UNIVERSITY OF CALICUT

Abstract

General and Academic - Faculty of Science - Scheme and Syllabus of MSc Applied Chemistry Programme under CCSS PG Regulations 2019 (University Teaching Departments) - Incorporating Outcome Based Education (OBE) with effect from 2020 Admission onwards - Implemented - Subject to ratification of Academic Council - Orders Issued.

G & A - IV - J

U.O.No. 5556/2021/Admn Dated, Calicut University.P.O, 25.05.2021

Read:-1. U.O.No. 9544/2019/Admn, Dated 19.07.2019.

2. Minutes of the meeting of Board of Studies in Applied Chemistry held on 11.05.2021 and 17.05.2021.
3. Remarks of Dean, Faculty of Science, Dated 20.05.2021.
4. Orders of Vice Chancellor in the file of even no, Dated 24.05.2021.

ORDER

1. Vide paper read as (1) above, the Scheme and Syllabus of MSc Applied Chemistry Programme in accordance with CCSS PG Regulations 2019 (University Teaching Departments), was implemented in the University with effect from 2019 Admission onwards.
2. Vide paper read as (2) above, the Board of Studies in Applied Chemistry , approved the Scheme and Syllabus of MSc Applied Chemistry Programme, incorporating Outcome Based Education (OBE) in the existing syllabus, in accordance with CCSS PG Regulations 2019 (University Teaching Departments), with effect from 2020 Admission onwards.
3. The decision of Board of Studies have approved by the Dean, Faculty of Science, vide paper read as (3) above and by the Vice Chancellor, subject to ratification by the Academic Council, vide paper read as (4) above.
4. The Scheme and Syllabus of MSc Applied Chemistry Programme, incorporating Outcome Based Education (OBE) in the existing syllabus, in accordance with CCSS PG Regulations 2019 (University Teaching Departments), is therefore implemented, with effect from 2020 Admission onwards, subject to ratification by the Academic Council.
5. Orders are issued accordingly. (Modified syllabus appended)

Ajitha P.P

Joint Registrar

To

Head, Dept.of Chemistry

Copy to: PS to VC/PA to PVC/ PA to Registrar/PA to CE/JCE I/JCE V/DoA/EX and EG Sections/GA I F/CHMK Library/Information Centres/SF/DF/FC

Forwarded / By Order

Section Officer

UNIVERSITY OF CALICUT

M.Sc. APPLIED CHEMISTRY

SYLLABUS

(*Under Choice Based Credit & Semester System)*

2020 admission onwards

DEAPARTMENT OF APPLIED CHEMISTRY

University of Calicut

Programme offered

MSc Applied Chemistry

Programme Objective

This post-graduate course in Applied Chemistry aims to provide integrated knowledge and training in various theoretical and applied aspects of Chemical Science leading to Masters Degree and to train competent manpower who can take challenges in Teaching, Research and Development.

Programme Specific Outcome

1. Demonstrate systematic understanding of fundamental concepts and principles of various branches of Chemistry and apply the knowledge to solve problems related to Chemical Science.
2. Explain and correlate the structure -property relationship of materials based on principles of Chemistry.
3. Design and perform the chemical synthesis and characterise the products, execute experimental routines for detection and quantification of chemical entities.
4. Apply the knowledge of classical and modern experimental techniques to perform experiments, interpret the results, thereby acquire the ability to plan and carry out independent projects.
5. Demonstrate the basic principles of instrumental methods of analysis and the operation of advanced instruments to execute in-depth analysis of chemical problems.
6. Employ the acquired time management skills in planning and executing experiments and to recognize importance of ethical and cultural values.
7. Demonstrate and communicate effectively how chemistry relate to the real world and their understanding of chemical principles to a layman and able to apply the knowledge when situation demands.

Course Code	***Title of the course***	***Type***	***Credits***
Semester 1			
ACH IC 01	Quantum Chemistry	Core	4
ACH IC 02	Inorganic Chemistry I	Core	4
ACH IC 03	Organic Chemistry I	Core	4
ACH IC 04	Physical Chemistry I	Core	4
ACH IP 01	Practical Inorganic I	Core	*

ACH IP 02	Practical Organic I	Core	*
ACH IP 03	Practical Physical I	Core	*
ACH IA 01	Ability Enhancement Course (AEC)	Audit	2#
Semester 2			
ACH 2C 05	Group Theory & Chemical Bonding	Core	3
ACH 2C 06	Inorganic Chemistry II	Core	3
ACH 2C 07	Organic Chemistry II	Core	3
ACH 2C 08	Physical Chemistry II	Core	3
ACH 1P 01& ACH 2P 04	Practical Inorganic I & II	Core	3
ACH 1P 02 & ACH 2P 05	Practical Organic I & II	Core	3
ACH 1P 03 & ACH 2P 06	Practical Physical I&II	Core	3
ACH 2A 02	Professional Competency Course (PCC)	Audit	2#
Semester 3			
ACH 3C 09	Inorganic Chemistry III	Core	3
ACH 3C 10	Organic Chemistry III	Core	3
ACH 3C 11	Physical Chemistry III	Core	3
ACH 3C 12	Instrumental Methods, Theory and Instrumentation	Core	3
ACH 3P 07	Practical-Instrumental methods of Analysis	Core	4
ACH 3E 01	Organometallic Chemistry	Elective	4
ACH 3E 02	Nanoscience & Technology	Elective	4
ACH 3E 03	Solid state Chemistry	Elective	4
ACH 3E 04	Synthetic Organic Chemistry	Elective	4
Semester 4			
ACH 4E 05	Bioinorganic Chemistry	Elective	4
ACH 4E 06	Computational Chemistry	Elective	4
ACH 4E 07	Chemistry of Natural Products	Elective	4
ACH 4E 08	Industrial Catalysis	Elective	4
ACH 4E 09	Chemistry of Polymers	Elective	4

ACH 4E 10	Green Chemistry	Elective	4
ACH 4E 11	Advanced Synthesis and Catalysis New Synthetic Methodologies	Elective	4
ACH 4PR 01	Project/Dissertation and Viva	Core	8

*****Examinations based on practicals of semesters I & II will be held at the end of semester II only. Credit will be 3 each for each examination. Practical Examination will be of six hours duration.

Every student should choose any four elective courses (offered) during the entire programme (two electives courses each during III and IV semester).

#Credit of this course will not be considered while calculating the SGPA/CGPA.

Core Courses (other than project/dissertation)	:	53
Elective Courses (4x4)	:	16
Project/Dissertation	:	8
Total	**:**	**77**

For more details:

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ACH 1C 01 Semester 1 Quantum Chemistry (4 Credits)

Course Outcome After completion of the entire course, the student should be able to:	Cognitive level
C.O.1: Examine the basic principles and concepts of quantum mechanics.	Analysis
C.O.2: Apply the postulates of quantum mechanics to simple systems with translational, vibrational and rotational motions such as-particle-in-a-box, harmonic oscillator, rigid rotor and hydrogen like atoms.	Application
C.O.3: Derive variational and perturbation principles and use them to calculate properties of simple systems of chemical interest.	Analysis
C.O.4: Define and explain the Hartree-Fock self-consistent field method.	Understand
C.O.5: Discuss the electron spin and atomic structure of simple chemical systems.	Understand

UNIT I Brief history of quantum mechanics

Plank's quantum Postulates, Einstein's quantum theory of radiation, Explanation of photo electric effect, Milliken's verification of Einstein's photoelectric equation, wave particle duality of radiation, wave particle duality of particles, de Broglie matter waves, Electron diffraction, Heisenberg's Matrix Mechanics (brief mention), Schrödinger wave mechanics, Deduction of Schrodinger equation from classical wave equation. Polar and spherical coordinates

UNIT II Formulation of quantum mechanics - The Postulates of quantum mechanics

State function postulate, Operator postulate, Eigen value postulate, Expectation value postulate, Postulate of time dependent Schrodinger Equation of motion, Conservative system and time-independent Schrodinger equation, Stationary states, Formulation of quantum mechanical problem. Rules of proper behavior of operators, Hermitian operators. Commutation of operators and their physical significance.

UNIT III

a) Particle in a one-dimensional box and in a three-dimensional box

The particle in a one-dimensional box-complete treatment. The particle in a three-dimensional box (consider rectangular and cubic boxes), Separation of variables,

Degeneracy, Symmetry breaking, Treatment of more than one particle (non-interacting) in a box. Applications. Introduction to Tunneling.

b) Harmonic Oscillators

Classical concepts. Derivation of Schrödinger equation. Harmonic oscillator (complete treatment): Wave functions and energies, important features of the problem, Harmonic oscillator and molecular vibrations, Three-dimensional harmonic oscillator.

UNIT IV Rigid Rotors

Rigid rotator (compete treatment).IR & Raman spectra. The wave equation in spherical polar coordinates. Planar rigid rotator (or Particle on a ring), The Phi-equation, Solution of the Phi-equation, Handling of Imaginary wave functions, Wave functions in the real form, Polar diagrams.

Nonplanar rigid rotator (or particle on a sphere), Separation of variables. The Phi-equation and the Theta-equation and their solutions, Legendre and Associated Legendre equations, Legendre and Associated Legendre polynomials, Spherical harmonics (imaginary and real forms). Polar diagrams of spherical harmonics. Spherical harmonics as eigen function of angular momentum operators L and L^2. Quantization of angular momentum, Angular momentum quantum numbers, Space quantization.

UNIT V Quantum Mechanics of Hydrogen-Like atoms

Potential energy of hydrogen-like systems. The wave equation in spherical polar coordinates, Separation of variables. The R. Theta and Phi equations and their solutions. Laguerre and Associate d Laguerre polynomials. Wave functions and energies of hydrogen-like atoms, Orbitals. Radial functions and Radial distribution of functions and their plots Angular functions (Spherical harmonics) and their plots, Orbital diagrams.

Explanation of Hydrogen spectrum, Fine structure, The postulate of spin by Unlebeck and Goldsmith, Dirac's Relativistic Schrodinger equation for hydrogen atom and discovery of spin, Hydrogen wave functions including spin or spin orbitals, construction of Spin orbitals from Orbitals and Spin functions.

UNIT VI

a) Many-electron atoms and approximation methods

Many-body problem. Approximation methods. Independent particle model, Distribution of electrons in many electrons atoms., Stoner's rule. Variation method. Variation theorem with proof, illustration of variation theorem using a trial function (e.g., x (a-x) for particle in ID-box. Variation treatment for the ground state of Helium atom, Effective nuclear charge. Perturbation method. Time-independent perturbation method (non-degenerate case only).

Illustration by application to particle in ID-box with slanted bottom, Perturbation treatment of the ground state of the helium atom. Hartree-Fock Self-Consistent Field (HF-SCF) method. Slater's treatment of complex atoms, Slater Orbitals, Slater's rules for calculating Slater orbitals.

b) Electron spin and atomic structure

Construction of wave functions including spin for many electron atoms, Symmetric and antisymmetric wave functions, Pauli's antisymmetry principle, Slater determinants, Pauli's exclusion principle.

Vector model of atoms and spectroscopic terms

Coupling of angular momenta, LS and jj-couplings, LS coupling and Spectroscopic term symbols for atoms. Brief mention of selection rule in atomic spectroscopy. Electronic spectrum of hydrogen atom-the fine structure of H□ line of the Blamer series. The electronic spectrum of Helium and Lithium atoms- Brief discussion.

REFERENCES

1. F.L. Pilar, *Elementary Quantum Chemistry*, McGraw Hill, 1968.
2. P. W. Atkins, R.S Friedman, Molecular Quantum Mechanics, 5th ed., OUP, Oxford, 2012.
3. M.W. Hanna, *Quantum mechanics in Chemistry*, 2nd Edition, W.X. Benjamin Inc. 1969.
4. I.N. Levine, *Quantum Chemistry*, 6th Edition, Pearson Education Inc. London, 2008.
5. D. A. McQuarrie, Quantum Chemistry, 3rd ed., Univ. Sci. Books, Mill Valley, California, 1983.
6. J. P. Lowe, Quantum Chemistry 3rd ed., Academic Press, New York, 2008.
7. A.K. Chandra, Introduction of *Quantum Chemistry*, Tata McGraw Hill, 1994.
8. R.K. Prasad, *Quantum Chemistry,* 3rd Edition, New Age International, 2006.
9. M.S. Pathania, *Quantum Chemistry and Spectroscopy (Problems & Solutions)*, Vishal Publications, 1984.
10. G. K. Vemulapally, Physical Chemistry, Prentice Hall of India

ACH 1C 02 Semester 1 INORGANIC CHEMISTRY 1 (4 Credits)

Course Outcome After completion of the full course the student should be able to:	**Cognitive level**
C.O.1: Analyze the electronic spectra of lanthanoids and actinoids and understand their general characteristics and magnetic properties.	Analysis
C.O.2: Evaluate the structure, bonding and reactions of carbonyl compounds, metal clusters and get an insight into heteropoly and isopoly	Analysis

anions of Mo, W	
C.O.3: Illustrate the stability and topology of non-metallic clusters as different polyhedral boranes and interpret the structure and properties of compounds of sulfur, nitrogen, phosphorous and group 14 elements.	Application
C.O.4: Describe nanomaterials, synthetic strategies and application of various nanomaterials	Understand
C.O.5: Compare the strength of various acids and bases and their reactivity and explain stereochemistry of coordination compounds and their stability	Analysis
C.O.6: Describe and explain the structure, bonding and stability in coordination compounds using bonding theories	Understand

UNIT I Chemistry of Lanthanoids and Actinoids

Periodic Table. Chemistry of Lanthanoides and Actinoides General characteristics of actinoids-difference between 4f and 5f orbitals, oxidation states. The lanthanoide-and actinoide contractions, separation of lanthanoides and actinoides electronic spectra and magnetic properties of lanthanoid complexes, Inorganic compounds and coordination complexes of the lanthanoids up to coordination No.12, Coordination compounds of the actinoids- sandwich complexes, coordination compounds of thorium and uranium-comparative account of coordination chemistry of lanthanoids and actinoids with special reference to electronic spectra and magnetic properties. Trans-actinide elements. Super heavy elements.

UNIT II Metal Clusters

Metal Clusters Metal – metal bond and metal clusters, General electronic aspects and bonding in metal-metal single, double, triple and quadruple bonded complexes of non carbonyl clusters, Carbonyl clusters - preparation, properties, structure and bonding of simple mono and binuclear metal carbonyls, Polynuclear metal carbonyls with and without bridging. Carbonyl clusters-LNCCS and HNCCS, Capping rule, Reactions of metal carbonyl clusters, Wade-Mingos rules, cluster valence electrons, IR spectral studies of bridging and non-bridging CO ligands, Isoelectronic and isolobal analogy, Isopoly and heteropoly anions of Mo and W.

UNIT III Non-Metallic Clusters

Non-Metallic Clusters Preparation, structure, bonding and reactions of Boron hydrides and borazine, styx numbers, closo, nido, arachno polyhedral strucutures, Boron cluster compounds, Wade's rule, synthesis, structure and bonding of carboranes, metalloboranes and metallao carboranes, Medical applications of boron clusters. Heterocyclic inorganic ring systems: Structure and bonding in phosphorous-sulphur and sulphur-nitrogen compounds. Homocyclic inorganic ring systems: Structure and bonding in sulphur, selenium and phosphorous compounds. Synthesis, structure and bonding of cage like structures of phosphorous. Synthesis structure and uses of Silicates, aluminosilicates, zeolites, Silcones, Carbides and silicides, Synthesis, structure, bonding and uses of phosphorous-nitrogen, sulphur-nitrogen compounds.

UNIT IV Chemistry of Nanomaterials

Fundamentals-Terminology and history, Bulk Vs nano size, Size-dependence of properties - Surface area to volume ratio and Quantum confinement, Novel optical and electronic properties of nanomaterials, Various types of nano materials - Metal and Semiconductor, Self-assembled nanostructures, Carbon nanostructures- Fullerenes and carbon nanotubes, Mesoporous nano materials - SiO_2 and TiO_2. Properties of metal and semiconductor nanoparticles-surface plasmon resonance, optical and electronic properties, Synthesis of Nanomaterials-Top down and bottom-up approach, Sol-gel synthesis of semiconducting oxide nanoparticles, Applications of semiconducting nanomaterials- Photocatalysis, superhydrophilicity, Self-cleaning applications, Dye sensitized solar cells and electrochromic device applications. Magnetic nanoparticles, super paramagnetism and biomedical applications of magnetic nanoparticles, Template-based synthesis of mesoporous nanomaterials (SiO2 and TiO2) and their applications.

UNIT V Acid-Base and Coordination Chemistry

Concepts of Acids and bases – Arrhenius to Pearson. Hard and soft acids and bases, Comparison of softness and hardness, charge/size effects. The Dargo-Wayland equation. Heterogeneous acid-base reactions. Symbiosis-hard and soft ligands Coordination compounds. Formation constants, Step-wise and overall stability constants- factors affecting stability- methods of determination of stability constants- solubility method-chromatographic method and spectrophotometric method. Chelate, macrocyclic and macro bicyclic effects. Geometrical and optical isomerism in octahedral complexes, resolution of optically active complexes, determination of absolute configuration of complexes by ORD and circular dichroism. Linkage isomerism: Electronic and steric factors affecting linkage isomerism, symbiosis-hard and soft ligands.

UNIT VI Bonding theories of coordination compounds

Valance bond theory and its limitations. Crystal Field and Ligand filed theories – Orbital splitting in octahedral, tetrahedral, cubic, square planar, square pyramidal and trigonal bipyramidal fields. Significance of 10Dq, factors affecting crystal field splitting, spectrochemical and nephelauxetic series, Jahn-Teller effect, Causes and consequences.

REFERENCES

1.D. J. Shriver and P. W. Atkins, Inorganic Chemistry, 5th edition, Oxford University press, 2010.

2. E. Huheey, E. A. Keiter, R. L. Keiter, Inorganic Chemistry: Principles of Structure and Reactivity, 4th ed., Harper Collin College Publishers, 1993.

3. F. A. Cotton, G. Wilkinson, C. A, Murillo, M. Bochmann, Advanced Inorganic Chemistry, 6 th ed., Wiley-Interscience: New York, 1999.

4. G. Wulfsberg, Inorganic Chemistry, Viva Books, 2002.

5.B.E. Douglas, D.H. Mc Daniel and J. J. Alexander, Concepts and models of Inorganic chemistry, 3rd edition, John Wiley, 1994.

6. F. A. Cotton, Basic Inorganic Chemistry, 3rd edition, John Wiley, 2004.

7.S. F. A. Kettle, Concise co-ordination chemistry, Nelson, 1969.

8.S. F. A. Kettle, Physical Inorganic Chemistry - A Co-ordination chemistry Approach, Spectrum academy publishers, 1996.

9. J. D. Lee, Concise Inorganic chemistry, 5th edition, Wiley India, 1996.

10.R. G. Person and F. Basolo, Mechanism of Inorganic Reactions, 2nd Edition, John Wiley, 1967.

11.T. Pradeep. The essentials of Nanotechnology, Tata Mc Graw Hill, New Delhi, 2007.

ACH IC 03 Semester 1 Organic Chemistry I (4 Credits)

COURSE OUTCOME After completion of the full course the student should be able to:	COGNITIVE LEVEL
C.O.1: Interpret structure and stability of reactive intermediates.	Application
C.O.2: Illustrate the mechanistic pathway of different rearrangements reactions and identify the products	Application
C.O.3: Discuss the concepts of isomerism and its classification, concepts of conformation and configuration.	Analysis
C.O.4: Illustrate modern synthetic methods and applications of reagents	Application
C.0.5: Identify the mechanism, structural and stereochemical implications of the product in a given reaction under	Analysis

photochemical condition**.**	
C.O.6: Compare the differences in reactivity of various oxidizing and reducing agents with mechanistic illustrations.	Analysis

UNIT I Reactive intermediates

Generation and characterization of free radicals, Stable and persistent free radicals -Factors affecting stability, Detection of free radical intermediates - Structural and stereochemical properties of radical intermediates - Free radical substitution and addition reactions - Intramolecular ractions. Rearrangement and fragmentation reactions of free radicals. Applications of free radicals. Gomberg-Bechmann reaction and Wohl-Zeigler reaction, Hunsdiecker reaction and Reed Reaction. Carbenes and nitrenes: generation, stability, addition, cyclisation, insertion and ring enlargement reactions, Skattebol rearrangement, Wolff rearrangement, Benzyne intermediates.

REFERENCES

1.N.S. Issac, Reactive Intermediates in Organic Chemistry, John wiley & Sons (1974)

2. P.S. Kalsi, Organic Reaction and their Mechanisms, Wiley Eastern Ltd, 2nd Edn. (2000)

3.F. A. Carey, R. J. Sundberg, Advanced Organic Chemistry (parts A and B), 5th ed., Springer, 2008.

UNIT II Molecular rearrangements I

Concepts, Types of Rearrangements, Rearrangement to electron deficient carbon: (carbon migration) Wagner-Meerwin rearrangement, Pinacol-Pinacolone rearrangement, Tiffeneau-Demjanov rearrangement, Benzilic acid rearrangement. Rearrangement to electron rich carbon: Stevens rearrangement, Sommelet-Hauser rearrangement, Wittig rearrangement, Favorskii rearrangement. Rearrangement to electron deficient nitrogen: Hofmann rearrangement, Curtius rearrangement, Schmidt rearrangement, Lossen rearrangement, Beckmann rearrangement. Rearrangement to electron deficient oxygen: Baeyer Villiger reaction, Hydroperoxide rearrangement, Dakin reaction. Intramolecular migration from nitrogen to carbon: Jacobsen rearrangement, Zinin-benzidine arrangement (semidine rearrangement)

REFERENCES

1. J. March, Advanced Organic Chemistry: Reactions, Mechanisms, and Structure, 7th ed., Wiley, 2013.

2.R.O.C. Norman and E.M. Coxon, Principles in Organic Synthesis, 2005, CRC Press, New York.

3.B. P. Mundy, M. G. Ellerd, and F. G. Favaloro Jr. Name reactions and reagents in Organic Synthesis, Wiley Interscience, New Jersey 2005

UNIT III Stereochemistry and conformations

Difference between configuration and conformation, Internal factors affecting the stability of molecules -dipole interaction, bond opposition strain, bond angle strain. Perspective and Newman projections - representation of different conformations. Conformation of acyclic compounds - Ethane, n-butane, alkane dihalides, glycols, chloro hydrines, tartaric acid, erythro and threo isomers, aldhydes and ketones (acetaldehyde, acetone). Introduction to isomerism, racemisation, resolution, asymmetric synthesis, atropisomersim, restricted rotation and asymmetry, reactivity in acylic compounds, non-carbon chiral centers, Introduction to stereochemistry of cyclohexane, fused rings and bridged compounds, Stereochemistry of organic compounds other than carbon center, Carbohydrate-Stereochemistry and configuration of glucose, mannose, xylose, galactose, arabinose and ribose.

REFERENCES

1.D. Nasipuri, Stereochemistry of Organic Compounds: Principles and Applications, 2nd ed., Wiley Eastern Limited, New Delhi, 1994

2.P. S. Kalsi, Stereochemistry, Conformation and Mechanism, 3rd ed., New Age Publications.

3.K.L. Eliel and S.H. Wilen, Stereochemistry of Organic compounds, Wiley Interscience.

4. P. S. Kalsi, Stereochemistry: Conformation and Mechanism, 10th ed., New Age Publications, 2019

UNIT IV Named Organic reactions I

Barbier coupling reactions, Castro-Stephens coupling, Baylis Hillman reaction, Corey-Fuchs alkyne synthesis, Dakin-West reaction, Eschenmoser methenylation, Evans Aldol reaction, Staudinger reaction,Horner-Wadsworth-Emmons reaction, Houben-Hoesh reaction, McMurry coupling, Nazarov cyclization, Nef reaction, Ritter reaction and Pauson-Khand reaction.

REFERENCES

1.T. H. Lowry, K. S. Richardson, Mechanism and Theory in Organic Chemistry, 3rd ed., Benjamin-Cummings Publishing Company, 1997

2. Jie Jack Li – Name Reactions: A Collection of Detailed Reaction Mechanisms.

3. Laszlo Kurti and Barbara Czako, Strategic Applications of named Reactions in Organic Synthesis, Elsevier Academic Press, 2005.

UNIT V Photochemistry

General principles, Photosensitization and PET reactions, Photochemistry of carbonyl compounds. Photochemistry of alkenes, Photochemistry of aromatic compounds, Norrish Type I and II, Patterno Buchi reaction, Barton reactions, atmospheric photochemistry, photosynthesis, industrial photochemistry, chemi and bioluminescence reactions, Photo chemical rearrangements- aromatic rearrangements, Dienone rearrangements, Di-pi methane rearrangements, Photo-Fries rearrangements.

REFERENCES

1.R.O. Kan- Organic Photochemistry, McGraw Hill

2.F. A. Carey, R. J. Sundberg, Advanced Organic Chemistry (parts A and B), 5th ed., Springer, 2008.

3.O. L. Chapman- Organic Photochemistry

4.R O C Norman & E M Coxon, Principles in Organic Synthesis, 2005, CRC Press, New York

UNIT VI Oxidation-Reduction Reactions

Oxidation of alcohols to aldehydes, Ketones or Carboxylic acids. Oxidation of aldehydes and ketones. Hydroxylation of alkenes, Oxidative cleavage of Carbon-Carbon double bonds, Addition of Oxygen to Carbon-Carbon double bonds, Oxidative cleavage of alkynes, reactions of alkenes with singlet oxygen. Allylic Oxidation, Muffat Oxidation, Swern oxidation, Oxidation coupling of Phenols. Reduction reactions. Reduction of double and triple bonds with catalytic hydrogenation, Stereochemistry and selectivity. Reductions using LAH, $NaBH_4$ and diimide.

REFERENCES

1. F. A. Carey, R. J. Sundberg, Advanced Organic Chemistry (parts A and B), 5th ed., Springer, 2008.

2. P.Y. Bruice, Organic Chemistry, Prentice Hall.

3. J. March, Advanced Organic Chemistry: Reactions, Mechanisms, and Structure, 7th ed., Wiley, 2013.

ACH 1C 04 PHYSICAL CHEMISTRY 1 (4 Credits)

Course Outcome After completion of the entire course, the student should be able to:	Cognitive Level
C.O.1: Apply the concepts of thermodynamics to derive relations between molecular properties and to predict spontaneity of processes. .	Application

C.O.2: Evaluate dependence of chemical equilibrium on pressure, temperature and concentration.	Evaluation
C.O.3: Describe the theories effecting ionic conductance and apply the concepts to calculate conductance behavior of a given system and understand the working principle and advancement in futuristic electrochemical devices.	Understand Application
C.O.4: Discuss the electronic conductance behaviour in charged interfaces	Analysis
C.O.5: Define the parameters of different crystal systems and apply it to understand crystal structure.	Understand Application
C.O.6 Analyze how diffraction patterns can be converted to structural information and interpret XRD pattern of solid samples	Analysis Application

UNIT 1 Thermodynamics I

Basic concepts-laws. Maxwells relations-derivation by method of Jacobians (The discussion to be confined to closed thermodynamic systems). Thermodynamics of solutions: partial molar quantities. Chemical potential. Variation of Chemical Potential with temperature and Pressure. Partial molar volume and its determination. Gibbs -Duhem equation. Ideal and non-ideal solutions. Fugacity of gases and its determination. Deviation from Raoul'ts laws. Gibbs-Duhem-Margules equation. Thermodynamics of mixing Excess thermodynamic functions. Excess free energy, excess entropy, excess enthalpy and excess volume.

UNIT II Thermodynamics II

Thermodynamics of irreversible process: Stationary state concept. Principle of local equilibrium. Simple examples of irreversible processes. Forces and fluxes. The phenomenological relations. Onsagar relations: Linear relations – Coupled flows. Reciprocal relation (no derivation). Entropy of production in simple irreversible system (closed systems). Application of reciprocal relation to diffusions. Thermal diffusion, thermo-osmosis and thermo-molecular pressure difference. Electro kinetic phenomena-entropy production, electro osmosis, streaming potential, streaming current, electro osmotic pressure.

REFERENCES

1.Donald A. Mc Quarrie, John D. Simon, Molecular thermodynamics

2. R.P. Rastogi and G.M. Misra, An Introduction to chemical Thermodynamics, Vikas

3.I Prigogine, An introduction to the Thermodynamics of Irreversible processes. Inrterscience.

4. Daniel and Alberty, Physical Chemistry, John Wiley.

5. Rajaram, Kuriacose, Thermodynamics for students of Chemistry,S.L.Nagin Chand&co

6. Gurdeepraj,Advanced Physical Chemistry,Goel Publishing House,Meerut

7. Kulu & Foster Lung, Physical Chemistry

UNIT III Electrochemistry I

Equilibrium properties of electrolyte solutions, Electrolytes of first and second kind, Activities and activity coefficients in electrolytic solutions. Mean ionic activity and ionic strength, Debye – Huckel Theory, Charge density near the central ion, Poisson equation, Debye- Falkenheigen equation, Debye-Huckel limiting law and its various forms (no derivation). Qualitative and quantitative tests of the Debye-Huckel limiting law. Debye-Huckel-Onsagar equation of conductivity. Validity of the Debye-Huckel-Onsagar equations, Deviations from the Onsagar equation. Conductance ratio and Onsagar equation. Dispersion of conductance with high potential gradients.

UNIT IV Electro Chemistry II

Thermodynamics of Electrochemical systems, Chemical, thermodynamic and practical reversibility, Reversibility and free energy, Free energy and EMF, EMF and concentration, Temperature coefficient of EMF and determination of G.H and S. Formal and standard electrode potentials, Concentration cells. Electrode - solution interface, Interfacial potential difference, Outer potential, Inner potential and surface potential, Electrochemical potential and absolute potential, Electrical double layer and its different models, Liquid junction potential and its determination. Fuel cells.

UNIT V Electro Chemistry III

Electrochemical cells and reactions, Energy levels of electrons and potential variation during redox processes, Current-potential curves, Irreversible electrode processes, Faradaic and non-Faradaic processes, Polarization phenomena and over potential, polarizable and non-polarizable electrodes and their *I-V* characteristics, Rate of electrode reaction, Factors affecting electrode reaction rate and current, Effect of electrode potential on Gibbs free energy of activation, Butler-Volmer equation, Exchange current density and activation over potential, Tafel equation and Tafel plots, Concentration polarization, Dissolution and decomposition potentials. Hydrogen over voltage, Ionic diffusion as the slow process, Ionic

discharge as the slow process. Principles of polarography, Voltammetry, Linear sweep, differential pulse and cyclic voltammetry (Brief mention only).

REFERENCES

1. S. Glsstone, Introduction to Electrochemistry, Van Nonstrand.

2. Bockris and Reddy, Modern Aspects and Electrochemistry Vol. I and II, Academic Press.

3. P.W. Atkins and Julio de Paula, Physical Chemistry (8th and 10^{th} Edition), ELBS Oxford University Press.

4.Allen J. Bard and Larry Faulkner, Electrochemical methods: Fundamentals and applications, Wiley

5.Gurdeepraj, Advanced Physical Chemistry, Goel Publishing

UNIT VI Crystalline state

Crystal symmetry, Symmetry elements and symmetry operations. Allowed combinations of operations leading to 32 crystal classes. Mathematical proof for the non-existence of 5-fold axis of symmetry for crystals. Hermann-Mauguin notations. Stereographic Projections of some simple crystal classes (e.g. 1, 1, 2/m, 222, mmm). X-rays and internal structure of crystals. XRD measurements. Laue method. Rotating crystal method. Powder diffraction method. Scattering factor. Electron density in crystals. Electron density maps (brief mention) Fourier synthesis.

REFERENCES

1.D.A McQuarrie and J.D. Simon, Physical Chemistry, a molecular approach, University Science Books.

2.G. K. Vemula Palli, Physical Chemistry, Prentice Hall.

3.P.W. Atkins, Physical Chemistry,10 th edn ELBS Oxford University Press.

4.L.V. Azaroff, Introduction to solids, Tata McGraw Hill

5.F.A. Cotton, Chemical applications of Group theory, Wiley.

6.Tareen and Kutty, Solid state chemistry.

7.Lesley Smart & Elaine Moore, SolidState Chemistry, nelson Thornes

8.R. West, Solid State Chemistry and its Applications, John Wiley, 1987.

9.N. B. Hannay, Solid State Chemistry, Prentice Hall of India, 1979.

10.R. J. D. Tiley, Defect Crystal Chemistry and its Applications, Chapman and Hall, NewYork, 1987

ACH 1P 01 Semester 1 PRACTICAL INORGANIC I

Objective of the Course

The learners should be able to apply the principles of qualitative and quantitative analytical techniques in inorganic chemistry for identification of ions and preparation and characterization of inorganic complexes

Course Outcome After completion of the full course the student should be able to:	**Cognitive level**
C.O.1: Understand safe laboratory practices of handling laboratory glassware, equipment and chemical reagents and develop basic laboratory skills	Knowledge
C.O.2: Identify the cations in a mixture of unknown salts.	**Analysis**
C.O.3: Estimate binary mixtures of metal ions by volumetry and gravimetry	**Analysis**

Part I

Separation and identification of a mixture of four cations (a mixture of ONE familiar ions such as Ag^{+}, $Hg^{2+,}$ $Pb^{2+,}$ Cu^{2+}, Bi^{2+}, $Cd^{2+,}$ As^{3+}, Sn^{2+}, Sb^{3+}, Fe^{2+}, $Fe^{3+,}$ $Al^{3+,}$ Cr^{3+}, Zn^{2+}, Mn^{2+}, Co^{2+}, $Ni^{2+,}$ Ca^{2+}, Sr^{2+}, Ba^{2+}, Mg^{2+}, Li+, Na^{+}, K^{+} and NH^{4+} and THREE less familiar metal ions such as Tl, W, Se, Mo, Ce, Th, Ti, Zr, V, U and Li). Anions which need elimination not to be given. Minimum 5mixtures to be analyzed and recorded

Part II

Estimation of simple binary mixtures (like Cu-Ni, Cu-Zn, Fe-Cr, Fe-Cu, Fe-Ni, Pb-Ca, Fe-Ca,) of metallic ions in solution by volumetric and gravimetric methods. Any three to recorded

ACH 1P 02 SEMESTER I PRACTICAL ORGANIC I

Course Outcome After completion of the full course the student should be able to:	**Cognitive Level**
C.O.1: Understand safe laboratory practices of handling laboratory glassware, equipment and chemical reagents and develop basic laboratory skills	Knowledge
C.O.2: Apply two synthetic procedures, chromatographic separation and purification of organic compounds.	Application
C.O.3: Analyze organic compounds from the organic binary	Analysis

mixture and identify the functional group(s) present	
C.O.4: Perform the quantitative analysis in organic chemistry	Application
C.O.5: Estimate given organic compounds	Analysis
C.O.6: Design experiments and validate the hypothesis of an independent research problem	Create (synthesis)

1.Laboratory Techniques: Method of separation and purification of organic compounds – fractions, steam and low-pressure distillation, fractional crystallization and sublimation.

2.Quantitative Organic Analysis: Quantitative Separation of organic binary mixtures by Semimicro analytical techniques. Measurements of Physical constants and preparation of derivatives.

3. Preparation of Organic Compounds: Preparation of about fifteen organic compounds in which at least five of them involves minimum two synthetic steps (including photochemical methods). Purification of products by crystallization, distillation and available chromatographic methods. Characterization of all isolated products by analytical and spectral methods (FT-IR, UV-Vis, GC-MS, Melting point/Boiling Point determination and TGA analysis). Illustrative examples: - Friedel-Crafts reaction. Perkin reaction Reimer-Tiemann reaction, Sandmeyer reaction Cannizzaro reaction, aldol reaction, Mannich reaction, Diazotization and Diazo coupling reactions, Benzoin condensation and selective reduction of polynitro aromatic compounds.

REFERENCES

1. A.I. Vogel, A Text Book of Practical Organic Chemistry, ELBS.
2. Fiester, Experiments in Organic Chemistry.
3. Mann and Saunders, practical Organic Chemistry.
4. Dey. Sitaraman and Govindachari, A Laboratory Manual of Organic Chemistry.
5. Cheronis and Fatrikin, Semi-micro-organic analysis.
6. P.G. Singh, D.S. Gupta and K.S. Bajpal, Experimental Organic Chemistry, Vols. I and II, 1980.
7. R. Srinivasan, Ed. Photochemical Synthesis Vols. I and II.

ACH 1P 03 SEMESTER I PRACTICAL PHYSICAL I

Course Outcome After completion of the full course the student should be able to:	Cognitive level
C.O.1: Understand safe laboratory practices of handling laboratory glassware, equipment and chemical reagents and develop basic laboratory skills	Knowledge
C.O.2: Perform experiments based on various laws of physical chemistry.	Application
C.O.3: Interpret the results obtained from various experiments.	Analysis
C.O.4: Practice various sophisticated instruments.	Application
C.O.5: Construct phase diagram of various eutectic systems having binary mixture.	Create (Synthesis)

1. Solubility

- Determination of Heat of solution from solubility data (Ammonium Oxalate and succinic acid).

2. Molecular weight

- Determination of molecular weight from depression in freezing point. Biphenyl-Naphthalene cooling curve method.
- Determination of molecular weight from depression in transition point. Cooling curve method.

3. Cryoscopic study

- Determination of cryoscopic constants of solvents and molecular weight of non-volatile substances using water and benzene as solvents.
- Cryoscopic study of the reaction. $2KI+Hgl_2$ □ K_2HgI_4, in water and determination of concentration of KI Solution.
- Determination of degree of dissociation and hence Vant Hoff factor of an electrolyte by cryoscopic method.
- Determination of activity coefficients of KCl in dilute solution by cryoscopic measurements

4. Polarography

- Determine the half wave potentials of Cd^{2+} and Zn^{2+} ions in 0.1 M KCl solution.
- To study the variation of diffusion current with concentration using Cd^{2+} ions. Construct a wave height concentration curve.

5. Conductometry

- Conductometry titrations of displacement and precipitation reactions - HCl vs NaOH (HCl + HOAc) vs NaOH, $AgNO_3$ vs KCl.
- Determination of Equivalent conductance of strong electrolytes (KCI). Verification of Onsagar equation.
- Determination of Equivalent conductance of weak acid-verification of Ostwald's dilution law-calculation of dissociation constant.
- Determination of Activity coefficient of Zn in 0.002JM $ZnZO_4$ using Debye-Huckel limiting law.
- Determination of solubility product of sparingly soluble salts (AgCl, $BaSO_4$).
- Determination of equivalent conductance of weak acids and hence the dissociation constant.
- Determination of pH of buffer solutions with a pH meter and evaluation of pK_a value of acids.

6. Refractometry

- Analysis of a binary mixture and determination of molar refraction of a solid and the composition of chloroform and acetone in its azeotropic mixture by refractometry
- Determine the refractive index of a given liquid by Abbe Refractometer and find the specific and molar refractions.
- Determine the electron polarisation and electron polarisability of a liquid refractometrically.

7. Viscometry

- Analysis of a binary mixture of two miscible liquids by viscometry and the relation between viscosity of a solution and the electrical conductivity
- Study of variation of viscosity of a liquid with temperature.

8. Distribution Law

- Distribution coefficient of 1_2 between CCl_4 and H_2O
- Study of equilibrium $Kl+1_2 \rightarrow KI_3$
- Determination of concentration of KI solution

- Determination of the association constant of a carboxylic acid in an organic solvent by the distribution method.

9. Density Measurements

- Determination of molar volume of ethanol and its partial molar volume at 25°C in dilute aqueous solution.

10. pH measurements and applications

- To determine the value of Dissociation constant, Ka of an unknown acid.
- To perform a pH titration (OPTIONAL, if time permits)
- To study the properties of buffer solutions.

11.Water Analysis

- Estimation of (i) total hardness (ii) permanent hardness and (iii) temporary hardness of a given sample of water.
- Determination of chloride ion concentration in a given sample of water by Mohr's method.
- Determination of dissolved oxygen present in a given sample of water by Winkler's method

REFERENCES

1. J.B.Yadav,Advanced Practical Physical Chemistry, Goel Publishing
2. Gurtu&Gurtu, Experimental Physical Chemistry, Prgti Prakashan
3. Gurdeep Raj,Experimental Physical,Krishna Prakasha
4. A Findlay, Practical Physical Chemistry, Longman's Green & Co., 1972.
5. D.F. Schomaker and C.W. Garland, Experiments in Physical Chemistry, McGraw Hill, 1974.

Practical Examination based on practicals of semesters I&II will be held at the end of semester II only. Credit will be 3 each for each examination. Each exam will be of six hours duration

ACH 1A 01 Semester I - Audit course (Credits: 2; Weightage: 30)

Ability Enhancement Course (AEC)

AEC aims to have hands on experience for the students in their respective field of study, both in the core and elective subject area. Also, it is a platform for the student community to have basic concepts of research and publication. Credit of this course will not be considered while

calculating the SGPA/CGPA. But the student has to obtain minimum pass requirements (weightage 15) in this course, which is compulsory for overall pass in the programme.

One particular AEC may be selected for all the students in a batch in the Department or each student in a batch may choose one AEC, among the pool of courses suggested below. Evaluation/examination on AEC must contain the following components: MCQ type written examination (weightage: 10), Report on AEC (weightage: 10), Presentation of AEC (weightage: 5), Viva voce on AEC (weightage: 10).

Course Outcome After completion of the entire course, the student should be able to any one of following C. O.:	**Cognitive level**
C.O.1: Describe the principles and concepts related to basic laboratory skills and research through industrial and research institution visit.	Understand
C.O.2: Develop skills related to presentation and publication of articles in seminar, book, journals *etc*	Application
C.O.3: Analyze research problems through internships.	Analysis
C.O.4: Solve problems related to various fields through hands on training in instruments.	Synthesis

- **Industrial/Research institution visit**: Basic concepts of research, motivation and objectives, research methodology, identification of research problem, data collection, descriptive research, analytical research, quantitative and qualitative research, research formulation.
- **Publication of a research article in journal**: review of literature, status of research problem, developments in research area, data analysis, presentation of results, writing articles, ethics in publishing articles, copy right- royalty- intellectual property rights- patent law, commercialization, national and international journals. Writing articles, bibliography.
- **Presentation of research paper/s in national level seminar/conference**: brief description of research problem and the result, presentation skill development, importance of seminar and conferences, significance of research problem, data presentation, illustration, PowerPoint preparation.

- **Presentation of Review article/s in seminar/conference**: importance of review of literature, knowledge of present status of research problem, developments in recent years, novel research topics.
- **Internships (at reputed research institutions/R&D centre/Industry)**: exposure in a new environment, development of research problem, data collection, analysis, conclusion, relevance of the study, presentation of results, commercialization, publication.

ACH 2C 05 SEMESTER II GROUP THEORY AND CHEMICAL BONDING (3 Credits)

Course Outcome After completion of the full course the student should be able to :	Cognitive level
C.O.1: Analyze the symmetrical aspects of any given molecule.	Analysis
C.O.2: Discuss applications of symmetry and Group Theory in Quantum mechanics and spectroscopy.	Application
C.O.3: Apply symmetry and group theory to study the bonding in chemical compounds (M.O and V.B theory).	Application
C.O.4: Describe the principles of chemical bonding in diatomic and polyatomic molecules.	Understand
C.O.5: Practice applications of Group theory to molecular orbital treatment and hybridization of various chemical systems.	Application
C.O.6: Construct character table of molecules and predict the spectral properties.	Analysis

UNIT I Molecular Symmetry

Symmetry elements and symmetry operations in molecules. Identity, Rotation, Reflection, Inversion and Improper rotation operation. Examples. Point Groups and their determination. Mathematical group-Definition, Examples, order of a group. Abelian and Cyclic groups, Group Multiplication table. Rearrangement theorem, Sub groups and classes in a group. Similarly transformation. Conjugate elements. Matrices, Addition and multiplication of matrices, Inverse of matrix. Character of matrix. Diagonal matrix, Direct sum and direct product of square matrices. Block diagonalized matrices. Solving linear equations by the method of matrices. Matrix form of symmetry operations. Basis.

UNIT II Theory of molecular symmetry

Representation of groups. Basis. Construction of representations using vectors and atomic orbitals as basis. The representation generated by using Cartesian co-ordinates positioned on the atoms of a molecule. (SO_2 and H_2O may be taken a examples). Reducible and irreducible representations. Construction of irreducible representations by reduction (similarity transformation). Great orthogonality theorem (GOT) and properties of irreducible representations using GOT, Construction of character Table (C_{2v}, C_{3v}, C_{2h}, C_{4v}). Nomenclature of irreducible representations - Mulliken symbols, Symmetry species. Derivation of reduction formular using GOT, Reduction of reducible representations (e.g. Γ_{cart}) using the reduction formula, Direct sum and direct product of irreducible representations. Connection between group theory and quantum mechanics.

UNIT II Application of group theory to Molecular vibrations

Molecular vibrations, symmetry species of normal modes of vibration, Construction of Γ_{cart}. Normal coordinates and drawings of normal modes (e.g., H_2O and NH_3), Selection of rules for IR and Raman activities, complementary character of IR and Raman spectra, Determination of IR active and Raman active modes of molecules (e.g., H_2O, NH_3, CH_4, SF_6).

UNIT IV Chemical Bonding I

i. Schrodinger equation for a molecule, Born-Oppenheimer approximation

ii. Molecular orbital (MO) theory

MO theory of H_2+. MO theory of H_2. MO treatment of homonuclear diatomic molecules Li_2, Be_2, C_2, N_2, O_2, F_2 and hetero nuclear diatomic molecules LiH, CO, NO, HF. Correlation diagrams, Non crossing rule. Spectroscopic term symbols for diatomic molecules.

iii. Valence Bond (VB) theory

VB Theory of H_2. VB theory of more complex molecules: Bonding in BeH_2, H_2O, NH_3, Orbital overlap. Molecular geometry, Hybridization, Examples: Methane, Water, Ethylene, and Acetylene, Multiple bonds. VSEPR theory.

UNIT V Chemical Bonding II

i) MO theory for more complex molecules - HMO theory of linear conjugated hydrocarbons (Ethylene, Butadiene, Allylic anion). Charge on an atom, bond order, Calculation of free valence. HMO theory of aromatic hydrocarbons (benzene). Formula for the rots of the Huckel determinantal equation. Frost-Huckel circle mnemonic device for cyclic polyenes.

ii) Inter molecular forces-Inter molecular forces - ion dipole, dipole-dipole, ion-induced dipole, dipole-induced dipole and dispersion interactions - mathematical expressions – donor-acceptor interactions - Lennard Jones potential

UNIT VI Application of Group theory to Chemical Bonding

i) Vanishing and non-vanishing integrals. Transition moment integral and selection rules. Overlap integrals and conditions for overlap.

ii) Molecular orbital treatment of molecules using Group theory. Treatment of H_2O, Classification of atomic orbital involved into symmetry species, Group orbital, Symmetry adapted linear combination (SALC), Projection Operator, Construction of MOs, Electronic Configuration of H_2O, Symmetries of the ground and excited states, Electronic transitions and selection rules, Laporte selection rule for centro symmetric molecules.

iii) Group theoretical treatment of hybridization, Construction of hybrid orbital in BF_3 and CH_4, Inverse transformation.

REFERENCES

1. F.A. Cotton, Chemical Applications of Group Theory, John Wiley & Sons, 3rd Ed. (2006).

2. R.L. Carter, Molecular Symmetry & Group Theory, John Wiley & Sons (2004).

3. K.V. Raman, Group Theory & its application to Chemistry, Tata McGraw Hill Publishing Co. Pvt. Ltd., New Delhi (1990).

4. I.N. Levine, *Quantum Chemistry*, 5th Edition, Pearson Education Inc.2003.

5. A McQuarrie, *Quantum Chemistry*, University Sciences Books, 1983.

6. J.P. Lowe, *Quantum Chemsitry*, 2nd Edition, Academic Press, Inc. 1993.

7. A.K. Chandra, Introduction of *Quantum Chemsitry*, Tata McGraw Hill,1994.

8. R.K. Prasad, *Quantum Chemistry,* 2nd Edition, New Age International, 2000.

9. M.S. Pathania, *Quantum Chemistry and Spectroscopy (Problems & Solutions)*, Vishal Publications, 1984.

10. G.K.Vemulapally,PhysicalChemistry,PrenticeHall of India

11.V. Ramakrishnan, M. S. Gopinathan, Group theory in Chemistry, Vishal Pub. New Delhi, 1996.

ACH 2C 06 SEMESTER II INORGANIC CHEMISTRY II (3 Credits)

Course Outcome After completion of the full course the student should be able to:	Cognitive level
C.O.1: Explain Molecular orbital formation and identify various d-d transitions and interpret the electronic spectra of any given coordination Compounds	Understand
C.O.2: Analyze magnetism in metal complexes and its applications	Analysis
C.O.3: Compare the stability of metal complexes, their reactivity, and the mechanisms of ligand substitution reactions.	Evaluation
C.O.4: Describe the mechanisms of redox reactions in coordination compounds	Analysis
C.O.5: Analyze the structure, bonding stability and reactions of organometallic compounds	Analysis
C.O.6: Illustrate mechanism of homogeneous catalytic processes by Organometallic complexes	Application

UNIT I Molecular Orbital Theory and Electronic Spectra of Coordination Compounds

Correlation diagrams. d^1 and d^2 systems. method of descending symmetry. Molecular Orbital Theory of Coordination Compounds. Transformation properties of atomic orbitals, hybridization schemes for sigma and pi bonding with examples, symmetry adapted linear combination of atomic orbitals in tetrahedral, octahedral, Square planar complexes, formation of symmetry adapted group of ligand, Charge transfer spectra. Charge Transfer spectra of $KMnO_4$. Electronic spectra of complexes – Terms of d^n configurations, selection rules for d-d transitions. Effect of ligand fields on RS terms in octahedral- and tetrahedral complexes. Orgal diagrams, spectra of 3d metal complexes, calculation of Dq, B and β. Correlation diagram. Tanabe and Sugano diagrams. Charge transfer spectra.

UNIT II Magnetic Properties of Coordination Compounds

Magnetic properties of transition metal complexes – Types of magnetic properties. Para magnetism - the Curie and Curie – Weiss law. The μJ, μL+S and μ spin-only expressions, temperature independent Para magnetism. Ant ferromagnetism types and exchange path

ways. Magnetic properties of f-block elements. Determination of magnetic moment by Gouy method. Applications of spectral and magnetic properties in co-ordination chemistry.

UNIT III Reaction Mechanism of Coordination Compounds

Reaction mechanisms of metal complexes, Classification, rate laws, Metal and ligand substitution reactions in octahedral complexes – A, D and I mechanisms and associated energetics aquation and base hydrolysis, stereochemical changes, isomerisation and recemisation. Fuoss-Eigen equation and factors determining A and D mechanisms. Lability and inertness of the complexes, trans-effect, its theories and applications, the cis-effect. Reactions of coordinated ligands: hydrolysis, acid dissociation, aldol condensation, transmination, template effect and macrocyclisation.

UNIT IV Redox Reactions of Coordination Compounds

Redox reaction mechanisms – classification, outer-sphere electron transfer, chemical activation, Marcus theory and thermodynamics. Inner-sphere electron transfer – kinetics, effect of the nature of metal and ligand, bridging group effects. Metal-ligand redox reactions. Two electrons, inner-sphere electron transfer processes.

UNIT V Organometallic Compounds-Synthesis, Structure and Bonding

Organometallic compounds, Various classification and hapto nomenclature of organometallic compounds, 16 and 18 electron rules, Electron counting methods-covalent and ionic model, Main group organometallics with alkyl and aryl ligands Groups 1, 2, 11, 12, 13, 14 and 15 – Synthesis, structure and applications, Organometallic complexes of 'f' block elements; σ-bonded complexes, cyclopentadienyl complexes and bis (arene) complexes. Transition metal to carbon multiple bond, metal carbenes – Synthesis, structure and reactions of Fischer and Schrock Carbenes, Tebbe's reagent. Intermediate carbene between Fischer and Schrock carbene, Synthesis, structure and reaction of metal-carbyne complexes, Transition metal complexes with chain π ligands – synthesis, structure, bonding and reactions of complexes of ethylene, acetylene, allyl and butadiene ligands. Complexes of ring π donor ligands – synthesis, structure, bonding and reactions of typical complexes of cyclobutadiene, C_5H_5, C_6H_6, C_7H_7 and $C_8H_8^{-2}$, Fluxional organometallic compounds.

UNIT VI Catalysis by Organometallic Compounds

Applications of organometallic compounds in organic synthesis and homogeneous catalysis, Complex formation and activation of H2, N2, O2, NO by transition metals. Catalytic steps, Oxidative addition, reductive elimination and insertion reactions Carbonylation by Collman's reagent. Hydrozirconation of alkenes and alkynes. Homogeneous catalysis-Hydrogenation, hydrosilation, isomerization of alkenes, alkyne, cycloadditions, Zeigler-Natta catalysis,

hydroformylation of alkenes, Monsanto acetic acid process and Wacker process. Metal complexes in enatioselective synthesis.

REFERENCES

1. D. J. Shriver, P. W. Atkins, Inorganic Chemistry, 5th edition, Oxford university press, 2010.

2. K.F. Purcell and J.C. Kotz, Inorganic Chemistry, W.B. Saunders Co.

3. E. Huheey, E. A. Keiter, R. L. Keiter, Inorganic Chemistry: Principles of Structure and Reactivity, 4th ed., Harper Collin College Publishers, 1993.

4.F.A. Cotton and G. Wilkinson, Advanced Inorganic Chemistry. 5th edition, John and Wiley, 1999. 5. G. Wulfsberg, Inorganic Chemistry, Viva Books, 2002.

5.R.L. Dutta and A. Shyamal, Elements of Magnetochemistry, 2nd edition, Affiliated east west press. 7. R.S. Drago. Physical Methods in Inorganic Chemistry, 2nd edition, Affiliated east west press.

6.P. Powell, Principles of Organomettalic Chemistry, 2nd edition, Chapman and Hall, London, 1998. 9. S.F.A. Kettle, Concise co-ordination chemistry, Nelson, 1969.

7.S.F.A. Kettle, Physical Inorganic Chemistry-A Co-ordination chemistry Approach, Spectrum academy publishers, 1996.

8. Ch. Elschenbroich, A. Salzer, Organometallics – A Concise Introduction, VCH Publishers, 1989.

9.B. D. Gupta, A. J. Elias, "Basic Organometallic Chemistry", University Press, 2010. 3. P. Powell, Principles of Organometallic Chemistry, 2nd ed., ELBS, 1991.

ACH 2C 07 Semester II Organic Chemistry II (3 Credits)

Course Outcome After completion of the full course the student should be able to:	Cognitive Level
C.O.1: Describe the reactivity, the stereo chemical aspects and various reactions possible with carbonyl compounds.	Analysis
C.O.2: Analyze mechanistic pathways of DA, sigmatropic and electrocyclic reactions	Analysis
C.O.3: Apply the concepts of Frontier orbital theory in the different types of pericyclic reactions.	Application

C.O.4: Illustrate the applications of some important name reactions.	Application
C.O.5: Describe the basic concepts and synthesis of different synthetic polymers in laboratory and in industries.	Understand
C.O.6: Able to explain classifications, mechanisms and applications of various intermolecular rearrangements involving migrations from nitrogen to carbon and nonaromatic heterocyclic organic compounds	Analysis

UNIT I Reactions of Carbonyl Compounds

Reactivity of carbonyl groups in aldehydes, ketones, carboxylic acids, esters and acid chlorides with nucleophilic reagents (Carbon, Hydrogen and Nitrogen nucleophiles). Carbonyl α-substitution reactions:- Keto- enol tautomerism. Reactivity of enols, mechanism of α-substitution reactions. α-Halogenation of aldehydes, ketons and carboxylic acids. Hell-Volhard- Zelinski reaction. Acidity of α hydrogen atom- enolate ion formation. Reactivity of enolate ions. Halogenation of enolate ions- haloform reaction. Alkylation of enolate ions. Aldol and related reactions, Claisen ester condensation, Darzen reaction, Dieckmann, Perkin and Prins reactions. Mannich reaction. Alkylation using enamine. Alkylation of carbon nucleophiles by conjugate addition, Michael reaction, Robinson anulation. The enamine and imine anion. Phosphorous ylides and Wittig reaction.

REFERENCES

1. F. A. Carey, R. J. Sundberg, Advanced Organic Chemistry (parts A and B), 5th ed., Springer, 2008.

2. Michael B. Smith, March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure 8th Edition McGraw Hill.

UNIT II Pericyclic Reactions

Definition and types of reactions classified as pericyclic actions - (a) Cycloaddition and cycloconversion (b) Electrocyclic ring closing and ring opening (c) Sigmatropic rearrangements (d) Cheletropic reactions (e) Group transfers, Stereochemistry of pericyclic reactions and theory of molecular orbital symmetry. Application of theory of M.O. Symmetry by the method of correlation diagram by both thermal and photochemical paths. Stereochemistry of Pericyclic reactions-thermal and photochemical by "Method of Transition state atomaticity". Basic principles of perturbation molecular orbital (PMO) theory,

significance of Frontier Molecular orbitals, Stereochemistry of pericyclic reactions by the "Frontier molecular orbital (FMO) method".

REFERENCES

1. J. Singh, Photochemistry and Pericyclic Reactions, New Age International, 2005.

2. Ian Fleming, Pericyclic Reactions (Oxford Chemistry Primers)

3. T. H. Lowry, K. S. Richardson, Mechanism and Theory in Organic Chemistry, 3rd ed., Benjamin-Cummings Publishing Company, 1997

UNIT III Name reactions II

Eschenmoser-Tanabe Fragmentation, Hofmann-Loffler-Freytag reaction, Julia-Lythogoe olefination, Koenig-Knorr glycosidation, Mitsunobu reaction, Mukaiyama aldol reaction, Peterson olefination, Hayashi reaction, Shapiro reaction, Sharpless asymmetric epoxidation, Sommelet reaction, Von Braun reaction, Hofmann-Loffler Freytag reaction, Ramburg-Backland reaction

REFERENCES

1. T. H. Lowry, K. S. Richardson, Mechanism and Theory in Organic Chemistry, 3rd ed., Benjamin-Cummings Publishing Company, 1997

2. Jie Jack Li – Name Reactions: A Collection of Detailed Reaction Mechanisms.

3. Laszlo Kurti and Barbara Czako, Strategic Applications of named Reactions in Organic Synthesis, Elsevier Academic Press, 2005.

UNIT IV Synthetic polymers I

Concept of polymers and macromolecules: definition, classifications, understanding the following terms - degree of polymerization, average degree of polymerization, number average and weight average molecular weights, poly-dispersity index, homopolymer and co-polymer, alternating, random and block polymers, linear, branched and network polymers. Chain growth (radical, anionic and cationic) polymerization, co-ordination polymerization and step growth polymerization-illustrated with suitable examples (Mechanism only). Crystalline and amorphous polymers, polymer chain flexibility- Factors affecting chain flexibility, glass transition temperature. Factors affecting glass transition temperature. Stereochemical configuration of polymers- Tacticity, isostatic, syndiotactic, atactic, illustrated with suitable examples.

REFERENCES

1. D. Feldman and A. Barbalata, Synthetic Polymers, Chapmann and Hall.
2. G. Odian, Principles of Polymerisation, McGraw Hill.
3. V.R. Gowarikar and N.V. Vishwanathan, Polymer Science, New Age international 2010

4. F. W. Billmayer, Text book of polymer science, 3rd ed., Willey, New York, 1991.
5. G.S. Misra, Introductory Polymer Chemistry, New Age International

UNIT V Molecular Rearrangements II

Intermolecular migration from nitrogen to carbon: Aromatic arrangements: Orton rearrangement, Fischer-Hepp rearrangement, Hofmann-Martius rearrangement, Bamberger Rearrangement, Other: Rupe rearrangement, Von-Richter Rearrangement, Neber rearrangement, Smiles rearrangement, Stieglitz rearrangement, Migratory aptitude in rearrangements, cross-over experiments and its significance.

REFERENCES

1. F. W. Billmayer, Text book of polymer science, 3rd ed., Willey, New York, 1991.Wiley Interscience New York.
2. R O C Norman and E M Coxon, Principles in Organic Synthesis, 2005, CRC Press, New York.
3. B. P. Mundy, M. G. Ellerd, and F. G. Favaloro Jr. Name reactions and reagents in Organic Synthesis, Wiley Interscience, New Jersey 2005

UNIT VI Heterocyclic Compounds

Aromatic heterocycles and nonaromatic heterocyclic compounds. Five membered ring compounds with one heteroatom. Synthesis, reactions and applications of Pyrrole, Furan, Thiophene, Benzofuran, Benzothiophene. Synthesis and reactions of six membered ring compounds. Isoquinoline, Pyrylium salts, 2H-pyran-2 ones, 4H-pyran-4 ones. Five and six membered rings with two or more heteroatoms-pyrimidines and purines, quinazoline, oxazine, Thiazine, Imidazole.

REFERENCES

1. J.A. Joule and K. Miller, Heterocyclic Chemistry
2. Gilchrist, Heterocyclic Chemistry.
3. P.Y. Brunice, Organic chemistry, prentice Hall.
4. I.L. Finar, Organic chemistry, Prentice Hall.

ACH 2C 08 SEMESTER II PHYSICAL CHEMISTRY II (3 Credits)

Course Outcome After completion of the full course the student should be able to:	**Cognitive level**
C.O.1: Distinguish different types of statistics and calculate the	Analysis

thermodynamic probability of any given thermodynamic system.	
C.O.2: Illustrate the partition function and thermodynamic properties from spectroscopic data and apply the principles of statistical thermodynamics to ideal gases, solids and metals.	Application
C.O.3: Analyze the electronic structure and properties of solids	Analysis
C.O.4: Explain the concepts and reactions in physical photochemistry	Understand
C.O.5: Understand the fundamentals of spectroscopy.	Understand
C.O.6: Interpret various spectral data.	Application

UNIT I Statistical Thermodynamics I

Basic principle, Permutations. Probability distribution of particles in energy states. Ensembles Micro states and macro states. Statistical weight. Most probable distribution. Thermodynamic probability and entropy. Maxwell-Boltzmann distribution law of energy for a system of distinguishable and indistinguishable particles. The partition function and its relation to the thermodynamics functions.

Factorization of the partition function in to the translational, rotational, vibrational and electronic parts. Evaluation of the thermodynamic functions and equilibrium constants using partition functions. The perfect gas-ideal monatomic and diatomic gases. Sackur-Tetrode equation. Heat capacity of gases. Classical and quantum theories. The anomalous heat capacity of hydrogen. Ortho and para hydrogen.

UNIT II Statistical Thermodynamics II

(a) The atomic crystal – Einstein theory of atomic crystals, Debyes modification of Einsteins model. (b) Imperfect gases, the virial expressions and the virial coefficients, relation between the virial coefficients and the cluster integrals.

Need for Quantum statistics-The ideal Fermi Gas. Fermi-Dirac distribution law. Gas Degeneracy. Application to electrons in metals. The ideal Bose gas. Bose-Einstein distribution law. Gas Degeneracy. Bose-Einstein condensation. Application to liquid helium. Comparison of the three statistics.

REFERENCES

1. G S Rush Brook Statistical Mechanics, Oxford University Press.

2. T L Hill, Introduction to Statistical Thermodynamics, Addison Wesley.

3. K. Huary, Statistical mechanics Thermodynamics and Kinetics, John Wiles.

4. F C. Andrew, equilibrium and Row, Statistical Thermodynamics.
5. O K Rice, Statistical Mechanics, Thermodynamics and Kinetics, W H Feeman and Co.
6. D A McQuarrie, Harper and Row, Statistical Thermodynamics.
7. Kistin and Dorfuran, A course on Statistical Thermodynamics, Academic Press. 1971.
8. L K Nash, Elements of Statistical Thermodynamics, Addison Wesley Publishing Co.
9. M C Gupta, Elements of Statistical Thermodynamics, New Age International.
10. Molewyn Hughes, Physical Chemistry, Cambridge University Press.
11. M C Gupta, Elements of Statistical Thermodynamics, New Age International.

UNIT III Solid State Chemistry

Theories of solid-free electron, MO band and zone theories. Classification of solids in to conductor, semiconductors and insulators. Preparation, properties and industrial importance of Semi conductors, Imperfections of solids, Point, line and plane defects and electrons and holes. New materials-zeolites, fullerenes, conducting polymers.

Imperfection and Physical properties of solids (Brief survey). Electrical properties-Electrical conductivity, Hall effect, dielectric properties, piezoelectricity, Ferro electricity and conductivity. Super conductivity-Type I and Type II superconductors, High T materials. Meissner effect, brief discussion of Cooper theory of superconductivity. Optical properties-Photoconductivity, luminescence, colour centers, laser, refraction, birefringence, Magnetic properties-diamagnetism, Para magnetism, ferromagnetism, antiferromagnetism. Thermal properties-thermal conductivity and specific heat. Mechanical properties: Strength of real crystals as compared with an ideal crystal, different strengthening mechanisms.

REFERENCES

1.L V Azaroff, Introduction to solids, McGraw Hill
2.A K Galway, Chemistry of Solids, Capman and Hall
3.N B Hanna, Solid State Chemistry, Prentice Hall
4.G M Barrow, Physical Chemistry., Mc Graw Hill
5.W J Moore, Physical Chemistry, Prentice Hall
6.A R West, Solid state chemistry, John Wiley.
7.D K Chakrabarthy, Solid state Chemistry, New Age Publications, 1996.
8.H V Keer, Principles of the Solid state, Wiley Eastern, 1993.
9.O P Khanna, Material Science and Metallurgy, Dhanpathraj Publications, 1987.
10.L Smart and E Moore. Solid State Chemistry-An Introduction, Nelson ThornesLtd.,

UNIT IV Photochemistry

Physical photochemistry: laws of Photochemistry, quantum yield and its determination. Effect of temperature, wavelength and intensity of radiation on photochemical reaction. Different types of photochemical reactions. Kinetics of photochemical chain reactions. H_2-Br_2 reaction H_2Cl reaction, polymerization, photosensitization, photo stationary states. Photolysis ammonia. Excimers and Exciplexes. Photosensitization by Hg. Photo-physical phenomena. Radiative and non-radiative transitions. Jablonski diagram. Fluorescence: quantum efficiency of fluorescence, Stern-Volmer equation; delayed fluorescence. E-type and P-type phosphorescence. Luminescence, chemiluminescences and thermo luminescence. Chemistry of photography. Principle of utilization of solar energy. Solar cells: Different types, working and applications (brief mention only)

REFERENCES

1. D A Mc Quarrie and J D Simon, Physical Chemistry, A molecular approach, University Science Books.

2. G K Vemulapalli, Physical Chemistry, Prentice-Hall of India.

3. K K Rhatgi and Mukherjee, Fundamental of Photochemistry, New Age International.

4. Dupoy and Chapmann, Molecular Reactions and Photochemistry, Prentice-Hall.

5. J Calvet and J Pitts, Photochemistry, John Wiley.

6. A Cox and T Camp, Introductory Photochemistry, Mc Graw Hill.

7. A W Adamson and PD Fleischauer; Concepts of Inorganic Photochemistry, Wiley.

UNIT V Spectroscopy

(i) General Theory of Spectra: Electromagnetic radiation and its different regions, Interaction of matter with radiation and its effect on the energy of the molecule. Origin of molecular spectra, Theory of the origin of rotational, vibrational and electronic spectra. Intensity of spectral lines, Dependence of intensity on population, transition probabilities, Transition moment integral, Selection rules. Line widths, Doppler broadening, Lifetime broadening.

(ii)Microwave spectroscopy: Rotation spectra of diatomic and poly atomic molecules, Rigid and non rigid rotator models, Asymmetric, symmetric and spherical tops. Isotope effect on rotation spectra, Stark effect, Nuclear and electron spin interactions. Rotational transitions and selection rules. Microwave spectrometer -Principles - Instrumentation (brief mention only). Applications.

(iii)Vibrational spectroscopy: Vibrational spectra of diatomic and poly atomic molecules, Harmonic oscillator model, Anharmonicity. Vibrational transitions and selection rules. Morse potential, Fundamentals, Overtones, Hot bands, Combination hands, Difference bands. Vibrational spectra of diatomic and polyatomic molecules, P, Q, R branches. IR and FTIR spectrophotometer - Principles - Instrumentation (brief mention only), Applications.

(iv)Raman Spectroscopy: Pure rational, pure vibrational Raman spectra, Vibrational-rotational Raman spectra, Selection rules, Mutual exclusion principle. Raman spectrophotometer - Principles - Instrumentation (brief mention only) Laser Raman spectroscopy, Applications.

(v) Electronic Spectroscopy: Basic principles, Beet-Lambert Law, Molar extinction coefficient, intensity of electronic transitions. Types of electronic transitions. Franck-Condon principle, Ground and excited electronic states of diatomic molecules. Electronic spectra of polyatomic molecules. Chromphores. The fate of electronically excited state species - Vibrational relaxation, External conversion, Internal conversion, Fluorescence, Phosphorescence, Jablonski diagram. Electronic spectra of conjugated molecules - Dissociation and predissociation spectra.

UV-Visible spectrophotometer - Principles - Instrumentation (brief mention only). Applications.

UNIT VI Resonance Spectroscopy

(i) NMR Spectroscopy: Magnetic properties of nuclei, Theory and measurement techniques, Solvents used, Chemical shift and factors influencing chemical shift, Shielding effects, Spin-Spin interaction coupling constant, factors influencing coupling constant, Effects of chemical exchange, Fluxional molecules, Hindered rotation on NMR spectrum, Karl's relationships, NMR spectrometer - Principles and instrumentation (brief mention only).Applications of NMR spectroscopy to structure elucidation of simple organic and inorganic molecules .FTNMR.

(ii) ESR Spectroscopy: Theory and measurement techniques, hyperfine interactions, Equivalent and nonequivalent protons, Kramer's theorem. ESR

REFERENCES

1.C.N. Banwell &E.N.McCash,Fundamentals of Molecular Spectroscopy,Tata, McGraw Hill

2. Aruldhas, Molecular Structure&Spectroscopy, Prentice Hall, India

3. F.W.Atkins,Physicl Chemistry,Oxford University Press

ACH 2P 04 SEMESTER II PRACTICAL INORGANIC II (3 Credits)

Course Outcome After completion of the full course the student should be able to:	Cognitive level
C.O.1: Understand safe laboratory practices of handling laboratory glassware, equipment and chemical reagents and develop basic laboratory skills	Knowledge
C.O.2: Analyze alloys and ores	Analysis
C.O.3: Estimate the amount of a given metal ion by colorimetry	Analysis
C.O.4: Synthesise metal complexes and characterize them by various physicochemical methods.	Synthesis
C.O.5: Interpret electronic spectrum of different metal complexes.	Application

Analysis of one of the alloys of brass, bronze and solder. Analysis of one of the ores from hematite, chromite, dolomite, monazite, ilmenite. Anyone to be analysed

OR

Colorimetric estimation of Fe, Cu, Ni, Mn, Cr, NH_4^+, nitrate and phosphate ions.

Any two to be recorded

OR

Preparation and characterization complexes using IR, NMR and electronic spectra. Any two complex to prepared

(a) Tris (thiourea)copper(I) complex

(b) Potassium tris (oxalate) aluminate (III).

(c) Hexammine cobalt (III) chloride.

(d) Tetrammine copper (II) sulphate.

(e) Schiff base complexes of various divalent metal ions.

(f) Bis(dimethylglyoximato)nickel (II)

(g) Prussian blue

OR

(b) Synthesize the following complexes of Ni(II) (a d^8 system) and prepare 0.05M solutions of the complexes in the solvents specified.

Complex Solvent and Blank. Concentration

1. $[Ni(bipy)_3]SO4.6H_2O$ Water 0.05M

2. $[Ni(en)_3]Cl_2.2H2O$ 20% en 0.05M

3. $[Ni(NH_3)_6]CI_2$ Aqueous NH3 0.05M

4. $[Ni(H_2O)6]SO_4$ Water 0.05M

5. $[Ni(DMSO)_6](CIO_4)_2$ DMSO 0.05M

6. $K4[Ni(NCS)_6]4H_2O$ 10M KSCN in water 0.05M

Record the electronic spectrum of each solution in the region 200 – 1100 nm. Calculate Δ values for all six complexes. Arrange the ligands in the spectrochemical series i.e. in the order of increasing Δ.

REFERENCES

1.A.I. Vogel, G. Svehla, Vogel's Qualitative Inorganic Analysis, 7thEdn., Longman,1996.

2.V.V. Ramanujam, Inorganic Semimicro Qualitative Analysis, The National, Pub.Co., 1974.

3.J. Singh, R. K. P. Singh, J. Singh, LDS Yadav, I. R. Siddiqui, J. Shrivastava, Advanced Practical Chemistry, PragatiPrakashan, 7th Edn., 2017.

4.A.I. Vogel, A Text Book of Quantitative Inorganic Analysis, Longman, 1966.

5.I.M. Koltoff, E.B. Sandell, Text Book of Quantitative Inorganic Analysis, 3rd Edn., McMillian, 1968.

6.G. Pass, H. Sutcliffe, Practical Inorganic Chemistry, Chapman & Hall, 1974.

7.N.H. Furman, Standard Methods of Chemical Analysis: Volume 1, Van Nostrand, 1966.

8.F.J. Welcher, Standard Methods of Chemical Analysis: Vol. 2, R.E. Kreiger Pub., 2006.

9.J. Singh, R. K. P. Singh, J. Singh, LDS Yadav, I. R. Siddiqui, J. Shrivastava, Advanced Practical Chemistry, PragatiPrakasan, 2014.

10.Journal of Chem. Ed, 1962, 39, 634.

11.Cotton, J. Chem. Educ.1964, 41, 466.

12.Sutton, J. Chem. Educ. 1960, 37, 498.

13. Manch&Fernelius, J. Chem. Educ. 1961, 38, 192.

ACH 2P 05 SEMESTER II PRACTICAL ORGANIC II (3 Credits)

Course Outcome After completion of the full course the student should be able to:	Cognitive Level
C.O.1: Understand safe laboratory practices of handling laboratory glassware, equipment and chemical reagents and develop basic laboratory skills.	Knowledge

C.O.2: Apply two synthetic procedures, chromatographic separation and purification of organic compounds.	Application
C.O.3: Analyze organic compounds from the organic binary mixture and identify the functional group(s) present	Analysis
C.O.4: Experiment the quantitative analysis in organic chemistry	Analysis
C.O.5: Practice the estimation of organic compounds	Application
C.O.6: Design experiments and validate the hypothesis of an independent research problem	Create (synthesis)

1. Quantitative Organic Analysis

Estimation of Nitrogen by Kjeldal methods, estimation of hydroxyl and carbonyl groups. Determination of Iodine number and Saponification value of oils. Estimations of reducing sugar, amines, pheols, esters, vitamins (A and C) and Drugs (Aspirin and Paracetamol).

2. Student-Designed Multistep Synthesis project

In the second semester each student will have to develop a multistep synthesis project, limited principally by cost, safety and availability of materials. The plan should contain at least four synthetic steps. Subsequently, the students should obtain their own literature protocols for the individual steps. After discussion with faculty members, they can start working on their own projects. The synthesis will be performed over three to four weeks. The students should conclude their project with a presentation of the results at the end of the semester. Evaluation of the student project will focus not only on the successful synthesis of the target molecule but also, their planning, skill and maturity they have shown in trouble shooting and the merit of the experimental and spectral techniques they have used for purification and characterization.

REFERENCES

1. A.I. Vogel, A Text Book of Practical Organic Chemistry
2. Fiester, Experiments in Organic Chemistry
3. Mann and Saunders, Practical Organic Chemistry
4. Dey, Sitaraman and Govindachari, A Laboratory Manual of Organic Chemistry.
5. Cheronis and Fatrikin, Semi-micro Organic Analysis
6. A.I. Voget. Quantitative Organic Analysis
7. P.G. Singh, D.S. Gupta and K.S. Bajpal, Experimental Organic Chemistry, Vols. I and II, 1980.

8. R. Srinivasan, Ed. Photochemical Synthesis Vols. I and II.

9. D. L. Pavia, G. M. Lampman, G. S. Kriz, Introduction to Organic laboratory Techniques, 3rd ed., Saunders Golden Sunburst Series

ACH 2P 06 SEMESTER II PRACTICAL PHYSICAL II (3 Credits)

Course Outcome After completion of the full course the student should be able to	**Cognitive level**
C.O.1: Understand safe laboratory practices of handling laboratory glassware, equipment and chemical reagents and develop basic laboratory skills	Knowledge
C.O.2: Analyze experiments based on various laws of physical chemistry.	Analysis
C.O.3: Interpret the results obtained from various experiments.	Application
C.O.4: Obtain and analyse data using various sophisticated instruments	Application
C.O.5: Construct phase diagram of various eutectic systems having binary mixture.	Create (Synthesis)

- **Chemical Kinetics**

  1. Kinetics of acid catalyzed hydrolysis of methyl acetate and determination of (a) order and rate constant, (b) Relative strength of two acids, (c) Energy of activation.

  2. Determination of temperature, coefficient and energy of activation of hydrolysis of methyl acetate. Determination of Arrhenius parameters.

  3. Saponification ethyl acetate (titration/conductance method).

  4. Inversion of cane sugar in presence of HCl by polarimetry

  5.Iodination of acetone in acid medium - Determination of order of reaction with respect to iodine and acetone.

  6. Determination of degree of hydrolysis of CH_3COONa and NH_4Cl.

  7. Determination of hydrolysis constant of aniline hydrochloride.

  8. First and second order kinetics of reaction between potassium persulphate and K1.

- **Adsorption**

  1. Verification of Freundich and Langmuir adsorption isotherms.

2. Determination of concentration of acetic acid/oxalic acid using Freundlich and Langmuir adsorption isotherms.

3. To study the adsorption of iodine on charcoal from alcoholic solution.

- **Phase equilibria**

1. Phase diagram of a simple eutectic system.

2. Phase diagram of a binary solid system forming a compound.

3. Mututal miscibility curve of a binary liquid system (phenol-water)-critical solution temperature (CST). Effect of impurities (NaCl, KCl, succinic acid, salicylic acid) on the CST of water-phenol system).

4. Ternary liquid system with one pair of partially miscible liquids, (DMSO)-benzene-water, acetone-chloroform-water etc.)

5. Construction of phase diagram of a two-component system by thermal analysis.

- **Potentiometry**

1. Potentiometric titrations of acid vs base in partial and non-aquous media.

2. Potentiometric titration of halides in mixtures (Cl^-, Br^- and I^-) with silver nitrate.

3. Determination of transport number of ions by emf method (Ag+, Cd^{2+}, NO_3^-, SO_4^{2}, etc).

4. Electrode potentials of Zn, Ag and Cu, in solutions of different molalities at room temperature and determination of their standard electrode potentials.

5. Mean activity coefficient of an electrolyte at different molalities by EMF method.

6. Dissociation constant of CH_3COOH in DMSO, DMF, acetone and dioxin by titrating with NaOH.

7. Determination of strength of the given HCL solution by differential potentiometric titration.

8. Dissociation constant of acetic acid by potentiometric titration method.

REFERENCES

1. A Findlay, Practical Physical Chemistry, Longman's Green & Co., 1972.

2. R.A Alberty et al., Experimental Physical Chemistry, McGraw Hill, 1956.

3. J.B.Yadav,Advanced Practical Physical Chemistry,Goel Publishing

4. Gurtu&Gurtu,Experimental Physical Chemistry,Prgti Prakashan

5. Gurdeep Raj, Experimental Physical Chemistry, Krishna Prakasha

Practical Examination based on practicals in semester I & II will be held at the end of Semester II only. Each paper will carry 3 credits. Each Exam will be of six hours duration

ACH 2A 02 II Semester Audit course (Credits: 2; Weightage: 30)

Professional Competency Course (PCC)

PCC particularly aims to improve the skill level of students, especially for using specific as well as nonspecific softwares useful in their respective field of study, both related to the core and elective subject area. Also, it is a platform for the student community to undertake socially committed projects and thereby developing a method of leaning process by through the involvement with society.

One particular PCC may be selected for all the students in a batch in the department or each student in a batch may choose one PCC, among the pool of courses suggested below. Credit of the PCC will not be considered while calculating the SGPA/CGPA. But the student has to obtain minimum pass requirements (weightage 15) in this course, which is compulsory for overall pass in the programme. Evaluation/examination on PCC must contain the following components: MCQ type written examination (weightage: 10), Report on PCC (weightage: 10), Presentation on PCC (weightage: 5), Viva voce on PCC (weightage: 5).

Course Outcome After completion of the entire course, the student should be able to :	**Cognitive level**
C.O.1: Describe the basic principles and concepts related to the application of computers in chemistry.	Understand
C.O.2: Discuss the main similarities and differences between various computational approaches.	Analysis
C.O.3: Develop skills for molecular modelling.	Application
C.O.4: Evaluate skill of using specific and nonspecific software to solve problems in chemistry.	Evaluation
C.O.5: Construct ability to conduct socially related projects.	Create (Synthesis)
C.O.6: Develop learning processes through the involvement of society.	Application
C.O.7: Develop solutions for e-security issues and system design.	Application

1. Applications of computers: History of development of computers, mainframe, mini, micro's and super computer systems, Personal computers, General awareness of computer hardware, CPU, input and output devices, memory, other peripheral devices, auxiliary storage devices, Basic knowledge of computer systems, softwares - System softwares and application softwares Programming languages: machine language, assembly language and high level languages, Interpreter and compiler, Flow charts and Algorithms, General awareness of operating systems: Disk operating system, Windows, MaCintosh, Linux.

2. Development of skills (using software's in chemistry): General awareness of Software and other scientific application packages, Applications and uses of common softwares in chemistry, Origin, Chemsketch, Chemdraw, GaussView, Gaussian 09, VASP, Autodock, Schrodinger, DataWarrior, etc. Basic ideas on the use of Internet in Chemistry education, Z-matrix, different computational tools, optimization of structures, global and local minimum, potential energy surfaces, molecular modelling, drug designing, drawing chemical structures, converting name to structure and vice versa, computing geometric parameters, calculation of molecular descriptors, analysis, plotting graphs, correlation study, advantages of computational chemistry.

3. Training on computational chemistry: introduction to computational chemistry, different computational methods: molecular mechanics, Ab initio methods, semi empirical methods, density functional theory methods, merits and demerits, computation *vs* experiment, computer aided drug designing, QSAR/QSPR studies, theoretical studies in various areas of chemistry, knowledge on z-matrix, advancement of computational tools in research: a brief review.

4. Case study and analysis on any relevant issues in the nearby society: water analysis: importance of water analysis, impurities in water, water contamination, removal of impurities and water purification, instruments in water analysis, references used in water analysis. soil analysis: important minerals in soil, references in soil analysis, instrumentation, pH analysis, acid/alkali content analysis, sugar content analysis: various methods for sugar testing, references.

5. Any community linking programme relevant to the area of study: Training for society-need and importance, soap/perfume making, waste disposal, plastic recycling, knowledge on pollution: pollutants, different types, awareness programs in decreasing pollution, surveys.

6. Cyber security: Security and system design, vulnerabilities, security challenges, social engineering, e-security issues, cryptography & digital signature, anti-spyware program, spread via Trojans, display fake security messages, privacy violation, compromise, computer

crime, cyber terrorism, cyber warfare, network sniffers, packet spoofing, hijacking, automated probes and scans, automated widespread attacks, email propagation of malicious code, hackers, white hat hackers, gray hat hackers, website hacking, security mechanisms selecting good password, authentication, antivirus softwares.

ACH 3C 09 SEMESTER III INORGANIC CHEMSITRY III (3 Credits)

Course Outcome After completion of the full course the student should be able to:	**Cognitive level**
C.O.1: Discuss the photochemical reactions of coordination compounds and its mechanisms	Understand
C.O.2: Interpret the structure of metal complexes using IR and NMR	Application
C.O. 3: Analyze the ESR spectra of any given transition metal complex and Mossbauer spectra of iron, tin complexes.	Analysis
C.O.4: Explain emergence of bioinorganic chemistry	Understand
C.O.5: Identify the role of metals in biological systems and the natural process taking place with the aid of metal ions in biological systems	Application

UNIT I Photochemistry of Coordination Compounds

Photochemical reactions of metal complexes. Prompt and delayed reactions. Excited states of metal complexes – intra ligand, ligand field, charge transfer and delocalized states. Charge ransfer excited states and redox processes, communication between excited states, radical pair models. Properties of ligand field excited states, rules for photo substitution, photo-aquation and ligand exchange reactions. Substitution and redox reactions of Cr (III), Co (III), Rh (III) and Ru (II) complexes. Photo-isomerization and photo-racemization. Metal complex sensitizers, chemical actinometry and photo-chromism. Semiconductor supported metal oxide systems. Water photolysis, nitrogen fixation and CO_2 reduction, dinitrogen splitting.

UNIT II IR and NMR spectroscopy of Coordination Compounds

Studies (IR and NMR) of simple inorganic compounds and metal complexes. Changes in ligand vibrations on coordination with metal ion. Metal ligand vibrations. Vibrational spectra of metal carbonyls. NMR spectroscopy for structural studies of diamagnetic metal complexes from chemical shift and spin-spin coupling.

UNIT III ESR and Mossbauer Spectroscopy of Coordination Compounds

ESR spectra of metal complexes-Hyperfine splitting and A parameter, g values, zero field splitting and Kramer's degeneracy, application to simple copper complexes. Mossbauer spectroscopy-the Mossbauer-effect, hyperfine interactions (qualitative treatment). Application to simple iron and tin complexes.

UNIT IV Bioinorganic Chemistry-I

Occurrence of inorganic elements in biological systems, bulk-and trace metal ions, emergence of bioinorganic chemistry. Co-ordination sites in biologically important ligands. Metal protein interactions. Role of metal ions in biological functions. Biochemistry of non metals. Biomineralization. Biological role of some trace nonmetals. (B, Si, S, Se, As, CI, Br, I). Biological importance of nitric oxide.

UNIT V Bioinorganic Chemistry-II

Ion transport across membranes. Role of alkali metal ions in biological systems. The sodium/potassium pump, structural role of calcium. Storage and transport of metal ions-ferritin, transferring and siderophores. Oxygen transport by heme proteins-hemoglobin and myoglobin, structure of the O2 binding site, nature of heme-dioxygen binding, cooperativity. Hemerythrin and hemocyanin.

UNIT VI Bioinorganic Chemistry-III

A brief idea on structure and function of copper proteins in electron transport process, cytochromes, iron-sulphur proteins, tyrosinase, superoxide, dismutase. Lewis acid role of Zn (II) and Mn (II containing enzymes, carboxy peptidase, vitamin B12 and coenzymes. Chlorophyll II-Photo systems I and II. Nitrogen fixation – Nitrogenase, Anticancer drugs.

REFERENCES

1. D. J. Shriver, P. W. Atkins, Inorganic Chemistry, 5th edition, Oxford university press, 2010.

2. K.F. Purcell and J.C. Kotz, Inorganic Chemistry, W.B. Saunders Co.

3. J. E. Huheey, Inorganic Chemistry – Principles of Structure and Reactivity, 4th edition, Pearson education, 1993.

4. F.A. Cotton and G. Wilkinson, Advanced Inorganic Chemistry. 5th edition, John Wiley, 1999.

5. A.E. Martell, Coordination Chemistry, Vol I and II, Van Nostrand Reinhold, New York, 1971.

6. D.E. Fenton, Bio co-ordination Chemistry, Oxford, 1995.

7. S.J. Lippard and J. M. Berg, 'Principles of Bioinorganic Chemistry', University Science Books, Mill Valley, 1995.

8. R.S. Drago. Physical Methods in Inorganic Chemistry, 2nd edition, Affiliated east west press, 1993. 9. Robert W. Hay, Bioinorganic Chemistry, Ellis Horwood Limited, UK, 1984. don Press, Oxford, 1976.

ACH 3C 10 ORGANIC CHEMISTRY III (3 Credits)

Course Outcome After completion of the full course the student should be able to:	Cognitive Level
C.O.1: Understand concepts and applications of UV-Vis, IR spectroscopy, NMR and Mass spectroscopy.	understand
C.O.2: Structure elucidation of Organic compounds by different spectroscopy techniques	Evaluate
C.O.3: Illustrate the different elements of synthesis and applications of protecting groups in chemistry.	Application
C.O.4: Analyze and design the strategies of the retrosynthetic approach to synthesize target organic molecules.	Analysis
C.0.5: Explain the structural features of molecular receptors and analyze the type of possible interactions in any given host guest assembly.	Knowledge
C.O.6: Analyze the concept of green chemistry and combinatorial chemistry	Analysis

UNIT I Organic Spectroscopy

Applications of UV, IR, ^{1}H & ^{13}C NMR and MS in the structural elucidation of organic compounds (Problem oriented approach only, instrumentation not required) UV-characteristic absorption of organic compounds - Empirical rules for calculating absorption maximum.

IR-Characteristic group absorption of organic molecules - Alkanes, Alkenes, Alkynes, Mononuclear aromatic Hydrocarbons, Alcohols, Phenols, Ethers, Carbonyl compounds, Amines and Amides, Nitriles, S-H and S=O groups.

^{1}H NMR - The chemical shift and shielding, chemical equivalence and Magnetic equivalence, local diamagnetic shielding, Magnetic anisotropy, Spin-spin coupling, coupling constants, the

mechanism of coupling, (One bond and two bonds coupling only). Protons on heteroatoms, coupling of protons to other nuclei, Quadrupole broadening. First and second order spectra. Aromatic compounds, Homotopic, enantiotopic and diastereotopic hydrogens. Spin decoupling-double resonance. High resolution NMR. Vicinal and Geminal coupling in rigid systems.

^{13}C NMR - ^{13}C chemical shifts, correlation charts, calculation of ^{13}C proton coupled ^{13}C spectra. Spin-spin splitting of ^{13}C signals, proton decoupled spectra, off resonance decouling. Mass Spectrometry-Mass Spectra, Determination of molecular weight, molecular formula from isotope ratio data, fragmentation pattern in differing classes of compounds. Modern techniques of ionization.

REFERENCES

1. Silverstein, Bassler, Monill - Spectroscopic Identification of Organic Compound-John Wiley & Sons, 1991.

2. Kemp- Organic Spectroscopy - McMillan, 1996.

3. Pavia, Spectroscopy of Organic Compounds, Sounde Publications.

4.J.B. Lambert, H.F., Shurvell, D.A. Lightner and R.G Cooks, Organic Structured Spectroscopy, Prentice Hall.

UNIT II Multistep Organic Synthesis

Elements of a synthesis (Reaction methods, reagents, catalysts, solvents, protecting groups (Hydroxyl, Amino Carbonyl and Carboxylic acid protecting groups), activating groups, leaving groups, synthons and synthetic equivalents. Types of selectivities (Chemo, Regio and Stereo selectivities). Synthetic Planning illustrated by simple molecules, disconnections and functional group inter conversions. Umpolung reactions and use in synthesis. Retrosynthetic analysis of a complex molecule-a case study.

REFERENCES

1. John McMurry, Organic Chemistry, 5 Ed., 2000 or newer.

2. Stuart Warren, Designing organic synthesis: programmed introduction to the synthon approach, 1994.

3. The Logic of Chemical Synthesis, E.J. Corey & Xue-Min Cheng, Wiley, 1989.

4. Classics in Total Synthesis, K.C. Nicolaou, E.J. Sorenson, V.C.H., 1996.

5. Organic Synthesis, Michael B. Smith, 2nd Edition, McGraw Hill, 2004.

6. F. A. Carey, R. J. Sundberg, Advanced Organic Chemistry (parts A and B), 5th ed., Springer, 2008.

7. R.O.C. Norman, Principles of Organic Synthesis.

8. R.S. Ward, Selectivity in Organic Synthesis, John Wiley and Sons.

UNIT III Synthetic Reagents

Synthetic reagents; synthetic applications of the following reagents: N-Bromosuccinimide (NBS), Diazomethane, Dicyclohexylcarbodiimide (DCC), Selenium dioxide, *m*-chloroperbenzoic acid, Dichloro-dicyano-benzoquinone(DDQ), Diisobutylaluminium hydride (DIBAL), Lithium diisopropylamide (LDA), Osmium tetroxide, Complex metal hydrides - ($NaBH_4$/$LiDH_4$ and $NaBH_4$/$AlCl_3$ only) Phase transfer catalysts.

REFERENCES

1. Carruthers, Modern Synthetic Methods, Cambridge.

2. Pizey, Synthetic Reagents, Vol. 1-4.

3. Fieser & Fieser, Synthetic Reagents, Vol. 1-4.

4. H.O. House, Modern Synthetic Reactions, Benjamin Cummins.

UNIT IV Molecular Recognition and Supramolecular Chemistry

The concept of recognition, host-guest receptor concept, Forces involved in molecular recognition- hydrogen bonding, Pi stacking, van der Walls and hydrophobic interactions and their significances. Supramolecular chemistry-molecular receptors like calixarenes, crown ethers, Cryptands, Cyclophanes, Cyclodextrins in detail. Self-assembly of supramolecular structures. Introductory study of Combinatorial chemistry.

REFERENCES

1. H. Vogtle, Supramolecular Chemistry, John Wiley and Sons

2. H.Dugas, Bioorganic Chemistry, Springer

3. Fenniri, Combinatorial Chemistry Oxford University Press

UNIT V Green Chemistry

Principles of Green Chemistry. Atom economy and E factor. Atom economic (Diels-Alder reaction, Claisen rearrangement and Michael addition), and atom uneconomic reactions (Wittig reaction, Mitsunobu reaction, and Amide formations). Alternative energy sources: Microwave assisted synthesis, sonochemical synthesis and photochemical synthesis. Emergence of solid acids and zeolites as green catalysts. Discussions on Solvent free Synthesis and Organic reactions in water. Use of super critical carbon dioxide and super critical water as a green media for organic reactions. Fluorous solvents in green organic chemistry. Immobilized Enzyme Catalysis in Green chemistry. Major methods for immobilization of enzymes. Ionic Liquids and Supported Catalysts/reagents. Green Chemistry in Core Organic Synthesis: Multicomponent, Domino and Tandem reactions)

REFERENCES

1. P.T. Anastas and J.C. Warner, *Green Chemistry: Theory and Practice,* Oxford University Press, Oxford, 1998.

2. James Clark and Duncan Macquarrie, Handbook of Green Chemistry and Technology, Blackwell Science, 2002.

3. J.H. Clark the Chemistry of Waste Minimization, Blackie Academic, London, 1995.

4. Multicomponent Reactions, Jieping Zhu and Hugues Bienayme, Eds. Wiley VCH Verlag GmbH & Co. KGaA, Weinheim 2005, ISBN:3-527-30896-7

UNIT VI Industrial Polymers

Brief study of the synthesis, structure, properties and application of the following polymers: - Styrene butadiene rubber, Natural rubber, Neoprene, Polyethylenes, Polypropylene, Polystyrene, PVC, Teflon, plexiglass, urea-formaldehyde resin, melamin-formaldehyde resins, polyethylene terephthalate, polycarbonate, polyurethanes foams, silicon elastomers.

REFERENCES

1. D. Feldman and A. Barbalata, Synthetic Polymers, Chapmann and Hall.

2. G. Odian, Principles of Polymerisation, McGraw Hill.

3. V.R. Gowarikar and N.V. Vishwanathan, Polymer Science, New Age international

4. F. W. Billmayer, Text book of polymer science, 3rd ed., Willey, New York, 1991.

5. R. J. Young, Principles of Polymer Science, 3rd ed., Chapman and Hall, New York, 1991

6. G.S. Misra, Introductory Polymer Chemistry, New Age International

ACH 3C 11 SEMESTER III PHYSICAL CHEMISTRY III (3 Credits)

Course Outcome After completion of the full course the student should be able to	**Cognitive level**
C.O.1: Distinguish the theories of chemical kinetics and gas phase kinetics	Analysis
C.O.2 Discuss control the reaction conditions to improve the reaction rate	Understand
C.O.3: Illustrate the power of photochemistry and radiation chemistry as individual technique and have a notion about their complementarity	Application
C.O.4: Describe the fundamental nature of catalysis, use of adsorption isotherms as a tool for obtaining the surface area and rate constants in the case of heterogeneous catalysis and apply the principles of catalysis to solve	Application Create

given kinetic data.	(synthesis)
C.O.5: Identify the types of nuclear reactions and their applications in the energy sector	Understand
C.O.6: Formulate various computational methods in terms of speed and accuracy for particular studies and perform virtual experiments of sorts with the help of computed molecular properties using quantum chemistry programs.	Synthesis Evaluate

UNIT I Fundamentals of Chemical Kinetics

Reaction dynamics. Theories of reaction rate. Effect of temperature on reaction rate. The Arrhenius equation. The energy of activation. Collision theory (Derivation). Reaction cross section. Transition state theory (Deviation). Comparison of the two theories. Thermodynamic treatment of reaction rates. Linear free energy relationships. Theoretical calculations of energy of activation. The London equation. Potential energy surfaces (brief treatment).

UNIT II Chemical Kinetics II

Kinetic of reaction in solution. Comparison of solution and gas kinetics. Diffusion controlled reactions. Influence of solvent on rate. Cage effect. Effect of dielectric constant on rate. Primary and secondary kinetic salt effects. Structural effects on rate. Hammett and Taft Equations. Study of fast reactions. Flash photolysis. Flow techniques. Relaxation methods.

UNIT III Photochemical and Radiation Chemical Reactions

Photochemical reactions – Primary process, Reactions of electronically excited species. Photochemical thresholds, Laws of photochemical equivalence. Rotator Sector techniques. Laser photochemistry, pulsed lasers. Multiphoton excitation. Photosensitization. Radiation-chemical reactions – primary processes, pulse radiolysis, hydrated electrons. Chemiluminescence.

REFERENCES

1. Fundamental Chemical Kinetics, Margaret Robson Wright. Horwood publishing Limited.
2. K. J. Laidler, Chemical Kinetics, McGraw Hill, New York, 1991.65
3. Kinetic and Mechanism by A.A. Frost and R. G. Pearson, John Wiley.
4. Physical Chemistry by F Daniels and R.A. Alberty, Wiley.

UNIT IV Catalysis

Homogenous and heterogeneous. Theories of homogeneous catalysis. Acid base catalysis, Bronsted catalysis law. Enzyme catalysis: features, Michaelis Menten Mechanism. Catalysis by co-ordination complexes (brief mention) Auto catalysis. Oscillating reactions. BZ reaction. Heterogeneous catalysis: Adsorption and catalysis. Kinetics and mechanism of surface catalyzed reactions. Unimolecular surface reaction: Eley- Rideal Mechanism. Bimolecular reactions: Langmuir-Hinshelwood Mechanism- Discussion on carbon monoxide oxidation reaction on catalyst surface. Industrial Applications (brief mention).

REFERENCES

1. E. K Rideal, Concepts in catalysis, academic press.

2. A. Clark, theory of adsorption and catalysis, Academic press.

3. R. Opearce and Patterson (Ed.) Catalysis and Chemical process, Blackie and sons Ltd (1981).

4. F. A. cotton and G. Wilkinson, Advanced Inorganic Chemistry, 4^{th} edition, John Wiley and sons (1980).

5. Jens Gagen, Industrial catalysis: A practical approach (Wiley VCH).

6. G. Etrl, H. Knozinger, J. Wltamp, Handbook of heterogeneous catalysis, Heterogenous catalysts Volumes 1-5, Wiley VCH (1997).

7. Physical Chemistry, Peter Atkins, Julio de Paula, Oxford University Press.

8. Reaction Kinetics, Vol. II by K.J. Laidler, Mc Graw Hill.

UNIT V Nuclear and Radiation Chemistry

Nuclear reactions: Types, conservation, reaction cross section compound nucleus theory, specific nuclear reactions, photonuclear the thermonuclear reactions, Nuclear fission: Fission Process, fission fragments, mass and charge distribution, fission energy, theory of nuclear fission.

Radio chemical techniques: Neutron activation analysis, Radiation chemistry: the interaction of radiation with matter-process responsible for energy less range and range energy relations, methods of detection and measurement of radiation. Elements of physical and chemical radiation effects in solids, radiation chemistry of water and aqueous ferrous sulphate solution. Radiation dosimetry – Fricks dosimeter-calculation of absorbed dose. Szilard -Chalmers effect.

REFERENCES

1.G. Friedlander and J.W. Kennedy, Nuclear and Radiation Chemistry.

2.S. Classtone, Source Book on atomic energy.

3.J.B. Rajam, Atomic physics

4.Vanderwerf, Radioactive Isotopes.

5.M. Haissinsky, Nuclear Chemistry and applications.

6.N.W.T. Spinks and R.K. Wonds, An Introduction to Radiation Chemistry.

7.Friedlander and J.W. Kennedy Nuclear and Radiation Chemistry.

8. H. J. Arnikar, Essentials of Nuclear Chemistry, 4th ed., New Age International, 2011.

9. W. D. Loveland, D. J. Morrissey, G. T. Seaborg, Modern Nuclear Chemistry, 2nd ed., Wiley, 2017.

10. K. H. Lieser, Nuclear and Radiochemistry, 2nd ed., Wiley VCH, 2001.

UNIT VI Introduction to Computational Chemistry

Computational Methods – Hartee Fock, SCF methods, Electronic structure of molecules, Basis sets, STO's and GTO's, nomenclature of basis sets, semi empirical and ab ignitio methods, calculations using Gaussian, Specification of molecular geometry using a) cartesian co-ordinates b) internal co-ordinates, The Z matrix. Z matrix of simple molecules: H_2O, formaldehyde, methanol.

REFERENCES

1.Jenson F, Introduction to Computational Chemistry – John Wiley

2. Cramer C.J., Essentials of Computational Chemistry – John Wiley

3. Young, Computational Chemistry – Wiley Inter Science

4. Andrews R. Leach, Molecular Modeling – Pearson

5. Ramachandran K.I et al computational Chemistry and Molecular Modeling Springer.

6. Schlick. T., Molecular Modeling and Simulations, Springer.

ACH 3C 12 SEMESTER III INSTRUMENTAL METHODS, THEORY AND INSTRUMENTATION (3 Credits)

Course Outcome After completion of the full course the student should be able to :	**Cognitive level**
C.O.1: Discuss statistical evaluation of experimental data during chemical analysis	Understand
C.O. 2: Demonstrate the concepts of various conventional analytical techniques	Application
C.O.3: Explain the theory, instrumentation and application of various electro-analytical techniques and optical methods of analysis	Understand

C.O.4: Analyze the instrumentation and applications of various surface characterization techniques.	Analysis
C.O.5: Illustrate the theory, instrumentation and applications of various thermal, radiochemical and chromatographic techniques of analysis.	Application

UNIT I Errors in Chemical Analysis (10hrs)

1.1 The basis and procedure of sampling, sampling statistics, sampling and the physical state, crushing and grinding, the gross sampling, size of the gross sample, sampling liquids, gas and solids (metals and alloys), preparation of a laboratory sample, moisture in samples-essential and non-essential water, absorbed and occluded water, determination of water (direct and indirect methods).

1.2 Systematic and random errors. Distribution of experimental results. Statistical treatment-standard deviation, variance, confidence limits, application of statistics to data treatment and evaluation, student-t and f tests, detection of gross errors, rejection of a result-Q test, estimation of detection limits.

Least square method, correlation coefficient and its determination, Hypothesis testing using statistical analysis. Using spread sheets for plotting calibration curves. Quality assurance and control charts.

UNIT II Conventional Analytical Procedures (9hrs)

2.1 Gravimetry: **s**olubility product and properties of precipitates-nucleation, growth and aging, co-precipitation and post precipitation, drying and ignition. Inorganic precipitating agents: NH_3, H_2S, H_2SO_4, $(NH_4)_2MoO_4$ and NH_4SCN.

Organic precipitating agents: oxine, cupron, cupferron, 1-nitroso-lnaphthol, dithiocarbamates,

2.2 Acid-Base and precipitation titrations: theory of neutralisation titrations, indicators for acid/base titrations, titration curves of strong acid, strong base, weak acid, weak base and polyprotic acids. Buffer solutions. Titrations in nonaqueous media. Different solvents and their selection for a titration. Indicators for non-aqueous titrations. Applications.

2.3 Variation of potential during a redox titration, formal potential during a redox titration, requirements and detection of the end point in redox titrations, typical titrants like $KMnO_4$, $K2Cr_2O_7$, Ce (IV), I^-, $S_2O_3^{2-}$. Precipitation reactions-titration curves, determination of end Points (colored precipitates, colored soluble compounds), adsorption indicators, turbidity methods. Typical examples.

2.4 Complexometric titrations: titration curves, types of EDTA titrations (direct, back, replacement, alkalimetric and exchange reactions), masking and demasking agents, selective demasking, metal ion indicators, theory of visual use of metal indicators, typical examples of titrants - murexide, eriochrome black T, Patton and Reeder's indicators, bromopyrogallol red, xylenol orange, variamine blue.

UNIT III Electro Analytical Methods (15hrs)

Potentiometry: techniques based on potential measurements, direct potentiometric systems, different types of indicator electrodes, limitations of glass electrode, applications in pH measurements, modern modifications, other types of ion selective electrodes, solid, liquid, gas sensing and specific types of electrodes, bio membrane, biological and biocatalytic electrodes as biosensors, importance of selectivity coefficients. Polarography and voltammetric techniques: micro electrode and their specialities, potential and current variations at the micro electrode systems, conventional techniques for concentration determination, limitations of detection at lower concentrations, techniques of improving detection limit-rapid scan, ac, pulse, differential pulse square wave polarographic techniques. Applications of polarography.

Amperometry: Biamperometry, amperometric titrations. Coulometry-primary and secondary coulometry, advantages of coulometric titrations, applications. Principle of chronopotentiometry. Anodic stripping voltammetry-different types of electrodes and improvements of lower detection limits. Voltammetric sensors. Organic polarography.

UNIT IV Optical Methods (10hrs)

Fundamental law of spectrophotometry, nephelometry and turbidometry and Fluorimetry. UV-visible and IR spectrophotometry – instrumentation, single and double beam instruments, Spectrophotometric titrations. Atomic emission spectrometry – excitation sources (flame, AC and DC arc), spark, inductively coupled plasma, glue discharge, laser microprobes, flame structure, instrumentation, and qualitative and quantitative analysis. Atomic absorption spectrometry: sample atomization techniques, instrumentation, interferences, background correction, and analytical applications. Atomic fluorescence spectrometry – theory, instrumentation and applications, X-ray methods: X-ray absorption and X-ray diffraction – photoelectron spectroscopy, Auger, ESCA. SEM, TEM, AFM.

UNIT V Thermal and Radiochemical Methods (6hrs)

Thermogravimetry (TG), Differential Thermal Analysis (DTA) and Differential Scanning Calorimetry (DSC) and their instrumentation. Thermometric Titrations. Measurement of

alpha, beta, and gamma radiations, neutron activation analysis and its applications. Principle and applications of isotope dilution methods.

UNIT VI Chromatography (10hrs.)

Classification, migration rates of solutes, important relationships Gas chromatography, GSC and GLC Instrumentation-preparation of column and column materials, temperature, effects, different types of detectors, capillary columns-bonded and crosslinked phases, chiral stationary phases, selectivity factors, applications. Liquid Chromatography: column efficiency, band broadening and the factors affecting it, particle size. HPLC-its instrumentation pumps, sample injection, columns, solvent selection and detectors. Partition chromatography-bonded phase. Ion exchange chromatography-ion exchange equilibria, packings, detectors, applications. Size Exclusion Chromatography- columns and limits of permeation and exclusion, applications. Planar Chromatography-methodology, materials for stationary phases, applications. Paper chromatography. Supercritical fluid chromatography: properties of supercritical fluids, operating variables in instrumentation, stationary and mobile phases, comparison with the techniques, applications, supercritical fluid extraction, advantages, applications.

REFERENCES

1. J.M. Mermet, M. Otto, R. Kellner, Analytical Chemistry, Wiley-VCH, 2004.

2. D.A. Skoog, D.M. West, F.J. Holler, S.R. Crouch, Fundamentals of AnalyticalChemistry, 8th Edn., Saunders College Pub., 2007.

3. J.G. Dick, Analytical Chemistry, R.E. Krieger Pub.,1978.50

4. J.H. Kennedy, Analytical Chemistry: Principles, Saunders College Pub., 1990.

5. G.H. Jeffery, J. Bassett, J. Mendham, R.C. Denney, Vogel's Text Book of

6. Quantitative Chemical Analysis, 5th Edn., John Wiley& sons,1989.

7. C.L. Wilson, D.W. Wilson, Comprehensive Analytical Chemistry, Elsevier, 1982.

8. G. D. Christian, Analytical Chemistry, 6th ed., John Wiley & Sons, 2007.

9. R.A. Day, A.L. Underwood, Quantitative Analysis, Prentice Hall, 1967.

10. A.I. Vogel, A Textbook of Practical Organic Chemistry, Longman,1974.

11. H.A. Laitinen, W.E. Harris, Chemical Analysis, McGraw Hill,1975.

12. J. M. Mermet, M. Otto, R. Kellne, Analytical Chemistry, Wiley-VCH, 2004.

13. V.K. Ahluwalia, Green Chemistry: Environmentally Benign Reactions, CRC,2008.

14. F.W. Fifield, D. Kealey, Principles and Practice of Analytical Chemistry, BlackwellScience, 2000.

ACH 3P 07 SEMESTER III PRACTICAL INSTRUMENTAL METHODS OF ANALYSIS (4 Credits)

Course Outcome After completion of the full course the student should be able to :	Cognitive level
C.O.1: Understand safe laboratory practices of handling laboratory glassware, equipment and chemical reagents and develop basic laboratory skills	Knowledge
C.O.2: Prepare and analyze metal complexes, characterization by spectroscopic and magnetic methods. Elemental analysis using AAS.	Synthesis Application
C.O.3: Examine Solvent extraction, chromatography techniques and electro analytical methods.	Analysis
C.O.4: Analyze Spectronalytical methods and simple titration using UV-Vis spectroscope. FT-IR spectra of samples	Analysis application
C.O.5: Experiment Potentiometric, conductometric and PH methods of titrations	Analysis
C.O.6: Interpret Thermal methods of investigation-TGA, DSC, DTA-Curve interpretation	Application

Section A: Analytical Chemistry

I. Preparation and elemental analysis of metal complexes, characterization by spectroscopic and magnetic methods. Elemental analysis using AAS.

II. Determinations by solvent extraction, ion-exchange and paper, thin layer and column chromatography.

III. Electro analytical methods: Analysis using electrogravimetry, coulometry, potentiometry, conductometry and polarography

IV. Spectronalytical methods: spectrophotometry, Fluriometry, Flame photometry, Nephelometry and turbidimetry, UV-Visible Spectroscopy. Simple titration using UV-Vis spectroscope. FT-IR spectra of samples and its characterization (two or three compounds should be prepared in this regard).

V. Potentiometric, conductometric and PH methods of titrations.

VI. Thermal methods of investigation-TGA, DSC, DTA, Simultaneous TG-DTA and TG-DSC. Determination of dehydration kinetics of simple oxalate hydrates by TGA and DSC. Isoconversional methods. Determination of kinetic parameters for the thermal dehydration reaction of simple oxalate hydrates using Isoconversional methods.

Section B: Computational Chemistry

[The experiment consists of computational chemistry experiment for calculating energy, bond lengths, bond angles of different forms of some simple compounds. Energy optimization of certain compounds using Gaussian software.

ACH 3E 01 ORGANOMETALLIC CHEMISTRY (4 Credits)

Course Outcome	Cognitive Level
C.O.1: Distinguish the different types of ligands with respect to the type of interaction with the metal	Analysis
C.O.2: Evaluate the structure, bonding and reactions of organometallic compounds and metal clusters	Evaluation
C.O.3: Identify synthesis, structure, reactivity and applications of main group organometallic compounds.	Understand
C.O.4: Understand the structure and properties of Organometallic π complexes –Metal-alkene complexes, and Metal-alkyne complexes	Understand
C.O.5: Illustrate various organometallic reactions	Application
C.O.6: Analyze organometallic reaction in homogeneous catalysis	Analysis

UNIT I

Organometallic compounds, Various classification and hapto nomenclature of organometallic compounds, 16 and 18 electron rules, Electron counting methods-covalent and ionic model, Main group organometallics with alkyl and aryl ligands Groups 1, 2, 11, 12, 13, 14 and 15 – Synthesis, structure and applications, Organometallic complexes of 'f' block elements; σ-bonded complexes, cyclopentadienyl complexes and bis (arene) complexes.

UNIT II

Metal carbonyls- Bonding modes of CO, IR spectroscopy as a tool to study bonding and structure of metal carbonyls, Synthesis of Metal carbonyls Direct and reductive Carbonylation, Reactions of Metal carbonyls-Activation of metal carbonyls, Disproportion, Nucleophilic addition, electrophilic addition to the carbonyl oxygen, Carbonyl cation, anions and hydrides, Collmann's reagent, Migratory insertion of carbonyls, Oxidative decarbonylation, Photochemical substitution, Microwave assisted substitution.

UNIT III

General aspects of synthesis, structure, reactivity and applications of main group organometallic compounds. Metal complexes of NO, H2, CS, RNC and Phosphines. Metal-carbon multiple bonds - Metal carbenes and carbyenes, bridging carbenes and carbynes, N-heterocyclic carbons, multiple bonds to hetero atoms.

UNIT IV

Organometallic π complexes – Synthesis and bonding models of Metal-alkene complexes, Synthesis and bonding models of Metal-alkyne complexes, Reactions of Metalalkene and Metal alkyne complexes, Pauson-Khand reaction. synthesis, structure, bonding and reactions of complexes of allyl and butadiene. Synthesis, structure bonding and reactions of typical ring π donor ligands complexes of butadiene, C5H5 (ferrocene structure, bonding and reactions), C_6H_6, C_7H_7 and $C_8H_8^2$, Polyalkyls, polyhydrides and f-block organometallic complexes, Fluxional organometallics.

UNIT V

Organometallic reactions – Oxidative addition, Reductive elimination and Insertion reaction - Concerted Additions, SN2 Reactions, Radical Mechanisms, Ionic Mechanisms, Reductive Elimination, σ-Bond Metathesis, Oxidative Coupling and Reductive Cleavage, Reactions Involving CO, Insertions Involving Alkenes, Other Insertions, α, β, γ and δ Elimination, De-insertion and Nucleophilic and electrophilic attack on co-ordinated ligand.

UNIT VI

Applications of organometallic reaction- Homogeneous catalysis- General features of catalysis, Types of catalyst, Catalytic steps, Hydrogenation of alkenes, Zeigler Natta polymerization of alkenes, Hydrocarbonylation of alkenes, Wacker process, Monsanto acetic acid process, Water-gas shift reaction, Fisher-Tropsch reaction, Hydrosilation of alkenes, Hydro cyanation of alkenes.

REFERENCES

1. B. D. Gupta, A.J. Elias, Basic Organometallic Chemistry - Concepts, Synthesis and Applications, Second edition, University Press, 2013.

2. R. H. Crabtree, The Organometallic Chemistry of the Transition Metals, Fourth edn. 2005, Wiley Interscience.

3. E. Huheey, Inorganic Chemistry – Principles of Structure and Reactivity, 4th edition, Pearson education, 1993.

4. F.A. Cotton & G. Wilkinson, Advanced Inorganic Chemistry. V ed, John and Wiley, 1999.

5. R.S. Drago. Physical Methods in Inorganic Chemistry, 2nd edition, Affiliated east west press, 1993.

6. P. Powell, Principles of Organomettalic Chemistry, 2nd edition, Chapman and Hall, London, 1998. 7. S. F. A. Kettle, Concise co-ordination chemistry, Nelson, 1969.

7. S. F. A. Kettle, Physical Inorganic Chemistry-A Co-ordination chemistry Approach, Spectrum academy publishers, 1996.

8. Purcell and Kotz, Inorganic Chemistry.

9. D. J. Shriver, P. W. Atkins, Inorganic Chemistry, 5th edition, Oxford university press, 2010.

ACH 3E 02 SEMESTER III NANOSCIENCE & TECHNOLOGY (4 Credits)

Course Outcome After completion of the full course the student should be able to	**Cognitive level**
C.O.1: Distinguish the various types of nano materials and its properties and the quantum mechanical explanation for the nanoscale behaviour.	Understand
C.O.2: Understand the structural aspects of nano materials using various theories and interpret the physiochemical properties with the aid of various spectroscopic techniques	Understand Application
C.O.3: Discuss the chemistry of various synthetic approach for the development of nano structures.	Knowledge
C.O.4: Analyze the electronic, optical and magnetic properties of various nano materials.	Analysis
C.O.5: Apply nano materials in the fields such as industrial catalysis, gas sensors, storage, drug delivery.	Application

UNIT I

Historical introduction, Bulk vs. nano: size dependence on material properties, quantum mechanical explanation for the nanoscale behaviour. Examples for nanoscale systems: Gas phase clusters, metal nanoparticles, semiconductor quantum dots, nanowires and nanotubes, magnetic nanoparticles, Carbon nanostructrues: fullerenes, carbon nanotubes etc., Nanoporous materials (meso and micro-porous materials), gas phase clusters (water etc). micelles, bilayers, bio-inspired materials.

UNIT 2

Structural aspects: Crystal structures and surfaces, Free electron theory, band and zone theory. Insulators, semiconductors, conductors, and superconductors. Effects of quantum confinement, its manifestations, selected examples (Coulomb blockade, band gap engineering). Surface energy and its importance in nanoparticles, phase transitions in nano systems.

UNIT 3

Tools for nanoscience: XRD, Photoelectron Spectroscopy, AUGER, Electronic and Vibrational Spectroscopy, magnetic resonance Microscopy: Optical electron (SEM, TEM), scanning probe (STM, AFM) techniques and their variations.

UNIT 4

Properties of nanoparticles: metal nanoparticles (magic numbers, electronic structure, reactivity, surface plasmon resonance, and bulk-to nano transitions), semiconductor quantum dots (optical properties, photo fragmentation, Coulomb explosion), magnetic nanoparticles (behavior of ferromagnetic nanoparticles, ferrofluids, anti-ferromagnetic nanoparticles), Electrical conduction in bulk nano structured materials.

UNIT 5

Chemistry of nanostructures chemical synthesis (solution synthesis, capped nanoclusters, sol-gel processing, electrochemical synthesis), physical vapor synthesis approach. Template-based synthesis of mesoporous metal oxides and their characterization. Synthesis of carbon nanostructures. Nanolithography.

UNIT 6

Applications: General applications of nano. Optical (Surface enhanced Raman Spectroscopy, Optical limiting etc), reactivity of metal nanoparticles and their applications in industrial catalysis, gas sensors, storage, drug delivery.

REFERENCES

1.C.P. Poole Jr. & F.J. Ownes. *Introduction to Nanotechnology*. Wiley India (2007), New Delhi.

2. T.Pradeep. *Nano*: *The Essentials*. Tata McGra Hill (2007). New Delhi.

3. K.J. Klabunde (Ed.) *Nanoscale Materials in Chemistry*, John Wiley & Sons (2001).

4. Springer Handbook of Nanotechnology.

5. Hari Singh Nalwa (Ed.), *Nanostructured materials and nanotechnology*, Academic Press, New York, 2002.

6. D. Vollath. *Nanomaterials*, QWiley-VCH (2008).

7. K.K. Cathopadhyay & A.N. Banerjee Introduction to Nanoscience and Technology. PHl Learning Pvt. Ltd. (2009).

ACH 3E 03 SEMESTER III SOLID STATE CHEMISTRY (4 Credits)

Course Outcome After completion of the full course the student should be able to	**Cognitive level**
C.O.1: Explain various theories of solid state and distinguish materials as metals, insulators, or semiconductors, and sketch a schematic band diagram for each one	Understand Analysis
C.O.2: Analyze thermal conductivity, electrical conductivity, magnetic behavior and other bulk properties of solids.	Analysis
C.O. 3: Illustrate the crystal defects and predict the consequences	Application
C.O.4: Interpret the kinetics and mechanisms of solid state reactions that occur on heating.	Application
C.O.5:Differentiate various thermoanalytical methods and discuss the practical applications of thermal analysis methods in material science	Analysis Understand

UNIT I: Theories of the solid state - Free electron theory zone theory band theory/classification of solids into conductors, insulators, semiconductors, super conductors. (10 Hrs.)

UNIT II: Electrical properties - conductivity in pure metals - super conductivity magnetic properties-diamagnetism, para magnetism, ferro magnetism anti-ferro magnetism - temperature effects - point defects, plane defects.

(10 Hrs.)

UNIT III: Thermodynamics of Schottky and Frenkel defects formation. Point defects equilibria. Interactions between dislocations (brief discussion). The movement of matter in solids.

(10 Hrs.)

Creation of defects - Doping, compression and irradiation, Control of the reactivity of solids (brief discussion). (10 Hrs.)

UNIT IV: Solid state reactions-Decomposition reactions of the type A(solid) → B(solid) + C(gas). Process limiting the rate of solid-state reactions. Nucleation, Nucleus growth (brief discussion).

UNIT V: Isothermal and non-isothermal decomposition reactions, kinetics analysis and elucidation of the mechanism of decomposition reactions (brief discussion). Kinetic Analysis with Coats-Redfern, Freemann-Carrol and Horrowitz-Metzger equations.

UNIT VI: Instrumental techniques - Thermogravimetry, Differential Thermal Analysis, Differential scanning calorimetry. Applications of infrared spectroscopy, mass spectroscopy and scanning electron microscopy in the study of solid-state reactions.

REFERENCES

1. L.V. Avaroff, Introduction to Solids, McGraw Hill, New York.

2. A.K. Galway, Chemistry of Solids, Science Paperbacks and Chapman and Hall Ltd., London 91967).

3. N. B. Hannay, Solid State Chemistry, Prentice Hall of India, 1979.

4. A.R. West, basic Solid State Chemsitry, John Wiley & Sons Ltd. (1991).

5. P.P. Budnikov and A.M. Ginstling, Principles of Solid State Chemistry, Reactions in Solids, Maclaren and Sons Ltd., London (1968).

6. D.A. Young, Physical Chemistry and Chemical Physics, Vol. I, Decomposition of Solids, Pergamon Press, Oxford (1996).

7. W.W.Wendlandt, Thermal Methods of Analysis, Inter-science, New York 91964).

8. B.S. Skoog and D.M. West, Principles of Instrumental Analysis, Sanndes College, Philadelphia (1980).

ACH 3E 04 SYNTHETIC ORGANIC CHEMISTRY (4 Credits)

Course Outcome After completion of the full course the student should be able to	Cognitive Level
C.O.1: Demonstrate strategies for the stereospecific/ stereoselective organic transformations towards chiral target molecules.	Application
C.O.2: Analyze different synthetic strategies for the formation of carbon-carbon, carbon- nitrogen and carbon-halogen bond	Analysis
C.O.3: Describe advantages and applications of biocatalysts.	Application
C.O.4: Understand multistep synthetic strategies of some natural products	Understand
C.0.5: Discuss phase transfer catalysis and polymer support reagents	Analysis
C.O.6:Analyze Structural characteristics and applications of speciality polymers	Analysis

UNIT I Asymmetric Synthesis

Enantiomeric excess and diastereomeric excess. Strategies and classification methods - Use of chiral substrates, auxilaris, reagents, and asymmetric catalysis in asymmetric synthesis. Use of enzymes in asymmetric synthesis.

REFERENCES

1. J. Clayden, N. Green, S. Warren, P. Wothers, Organic Chemistry, 2nd ed., Oxford University Press, 2012.

2. K.K. Maceie, D.M. Smith and R.A. Atkin, Guide to Organic Synthesis, pp.311-344, Longman.

3. E.L. Eliel, S.H. Wilen, Stereochemistry of Organic Compounds, John Wiley and Sons.

UNIT II Synthetic Strategy

Formation of Carbon-Carbon bonds: Principles, disconnections and synthons, electrophilic and mucleophilic carbon species, Base catalyzed condensations: Mannich Base as

intermediates in organic synthesis. Four centre reactions. Diels-Alder Reaction, 1,3- Dipolar additions.

Formation of carbon-nitrogen bonds: Nucleophilic nitrogen and electrophilic carbon, electrophilic nitrogen and nucelophilic carbon, Beckmann rearrangements, Skraup synthesis, Bischler-Nappieralski reaction.

Formation of Carbon-Halogen bond - Allylic halogenation by NBS and NCS Electrochemical methods in organic synthesis like electro polymerization, electro-oxidation and electro reduction reactions.

REFERENCES

1. R.O.C. Norman, Principles of Organic Synthesis.

2. March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure 8th Edition, Michael B. Smith

UNIT III Biotransformations in Organic Chemistry

Introduction to biocatalysis, Advantages and disadvantages of Biocatalysts. Biocatalytic applications, Enzymes commonly used in organic transformations and prominent enzymatic transformations. Immobilized biocatalysts, Different immobilization methods, prominent solid supports for immobilization. Advantages and disadvantages of immobilized biocatalysts.

RERERENCES

1. K. Fabrer, Biotransformations in Organic Chemistry, Springer

2. P.Y. Brice, Organic Chemistry, Prentice Hall.

3. R.B. Silverman, Organic Chemistry of Enzyme Catalyzed Reactions, Academic Press.

UNIT IV Multistep Synthetic Strategies

Synthetic studies on Reserpine, Altropine, 11-Oxoprogesterone, Prostaglandin E2, Penicillin V, Cephalosporin, Polyoxygenated flavones, Caryophyllene, Edulance, Ibogamine.

REFERENCES

1. Norman, R.O.C., Principles of Organic Synthesis.

2. Finar Vol. 2, Longman.

3. N.R. Krishnaswamy, Chemistry of Natural Products, University Press.

UNIT V Catalysis

Use of solid acids and supported catalysts in Organic Synthesis, Phase Transfer Catalysis, Organic Reactions in Organized media (Organic reactions in Zeolites, Clays, Mesoporous Materials, Nafion H, Illustrative examples), Polymer supported Reagents. Use of polymer

supported reagents in Organic synthesis (Illustrative examples). Introduction to Solid Phase Organic Synthesis.

REFERENCES

1. J.H. Clark, *Catalysis of Organic Reactions by Supported Inorganic Reagents*, VCH: New York, 1994.

2. Narang, Mathur and Williams, Polymer as Aid in Organic Chemistry, Academic Press.

3. D.C. Sherrington and A.P. Kybett, Supported Catalysts and their Applications, Royal Society of Chemistry, 2001.

UNIT VI Specialty Polymers

Atom Transfer Radical Polymerization (ATRP), Nitroxide mediated Polymerization (NMP), Reversible Addition Fragmentation Termination (RAFT). High temperature polymers, Liquid crystal polymer, Polymer composites, Polymer nanocomposites, Polymer blends, Polymers in medicine (PE, PU, Polysiloxanes only).

REFERENCES

1. Polymer Chemistry – An Introduction R. B. Seymour and C. E. Carraher, Jr. Marcel Dekker, Inc. New York.

2. Organic Chemistry of Synthetic High Polymers W.Lenz Interscience Publishers, New York (1967)

3. High performance polymers, their origin and development, by Seymour R. B. and Kirshenbaum G. S. Elservier.

4. Nicolay Tsarevsky, Brent S Sumerlin, Fundamentals of Controlled/Living Radical Polymerization, RSC publishing, 2013.

ACH 4E 05 BIOINORGANIC CHEMISTRY (4 Credits)

Course Outcome After completion of the full course the student should be able to	Cognitive Level
C.O.1: Explain emergence of bioinorganic chemistry and model compounds in biochemical processes	Understand
C.O.2: Illustrate the role of metals in biological systems and identify the natural process taking place with the aid of iron in biological systems	Application
C.O.3: Identify the biochemical processes taking place with the aid of copper ions in biological systems	Understand
C.O.4: Analyze the use of metals in medicine, their applications	Analysis

and toxicity	
C.O.5: Describe bioenergetics and identification of the natural process taking place with the aid of metal ions in biological systems	Application

UNIT I

Elementary cell biology: cell membrane - Ribosomes. Elements of life: water, phosphates, organic acids, sugars, amino acids, peptides, proteins, purine and pyrimidine bases, DNA, RNA and Lipids. Protein synthesis. DNA replication. Metal ions in biological system. Bulk trace and ultra-trace metal ions. Coordination sites in biologically important ligands, factors affecting the stability of metal complexes, mixed ligand complexes, labile and inert complexes. Trans effect, reactions on coordinated ligands. Chelate effect and macrocyclic effect. Model compounds in biochemical studies.

UNIT II

Role of alkali and alkaline earth metals in biological systems. Ionophores. Active and passive transport. Sodium-potassium pump. Structural role of calcium. Transport of calcium, intra and extra cellular calcium binding proteins. Calcium pump Metalloenzymes and electron carrier metalloproteins. Direct and indirect roles of Magnesium. Diverse role of zinc in biological systems. Zn (II) and Mg (II) containing enzymes, carbonic anhydrase, alcohol dehydrogenase, catalyses, peroxidase DNA and RNA polymerases. Redox enzymes. Vitamins and coenzymes. Vitamin B12.

UNIT III

Iron in biological systems, hemoglobin and myoglobin. Transport of oxygen by heme proteins, Non-heme oxygen carriers, heme-erythrin and hemovanadium. Model synthetic complexes of iron as oxygen carriers. Storage and transport of metal ions. Ferritin, transferrin and siderophores. Ceruloplasmin. Iron enzymes, Ferridoxins, cytochromes bf, cytochrome P450.

UNIT IV

Copper in biochemical systems. Oxidase activity, super oxide dismutase activity. Electron transport in biology. Structure and function of copper proteins in electron transport process. Oxygen transport copper proteins. Hemocyanin-copper transport, copper enzymes - Azurin, plastocyanin.

UNIT V

Inorganic medicinal chemistry. Metals in medicine (MIM). Metal toxicity and homeostasis. Metal deficiency and diseases. Toxic effects of metals. Effect of deficiency and excess of essential metal ions. Toxicity due to non-essential elements. Speciation of metal ions. Detoxification mechanism. Role of lithium and aluminium in biological systems. Chelation therapy and chemotherapy. Metal complexes as drugs. Anticancer drugs and Vanadium based diabetics drugs. Inorganic pollutants in natural water. Plants as accumulators of elements. Indicator plants and biominerals.

UNIT VI

Bio energetics. ATP cycle. Glucose storage. Phosphate transfer. Pyruvate kinase. Creatine kinase. ATP as molybdoenzymes. Chlorophyll, Photosystem I and photosystem II, Model systems of water splitting and CO2 reduction. Biological nitrogen fixation, Nitrogenases, structure and activity of Fe and Fe-Mo nitrogenases. Nitrogenase model systems.

REFERENCES

1. F. A. Cotton, G. Wilkinson, C. A, Murillo, M. Bochmann, Advanced Inorganic Chemistry, 6 th ed., Wiley-Interscience: New York, 1999.

2. E. Huheey, E. A. Keiter, R. L. Keiter, Inorganic Chemistry: Principles of Structure and Reactivity, 4th ed., Harper Collin College Publishers, 1993.

3. K.f. Purcell and K.C. Kotz, Inorganic Chemistry.

4. D.E. Fenton, Bioinorganic Chemistry.5. S.J. Lippard and J.M. berg, Principles of Bioinorganic Chemistry.

5. Robert W. Hay, Bioinorganic Chemistry.7. Rosette M. Roat-Malone, Bioinorganic Chemistry.

6. D.A. Phipps, Metals and Metabolism, Clarendon Press, oxford, 1976.

7. G.I. Eichhon, (ed.), Inorganic Biochemistry, Elsevier.

8. I. Bertini, H.B. Gray, S.J. Lippard & J.S. Valentine, BioinorganicChemistry.

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9. Lehninger, Principles of Biochemistry.

10. Philip Nelson, Biological Physics Energy, Information, Life.UNIT

ACH 4E 06 Computational Chemistry (4 credits)

Course Outcome	Cognitive level
After completion of the full course the student should be able to	

C.O.1: Describe the basic concepts of the various theoretical models and methods.	Understand
C.O. 2: Analyze the different basis sets used in the computational calculations.	Analysis
C.O.3: Explain the quantum mechanical nature of the chemical bond.	Understand
C.O.4: Describe the main similarities and differences between theoretical approaches and identify advantages and disadvantages for modelling various chemical problems.	Analysis
C.O.5: Apply computational chemistry software to perform and interpret electronic structure calculations.	Application Evaluate

UNIT I Introduction

Theory, Computation, and Modeling-Definition of terms. Need of approximate methods in quantum mechanics. Computable Quantities-Structure, Potential Energy Surfaces and Chemical Properties. Cost and Efficiency. Relative CPU time. Software and Hardware. Molecular Mechanics-Force fields (Introductory remarks only). Electronic Structure Methods-Semi Empirical and ab initio methods. Applications of semi empirical methods. Limitations of semi empirical methods.

UNIT II Hartree-Fock theory

Review of Hartee- Fock SCF method for atoms. SCF treatment of polyatomic molecules. Closed shell systems - Restricted HF calculations. Open shell systems - ROHF and UHF calculations. The Roothan - hall equations. Koopmans theorem.

UNIT III Density Functional Methods

Introduction to density matrices. N-representability and V-representability problems. Hohenberg - Kohn theorems. Kohn-Sham orbitals. Exchange correlation functionals. Thomas-Fermi-Dirac Model. Local density approximation. Generalised Gradient approximation. Hybrid functionals. Comparison between DFT and HF methods.

UNIT IV The Basis set approximation

Slater and Gaussian type orbitals. Classification of basis sets. Minimal, double zeta and triple zeta basis sets. Split valence basis sets. Contracted basis sets-Pople style Dunning Huzinaga, MINI, MIDI and MAXI basis sets. Polarisation and diffuse functions, Correlation

consistent basis sets. Basis set truncation error. Effect of choice of method/basis set (model chemistries) on cpu time.

UNIT V Introduction of Gaussian programme (e.g., G03)

Input files. Converting a structure from a graphics program. Main features of Guassian output files. Use of graphics programs like Gaussiview, Chemcraft, Molda and Moden in analyzing Gaussian output data. Identification and visualization of normal modes of vibration. Calculation and interpretation molecular orbitals.

UNIT VI Simple calculations using Gaussian programme

Single point energy calculations, Geometry optimization. Frequency claculations. Locating local minima and saddle points on Potential energy surfaces. Scaling frequencies and zero-point energies. Transition state optimizations. Characterizing transition states. The normal mode and IRC analyses.

REFERENCES

1.C.J. Cramer, "Essentials of computational chemistry-Theories and models" John Wiley & Sons LTD 2002.

2. Frank Jensen, "Introduction to Computational Chemistry", John Wiley & LTD 1999.

3. E. Lewars, "Introduction to the theory and applications of molecular quantum mechanics", Kluwer Academic Publishers 2003.

4. Ira.N. Levine: "Quantum Chemistry 5th ed., Prentice Hall 2000.

5. P.W. Atkins & R.S. Friedman: 'Molecular Quantum Mechanics", 3rd ed., Oxford University Press 1997.

6. J. Foresman & Aelieen Frisch, "Exploring Chemistry with Electronic Structure Methods", Gaussian, Inc.

7. W.J. Hehre. L.D. Burke, A.J., Shusterman, W.J. Pietro, "Experiments in Computational Organic Chemistry", Wave function, Inc. 1993.

8. David.C. Young, "COMPUTATIONAL CHEMISTRY-A Practical Guide for Applying Techniques to Real-World Problems", John Wiley & Sons LTD 2001.

9. W. Koch. M.C. Holthausen, "A Chemist's Guide to Density Functional Theory", Wiley-VCH Verlag, 2000.

ACH 4E 07 CHEMISTRY OF NATURAL PRODUCTS (4 Credits)

Course Outcome After completion of the full course the student should be able to	Cognitive Level
C.O.1: understand chemistry and reactions of natural products	Understand

C.O.2: Analyze structure and device synthesis for important natural products.	Analysis
C.O.3: Recognize the chemistry of prostaglandins	Understand
C.O.4: Develop an understanding about the historical development, classification and mode of action of antibacterial**.**	Analysis
C.0.5: Illustrate occurrence, isolation, biological significance and synthesis of certain vitamins.	Application

UNIT I

Essential oils and aromatics: Cultivation, collection, storage and uses of plants of medicinal importance. Isolation and study of the important constituents of: lemon grass oil, citronella oil, ajowan, oil, palmarosa lil, rosemary oil, patchouli oil, peppermint oil, turpentine oil, sandalwood oil lavender oil, geranium oil, vetiver oil and rose oil. Essential oils of turmeric and ginger.

Oleoresins of pepper chilly, ginger and turmeric. Uses of essential oil in medicine.

REFERENCES

1. The essential oils, The constituents of essential oils by Ernest Guenther (1975).

2. Organic Chemistry by I.L. Finar, Vol. II

3. Kirk Othmer encyclopedia of Science and Technology.

UNIT II

Tepenoids: Chemistry and structure of the following (synthesis and structural elucidation excluded). Classification of terpenoids-isoprene rule. Carvone, menthol, limonene, zingiberine, alphathujene, car-3-ene, car-2-ene, carone, caryophylline, alpha-pinene, camphor, citral, farnesol, bisaboline, eugenol, abietic acid and squalene.

REFERENCES

1. Organic Chemistry by I.L. Finar, Vol. II.

2. A fragrant introduction to terpeniod chemistry by C.S.Sell (2003).

3. The chemistry of terpeniods, by A.R. Pinder.

UNIT III

Alkaloids: Nomenclature, classification, isolation, purification, and pharmaceutical applications of alkaloids. Sources and synthesis of the following: Morphine, strychnine, nicotine, atropine, cocaine, ephedrine, caffeine and arecaidine.

REFERENCES

1.Organic Chemistry by I.L. Finar, Vol. II.

2.Chemistry of Natural Products by Bhat, Nagasampagi and Sivakumar, 2005, Narosa Publishing.

3.Principles of Organic synthesis by Norman and Coxon (1993).

UNIT IV

Prostaglandins: Chemistry of Prostaglandins - Occurrence, isolation, classification and nomenclature. Synthesis of PGA, PGE, PGF and PGB groups of prostaglandins.

REFERENCES

1. Principles of Organic synthesis by Norman and Coxon (1993).

2. Chemistry of Natural Products by Bhat, Nagasampagi and Sivakumar, 2005, Narosa Publishing.

3. Organic chemistry by Clayden et al., Oxford University Press, 2011.

UNIT V

Antibacterials: Historical development and modes of action and resistance. Classification of antibacterials. Syntheses of Penicillin V, Chloramphenicoal, griseofulvin, sulphamethazine, sulphadoxine. Structure activity relationships of penicillin. Semisynthetic penicillins (brief idea only).

REFERENCES

1. Chemistry of Natural Products by Bhat, Nagasampagi and Sivakumar, 2005, Narosa Publishing.

2. Organic Chemistry by I.L. Finar, Vol. II.

UNIT VI

Vitamins: Occurrence, isolation, biological significance (brief idea only) and synthesis of the following vitamins: Vitamin A, E, K1, Thiamine, Riboflavin, Pyridoxine, Niacin, Pantothenic acid and Ascorbic acid.

REFERENCES:

1.Organic Chemistry by I.L. Finar, Vol.II

2.Chemistry of Natural Products by Bhat, Nagasampagi and Sivakumar, 2005, Narosa Publishing.

ACH 4E 08 INDUSTRIAL CATALYSIS (4 Credits)

Course Outcome After completion of the full course the student should be able to	Cognitive level
C.O.1: Describe catalysis, adsorption and various kinds of adsorption isotherms.	Understand
C.O.2: Analyze the preparation of various types of catalyst, spectroscopic characterization and activity studies.	Analysis
C.O.3: Interpret Surface and structural investigation of catalysts using various spectroscopic techniques	Application
C.O. 4: Evaluate adsorption isotherms as a tool for obtaining the surface area and rate constants in case of heterogeneous catalysis.	Evaluation
C.O.5: Recall the previous knowledge about the development of catalysts and the general characteristics of a catalyst.	Knowledge
C.O.6: Illustrate novel catalytic materials including their structure and preparation and explain the application of organometallic catalyst in various catalytic processes.	Application

UNIT I General Introduction to adsorption and catalysis (10hrs)

General characterizes of catalysis, classification-heterogeneous catalysts, theory, adsorption-physical, chemical activated and non-activated chemisorption, potential energy level diagrams, kinetics of chemisorptions, Langmuir adsorption isotherm, BET theory and adsorption isotherm-applications, unimolecular and bimolecular surface rations and kinetics, Langmuir – Rideal and Langmuir Hinshellwood models. Adsorption and catalysis on metals and semiconductor oxide surfaces, electronic factors in adsorption and catalysis by metals-Band concept. Valence band theory by Pauling, percentage character – involvement of heat of adsorption and heat of sublimation. Electronic factors in adsorption and catalysis by semiconductors charge transfer and Wolkensteins theories of adsorption and catalysis.

UNIT II Catalyst: Preparation and physico-chemical characterization methodologies

Experimental aspects in catalyst preparation, characterization and activity studies. X-ray diffraction study, FTIR spectral analysis, UV -Vis spectra, surface area and pore volume measurements, acid base property studies – Hammett indicator method and temperature

programmed desorption of probe molecules. Liquid and gas phase reactions, Different types of reactors, tubular reactors.

UNIT III Surface Structure and Techniques for surface investigation

Structure of surfaces-techniques for the study of surfaces-low energy electron diffraction, field electron emission, photoelectron spectroscopy-ESCA, Auger, Mossbauer spectroscopy, Electron diffraction, scanning tunneling microscopy (STM), high resolution electron energy loss spectroscopy (HREELS), Ultraviolet photoelectron spectroscopy, inverse photo emission, ion scattering (LEIS) and SIMS).

UNIT IV Development and performance criteria of Industrial catalysts

Development of Industrial catalysts – brief history. Catalytic performance, activity, turn over number, selectivity, catalyst life, stability, accessibility, mechanical strength. Deactivation of catalysis – fouling cocking, thermal deactivation. Reusability of catalysts, regeneration and recycling.

UNIT V Novel catalytic materials

Shape selective catalysts-zeolites, mesoporous materials, various synthesis methods, nanoparticles, super acid catalysts, redox catalyst systems, supported catalysts-merits, features of supports, role of supports, Preparation and structure of supports like silica, alumina, zeolites, carbon, immobilized systems. Metal organic frame works (MOF). Electrocatalysis and photocatalysis.

UNIT VI Industrially significant catalyzed reactions

Catalysis by organometallics – cracking, hydro treatment, discher Tropch process, Mobil process, Monsanto process, Oxo process, Ziegler Natta reaction, Oxidation and ammoxidation catalysts, alkylation catalysts. Pollution by automobiles-Applications of catalysts in abating pollution – CO oxidation and NO reduction catalysts.

REFERENCES

1. E.K. Rideal, Concepts in catalysis, academic press (1968)

2. A. Clark, Theory of adsorption and catalysis, Academic press (1970).

3. Surface Analysis: The Principal Techniques John. C. Vickerman, Ian Gilmore (Eds)

4. R. Opearce and Patterson (Ed). Catalysis and Chemical process, Blackie and sons Ltd (1981).

5. F.A. Coton and G. Wilkinson, Advanced Inorganic Chemistry, 4th edition. John Wiley and sons (1980)

6. W.B. Innes, Experimental methods in catalytic research, vol. I. ed. By R.B. Anderson (AP).

7. Jens Hagen, Industrial catalysis: A practical approach (Wiley VCH)

8. G. Etrl, H. Knozinger, J. Wltamp, Handbook of heterogeneous catalysis, Heterogeneous catalysts volumes 1-5, Wiley VCH (1997)

ACH 4E 09 Chemistry of Polymers (4 credits)

Course Outcome After completion of the full course the student should be able to	**Cognitive level**
C.O.1: Describe the fundamentals of polymers and its classification.	Knowledge
C.O.2: Discuss the various polymerization processes.	Understand
C.O.3: Analyse the polymerization in homogeneous and heterogeneous systems	Analysis
C.O.4: Illustrate the structure and applications of some biologically and industrially important polymers.	Application
C.O.5: Interpret the use of various polymerization process in newer areas of polymerization processes like ATRP, NMP, RAFT etc.	Application
C.O.6: Understand the kinetics and mechanisms of various polymerization processes.	Understand

UNIT I Classification of polymers:

Plastics, rubbers and fibers, Thermosets and thermoplastic, Linear, Branched and cross-linked polymers. Random, block and graft co-polymers and stereo specific polymers.

UNIT II Methods of Polymerization I

(a) Step reaction (condensation) Polymerization: Mechanism, types and Kinetics of condensation polymerization. Interfacial condensation. Ring versus chain formation. Bifunctional & Polyfunctional step reaction polymerization-gelation, gelpoint-experimental, observation, Ring scission polymerization.

(b) Radical Chain (Addition) Polymerization: Vinyl polymerization, Vinyl monomers, Mechanism of Vinyl polymerization, Experimental methods in Vinyl polymerization. Kinetics of free radical polymerization, Molecular weights and its distribution.

UNIT III Method of Polymerization II

Polymerization in homogenous and heterogeneous systems. Gas phase polymerization, Bulk polymerization and polymer precipitation. Suspension and emulsion polymerization of mono and hetero-disperse polymers. Co-polymerization: Different types of copolymers, kinetics of co-polymerization. The co-polymerization equations, composition of copolymers, Mechanism of co-polymerization-monomer reactivity ratios.

UNIT IV Structure, Properties and Characterization of Polymers:

Glass transition temperature, Melting Temperature-Experimental and method of their determinations. Method for molecular weight determination of polymers. End-group analysis, Solution viscosity methods. Empirical correlations between intrinsic viscosity and molecular size of polymer structure. Gel permeation chromatographic techniques in the fractionation of polymers.

UNIT V Structure, Synthesis and applications of the following

a) Cellulose and cellulose based polymers- Cellulose nitrate, cellulose acetate.
b) Polyolefins - Polyethylene and Polypropylene.
c) Vinyl polymers - PVC, Polystyrene, acrylic polymers.
d) Flurocarbon polymers - Teflon.
e) Phenol formaldehyde and urea formaldehyde resins.
f) Polyamides (Nylon) and polyesters (Terylenes)
g) Caprolactam based polymers.

UNIT VI Newer Areas of Polymer Chemistry

Atom Transfer Radical Polymerization (ATRP), Nitroxide mediated Polymerization (NMP), Reversible Addition Fragmentation Termination (RAFT). Anionic polymerization - Initiation and Propagation, mechanisms of living polymerization. Molar mass distribution. Transfer and termination, cationic polymerization – Mechanism.

REFERENCES

1.F. W. Billmayer, Text book of polymer science, 3rd ed., Willey, New York, 1991

2. G. Odian, 'Principles of Polymerization' McGraw Hill 1970.

3. Eiias "Macromolecules', Plenum Press (1980).

4. M.L. Miller 'The structure of Polymers Reinhold (1968).

5. C.M. Blow and C. Hepbrun (eds). 'Rubber Technology and Manufacture', Butterworth's (1982).

6. I.M. Campbell, "Introduction to polymers" Oxford Scientific publications, 1994.

7. K.J. Saunders 'Organic Polymer Chemistry Chapman and Hall, London, Mathur, Narang and Williams, "Polymers as Aids in Organic Chemistry, Academic Press, London.
8. R. J. Young, Principles of Polymer Science, 3rd ed., Chapman and Hall, New York, 1991.

ACH 4E 10 Green Chemistry (4 credits)

Course Outcome After completion of the full course the student should be able to	**Cognitive level**
C.O.1: Understand the basic principles and concepts of green chemistry	Understand
C.O.2: Apply green technology in various chemical reactions	Application
C.O.3: Illustrate the green catalytic processes for industrial applications	Application
C.O.4: Evaluate the use of supported catalysts as an alternative for hazardous homogeneous catalysts in some common chemical transformations.	Evaluation
C.O.5: Describe homogeneous and heterogeneous biocatalysts and its application in the production of bulk chemicals synthesis, pharmaceuticals, flavor and fragrance compounds etc.	Application
C.O.6: Discuss the use of green solvents in organic reactions.	Understand
C.O.7: Analyze various green chemistry methodologies such as microwave assisted synthesis, solvent free reactions, green solvents, phase transfer catalyst etc.	Analysis

UNIT I The Concept and Content of Green Chemistry

Definition of Green Chemistry, Green Chemistry Why Now? The historical context of Green Chemistry. Principles of Sustainable and Green Chemistry.

Areas of Green Chemistry:- alternative feed stocks, benign reagents/synthetic pathways, synthetic transformations, solvents/reaction conditions, products/design of safer chemicals, minimization of energy consumption, (Discussion about alternative energy sources) Atom Economy, Inherently atom economic reactions (Diels-Alder reaction, Claisen rearrangement and Michael addition-Introductory examples only), inherently atom uneconomic reactions and its green chemical solutions (Witting reaction, Mitsunobu reaction, Amide formations). (10 Hrs)

UNIT II Industrial process Using solid Acid Catalysts

Concept of Acidity and Solid Acid Catalysts. Industrial applications of solid acid Catalysts:- Zeolite-based Solid Acid Catalysts (H-ZSM-5, Zeolote Y, HY Zeolite, and Zeolite). Heteropolyacids (Super acids)-based solid acid catalysts. Sulfated Zirconia, Ion0ecchange resis, Acidic and Pillard Clays (Calcined Kaolin, Mont K10, Bentonite clay and Filtrol-24). Nafiron$^{(R)}$/Slica manocompsites. Recent developments in green Catalytic process using Solid Acids:- a) The 'Kvaerner Process' and Esterification Chemistry, b) Halder-Topsoe alkylation process to High Octane fuels, c) Mobil-Badger Cumene Process and d) Isodewaxing process (Production of base oils-Chevron process).

(10 hrs)

UNIT III Polymer Supported Reagents-A Green Chemical Perceptive

Polymeric tools for organic chemistry:- Polymeric reagents, polymeric carriers, Polymeric catalysts. Advantages of polymeric reagents and catalysts, required properties of a polymeric material will be used as a carrier. Making functional polymers-copolymerization. Examples of polymeric carriers and reagents - a) Polystyrenes, b) polyacrylate, c) polyvinyl pyridines, d) polybenzimidazoles, e) polyphosphazenes and f) Chlorofluropolymers. Synthesis with polymer supported reagents: Conversion of Carboxylic acids to Acid chlorides and anhydrides. Hydrolysis of Alkyl halides to alcohols, Oxidation of alcohols to aldehydes and ketones, Reduction of imines to amines. Conversion of alkyl and benzyl halides to Azides. Epoxidation of Alkenes. Wittig and related reactions.

(10 Hrs)

UNIT IV Biocatalysis

Introduction to biocatalysts, Advantages and disadvantages of Biocatalysts. Biocatalytic applications, Enzymes commonly used in organic transformations and prominent enzymatic transformations. Immobilized biocatalysts. Different immobilization methods, prominent solid supports for immobilization. Advantages and disadvantages of immobilized biocatalysts. Chemicals production by Biocatalysis, 1. Bulk Chemicals (Conversion of acrylonitrile to acrylamide, Production of nicotinic acids, Glucose to Fructose, Lactose to glucose, Penicillin G to 6-aminopenicillanic acid production of picolinic acids and lactams. 2. Production of Parmaceuticals-Production of Cortisones (Anti-inflammatory steroids), Production of trimegestrone using bakers east. 3. Production of Flavour and Fragrance compounds-Biocatalytic route for the formation of Vanilin, Production of methyl anthranilate. Production of carbohydrates.

(10 hrs)

UNIT V Green Solvents

Organic reactions in Supercritical Carbon Diozide-Phase behaviour and solubility in supercritical reaction mixtures, Supercritical Carbon Dioxide as a replacement for organic solvents-examples. Use of Supercritical Carbon Dioxide for product separation and catalyst recycling-examples: - Chemistry of Fluorous Biphase Systems- The fluorous Biphase concept, Fluorous Solvents, Synthesis of Fluorous Compounds. Fluorous Synthesis-examples, Fluorous Tags. Relationship between Fluorous and Supercritical Carbon Dioxide media. Organic reactions in Super heated water. Extraction of natural products with super heated water-examples only.

UNIT VI Alternative Energy Sources

Applications of Microwaves for Environmentally Benign reactions - Properties of Microwaves. Influence of Microwave heating on chemical reactions. Approaches to microwave assisted Organic Chemistry-general advantages. Microwave assisted synthesis-Solvent-free methods (Neat reactions in an open container, Dry media reactions, phase transfer catalysed reactions under microwave conditions-Advantageous and disadvantageous of solvent free methods). Methods with solvents-MORE chemistry (Microwave-induced organic reaction enhancement), super heated solvents and reactions at reflux. Sonochemistry-Definition, Power ultrasound, some industrial use of Power ultrasound, Transducers-Liquid driven Transducers, Magnetostrictive transducers, Piezolectric Transducers. In Homogenous reactions, In heterogeneous liquid-liquid or liquid-solid ionic reactions, In heterogeneous reactions. Examples of Sonochemical Reactions.

(10 Hrs)

REFERENCES

1. P.R. Anastas and J.C. Warner, *Green Chemistry: Theory and Practice,* Oxford University Press, Oxford, 1998.

2.James Clark and Duncan Macquarrie, handbook of Green Chemistry and Technology, Blackwell Science, 2002.

3. J.H. Clark, *Catalysis of Organic Reactions by Supported Inorganic Reagents*: VCH: New York, 1994.

4. T.J., Mason Sonochemistry, The Use of ultrasound in Chemistry, Royal Society of Chemistry London, 1990.

ACH 4E 11 Advanced Synthesis and Catalysis-New Synthetic Methodologies (4 Credits)

Course Outcome After completion of the full course the student should be able to	Cognitive Level
C.O.1: Illustrate the applications of various multi component reactions	Application
C.O.2: Analyze the mechanism and synthetic applications of palladium catalysed coupling reactions	Analysis
C.O.3: Examine metathesis catalysts and their applications	Analysis

UNIT I Multicomponent Reactions (MCR) Part 1

An introduction to Multicomponent reactions. Synthesis and Chemistry of isocyanides. Passerini reaction (Mechanistic aspects, reaction conditions and building blocks), Ugi reaction - general conditions, Mechanistic aspects, building blocks and solid phase variations. Applications of Ugi and Passerini reactions in developing linear and cyclic small peptide molecules. Biginelli reactions (Mechanistic studies, Reaction conditions, building blocks, Solids phase variations.

UNIT II Multicomponent Reactions (MCR) Part 2

Mannich and Mannich type reactions and their chemistry and applications. The Petasis reaction, its chemistry and applications. Chemistry and applications of Strecker reaction, van Leusen Reaction and Hantzsch reaction. Multicomponent synthesis based on Knoevenagel reaction and Michael reaction.

REFERENCES

1. Multicomponent Reactions, Jieping Zhu and Hugues Bienayme, Eds.; Wiley-VCH Verlag GmbH & Co. KGaA, Weinheim 2005, ISBN; 3-527-30806-7.

2. Laszlo Kurti and Barbara Czako, Strategic Applications of Named Reactions kin Organic Synthesis, Elsevier Academic Press, 2005.

UNIT III Palladium Catalyzed Coupling Reactions Part I

Heck reaction: Mechanism and applications. Suzuki cross-coupling reactions (Mechanism and synthetic applications). Kumauda cross-Coupling reactions (Mechanism and Synthetic applications). Sonogashira cross-coupling reaction (Mechanism and Synthetic applications in organic electronics and cyclic peptides).

UNIT IV Palladium Catalyzed Coupling Reactions Part II

Stille carbonylative cross-coupling reaction (Mechanism and Synthetic applications). Negishi coupling: mechanism and applications. Buchwald-Hartwig coupling in Carbon –hetero atom bond formations. Stille Cross coupling reaction (Mechanism and Synthetic applications). Stille Kelly Coupling (Mechanism and Synthetic applications).

REFERENCES

1. Metal catalyzed Cross-Coupling reactions, Diederich, F, and Stang P.J. Eds.; Wiley-VCH: New York: 1998.

2. V. Farina, V. Krishnamurthy; Scott, W.J. *the Stille Reaction:* John Wiley & Sons: New York, 1998.

3. Laszle Kurti and Barbara Czako, Strategic Applications of Named Reactions in Organic Synthesis, Elsevier Academic Press, 2005.

UNIT V Metathesis Reactions Part I

An introduction to various metathesis catalysts a) First-generation Grubb Catalysts, Second generation Grubb Catalysts and Schrock Catalysts. Alkene Metathesis - Ring closing Metathesis (RCM)

UNIT VI Metathesis Reactions Part II

Ring opening Metathesis (ROMP), Cross Metathesis (CM), Acyclic Diene Metathesis (ADMP) - (Catalysts, Mechanism, Conditions and Synthetic Applications), Applications of Ene Metathesis and Yne metathesis reactions in the synthesis of bio-active molecules.

REFERENCES

1. Laszlo Kurti and Barbara Czako, Strategic Applications of Names Reactions in Organic Synthesis, Elsevier Academic Press, 2005.

SEMESTER IV

ACH 4PR 01-Research Project & Viva Voice (Credit- 8)

Course Outcome

Course Outcome On completion of the research project the student should be able to	**Cognitive level**
C.O.1: Identify a research problem and to make an hypothesis/experimental solution to the above research problem.	Create (synthesis)
C.O.2: Design experiments and validate the hypothesis/ experimental solution of the research problem.	Create (synthesis)

1. The students shall carry out research project at various National and State Research laboratory.
2. The students shall submit a project report on the research work carried out.
3. The students will have to present the results of the research project in a seminar and appear for a comprehensive viva-voce