groups from metal to ligand - insertion reaction - reactions of coordinated ligands - catalytic reactions of alkenes - isomerisation of alkenes - hydrogenation - hydroformylation and hydrosilation of alkenes - alkene polymerisation and oligomerisation - fluxional molecules - The Nobel Prize in Chemistry 2001- Assymetric synthesis, 2005- Olefins metathesis in organic synthesis and 2010 – Palladium catalysed cross coupling reactions in organic synthesis

Power point Presentations, Group discussions, Seminar ,Quiz, Assignment, Experience Discussion, Brain storming, Activity, Case study

Assignment: Types of bonding in organometallic chemistry and Nobel Prizes in chemistry. **Power point presentation**: Bondings in metal carbonyls and metallocene complexes, nucleophilic reactions on coordinated ligands.

Seminar: Important catalytic reactions of various organometallic complexes.

Books for Study

- 1. Organometallics 1, Complexes with transition metal-carbon σ -bonds, Manfred Bochmann, Oxford science publications, Oxford, 1994.
- 2. Organometallics 2, Complexes with transition metal-carbon π -bonds, Manfred Bochmann, Oxford science publications, Oxford, 1994.

Books for References

- 1. *Basic organometallic chemistry*, J. Haiduc and J. J. Zuckerman, Walter de Gruyter, Brelin, 1985.
- 2. *Inorganic Chemistry Priciples of structure and reactivity*, J. E. Huheey Harper International Edition, Harper and Rone New York, 1978.
- 3. *Advanced Inorganic Chemistry*, F. A. Cotton and G. Wilkinson, Fourth Edition.

Course Outcomes (CO)

| K1 | CO1 | Understand the historical development of Organometallic chemistry and |
|----|-----|---|
| | | uniqueness in various bonding behaviour of organometallic compounds. |
| K2 | CO2 | Gaining the knowledge on metal carbonyl compounds, various types of |

| | | insertion reactions in carbonyl chemistry and their applications |
|----|-----|--|
| K3 | CO3 | Organometallic alkyl, alkylidene and alkylidyne, alkene and alkyne |
| | | chemistry and application of them in insertion, double carbonylation, |
| | | olefin metathesis, hydrogenation, hydrosilation, oxidation and |
| | | polymerisation reactions. |
| K4 | CO4 | Inferring the importance of metallocene chemistry and the applications of metallocenes in stereospecific polymerisation of 1-alkenes and fluxional behaviour of π -electron systems and importance of organometallic chemistry in catalysis and recognition of Noble prizes 2001, 2005 and 2010. |

Prepared by : Dr. R. Prabhakaran

Title of the Subject : PHYSICAL CHEMISTRY – IV Number of credits :4

Code No. : CHMA43C

Number of Teaching hours : 60

Course Objectives :

- To present the laws of classical and statistical thermodynamics.
- To learn various co-efficient involved in thermodynamics.
- To develop a vast knowledge in the interpretation of various physical quantities involved in thermodynamics.

Unit – I THERMODYNAMICS AND NON-IDEAL SYSTEMS

Chemical potential and the definition of fugacity – Determination of fugacity of gases by graphical method and from equations of state – Variation of fugacity with temperature – Fugacity and the standard state for non-ideal gases – Fugacity (or activity) coefficient – Fugacity and mixtures of non-ideal gases, chemical equilibrium involving non-ideal gases.

Definition of activity. Activity coefficient. Temperature coefficient of activity. Standard states – Application of activity concept to solutions – The rational and practical approaches – Measurement of solvent activity from colligative properties – Determination of activity of solute – Use of activities in the formation of reaction potentials.

Unit – II THIRD LAW OF THERMODYNAMICS

Probability and third law – Need for the third law – Nernst heat theorem and other forms stating third law – Thermodynamic quantities at absolute zero – Statistical meaning of third law and apparent exception.

Mathematical introduction - Theories of permutations and combinations – Laws of probability – Distribution laws – Gaussian distribution.

Unit – III STATISTICAL THERMODYNAMICS - I

Maxwell-Boltzmann statistics – Thermodynamic probability – Thermodynamic probabilities of system in equilibrium – Boltzmann expression for entropy – Sterling's approximation – State of maximum thermodynamic probability – Legrangian multipliers – Thermodynamics probabilities of systems involving energy levels – Maxwell-Boltzmann distribution law – Evaluation of alpha and beta in M-B distribution law.

Unit – IV STATISTICAL THERMODYNAMICS - II

Partition function – definition, justification of nomenclature, microcanonical and canonical ensembles – Molecular partition function and canonical partition function – The relation between the total partition function of a molecule and the separate partition functions – Translational and rotational partition functions – Effect of molecular symmetry on rotational partition function – Ortho and para hydrogen – Vibrational partition function. Electronic partition function. Evaluation of thermodynamic properties E, H, S, A, G, Cv and Cp from monoatomic and diatomic ideal gases – Calculation of equilibrium constants of reactions involving ideal gases from partition functions.

Unit – V: STATISTICAL THERMODYNAMICS - III

Bose-Einstein and Fermi-Dirac Statistics: Bose-Einstein distribution law – Entropy of Bose-Einstein gas -Plank distribution law for black body radiation – Fermi-Dirac distribution law – Entropy of a Fermi-Dirac gas – Heat capacity of electron gas and the heat capacity of metals – Helium at low temperature – Negative absolute temperature.

Heat capacities of Solids: Einstein's and Debye's theories of heat capacities of solids.

References:

- 1. F.T. Wall Chemical Thermodynamics, Freeman and Company, 3rd Ed., 1974.
- 2. S. Glasstone Thermodynamics for Chemists, East West Press, 1st Ed., 2008.
- 3. J.F. Lee, F.W. Sears and D.L. Turcottee Statistical Thermodynamics, 2nd Ed., 1973.
- 4. M.C.Gupta Statistical Thermodynamics, New Age International, 2007.
- 5. G.W. Castellan Physical Chemistry, 1983.

Course Outcomes:

On successful completion of the course, the students will be able to

- CO 1 Understand the concepts of classical and statistical thermodynamics.
- CO 2 Comprehend the quantum statistics and partition function.
- CO 3 Analyze the variation of fugacity, heat capacities and various quantum statistics in determination of probability.
- CO 4 Apply third law of thermodynamics

Course prepared by : Dr.M.Illanchelian

| Title of the Subject : | Analytical Chemistry | No. of Credits: | 4 | |
|------------------------|-------------------------|-----------------|----|--|
| Code No | CHMA43D | No. of Teaching | 60 | |
| | | Hours | | |

Course Objectives:

- To study the various methods involved in analytical techniques
- To learn the statistical analysis
- To learn qualitative and quantitative measurements in the absorption and emission spectroscopy
- To apply the knowledge of electrochemistry in practical applications
- To learn the separation process using various chromatographic techniques

Unit I : Quantitative Inorganic Analysis

Theoretical basis of quantitative inorganic analysis-common ion effect solubility product, effect of acid, temperature and solvent upon the solubility of a precipitate. Super saturation-Von Weimarn concept. Formation and treatment of precipitates-co precipitation and post-precipitation. Precipitation from homogeneous solution. Specific and selective precipitants.

Principles of acid-base, oxidation-reduction, precipitation and complexometric titrations-indicators used in such titrations. Uses of organic reagents in inorganic quantitative and qualitative analysis.

Unit-II : Data Analysis

Errors in chemical analysis – Defining terms: mean, median, accuracy and precision – classification of errors: Systematic errors and random errors. Improving accuracy of analysis – mean, standard deviation and Q-test. Comparison of results – Least square, 't'-teat, 'F'-test and 'Chi' square test.

Unit-III: Techniques in Inorganic Chemistry

Colorimetry: Theoretical and practical aspects of colorimetric analysis. Flame emission and atomic absorption spectroscopy – types of atomic spectroscopy – emission methods – absorption methods – fluorescence methods – source and atomizers for atomic spectroscopy – flame atomizers – Eletrothermal atomizers – principle and applications of atomic absorption spectroscopy. Advantages of atomic absorption spectrometry over flame photometry.

Unit-IV : Electrochemical Methods of Analysis

Cyclic Voltammetry, coulometry and amperometry-principle and applications.Thermal Characterization techniques, Principle and applications of Differential Thermal Analysis (DTA), Differentials Scanning Calorimetry (DSC) and Thermogravimetric Analysis (TGA) Thermometric titration.

Unit- V : Chromatographic methods

Classification – techniques and applications in column, size-exclusion, ion exchange, paper and thin layer chromatography. Gas chromatography and high performance liquid chromatography (HPLC) – principle, equipment design, sample injection system, columns, detectors and applications.

References:

- 1. A.T. Vogel A text book of Quantitative Inorganic Analysis.
- 2. G.D. Christian Analytical Chemistry
- 3. D.A.Skoog and D.M.West Fundamentals of Analytical Chemistry.
- 4. *Willard*, H.H., *Merit* L.L., *Dean* J.A Seattle F.L., Instrumental Methods of Analysis, CBS publishing and Distribution, 2004.
- 5. Skoog, West, Holler and Crouch Analytical Chemistry An Introduction.

Course Outcomes (CO)

On successful completion of the course, the student will

| CO1 | Learnt to interpret the results of the quantitative and qualitative measurments |
|-----|---|
| CO2 | Evolved the verification strategy in the error analysis |
| CO3 | Studied the detection of various metal ions in biological systems |
| CO4 | Gained the knowledge on redox system |
| CO5 | Expertise in the detection and quantitative analysis by using various chromatographic methods |

Mapping

| PSO CO | PSO1 | PSO2 | PSO3 | PSO4 | PSO5 |
|-----------|------|------|------|------|------|
| CO1 | S | Н | S | S | М |
| CO2 | S | S | S | S | Н |
| CO3 | S | S | S | Н | Н |
| CO4 | S | S | S | Н | М |
| CO5 | S | S | S | Н | М |

S-Strong; H-High; M-Medium; L-Low

Course Prepared by

Dr.M.V. Kaveri

Course Approved by

Professor and Head