UNIVERSITY OF CALICUT

Abstract

General and Academic IV - Faculty of Science - Scheme and Syllabus of MSc Applied Chemistry Programme under CCSS PG Regulations 2022 (University Teaching Departments) - With effect from 2022 Admission - Implemented - Subject to ratification by the Academic Council - Orders Issued.

G & A - IV - J

U.O.No. 17569/2022/Admn Dated, Calicut University.P.O, 16.09.2022

Read:-1. U.O.No. 8479/2022/Admn dated 11.04.2022
2. Minutes of the meeting of Board of Studies in Applied Chemistry held on 01.09.2022
3. Remarks of Dean, Faculty of Science dated 14.09.2022

ORDER

1. Vide paper read as (1) above, the Regulations under Choice-based Credit Semester System for Post Graduate Programmes (CCSS PG-2022) of all Teaching Departments / Schools of the University of Calicut, were implemented with effect from 2022 admission.
2. Vide paper read as (2) above, Board of Studies in Applied Chemistry approved the Scheme and Syllabus of MSc Applied Chemistry Programme (CCSS), in accordance with CCSS PG Regulations 2022 (University Teaching Departments), with effect from 2022 admission.
3. The decision of Board of Studies have been approved by the Dean, Faculty of Science, vide paper read as (3) above and by the Vice-Chancellor on 15.09.2022, subject to ratification by the Academic Council.
4. The Scheme and Syllabus of MSc Applied Chemistry Programme (CCSS PG), in accordance with CCSS PG Regulations 2022 (University Teaching Departments), is therefore implemented, with effect from 2022 admission, subject to ratification by the Academic Council.
5. Orders are issued accordingly. (Scheme and Syllabus appended)

Abdussamad M

Assistant Registrar

To

Head, Dept.of Chemistry, University of Calicut
Copy to: PS to VC/PA to PVC/ PA to R/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

DEPARTMENT OF CHEMISTRY
UNIVERSITY OF CALICUT

SYLLABUS

M.Sc. APPLIED CHEMISTRY
(*Choice based credit semester system)*

2022 Admission onwards

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 ChemicalScience leading to master's 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			
ACH1C01	Group Theory & Quantum Chemistry	Core	3
ACH1C02	Inorganic Chemistry I	Core	3
ACH1C03	Organic Chemistry I	Core	3
ACH1C04	Physical Chemistry I	Core	3
ACH1C05	Analytical Chemistry	Core	3
ACH1P01	Inorganic Chemistry – Practical I	Core	2

ACH 1P02	Organic Chemistry – Practical I	Core	2
ACH 1P03	Physical Chemistry – Practical I	Core	2
ACH1A01	Ability Enhancement Course (AEC)	Audit	2#
Semester 2			
ACH2C06	Chemical Bonding & Chemical Applications of Group Theory	Core	3
ACH2C07	Inorganic Chemistry II	Core	3
ACH2C08	Organic Chemistry II	Core	3
ACH2C09	Physical Chemistry II	Core	3
ACH2C10	Molecular Spectroscopy & Photochemistry	Core	3
ACH2P04	Inorganic Chemistry – Practical II	Core	2
ACH2P05	Organic Chemistry – Practical II	Core	2
ACH2P06	Physical Chemistry – Practical II	Core	2
ACH2A02	Professional Competency Course (PCC)	Audit	2#
Semester 3			
ACH3C11	Inorganic Chemistry III	Core	3
ACH3C12	Organic Chemistry III	Core	3
ACH3C13	Physical Chemistry III	Core	3
ACH3C14	Instrumental Methods - Theory and Instrumentation	Core	3
ACH3P07	Instrumental methods of Analysis – Practical	Core	2
ACH3E01	Organometallic Chemistry	Elective	4
ACH3E02	Nanomaterials & Nanotechnology	Elective	4*
ACH3E03	Advanced Organic Chemistry	Elective	4
ACH3E04	Advanced Electrochemistry	Elective	4
ACH3E05	Orbital Interactions in Chemistry	Elective	4
Semester 4			
ACH4E06	Bioorganic & Bio-coordination Chemistry	Elective	4
ACH4E07	Essentials of Computational Chemistry	Elective	4
ACH4E08	Medicinal Chemistry	Elective	4*
ACH4E09	Solid state Chemistry	Elective	4
ACH4E10	Industrial Catalysis	Elective	4
ACH4E11	Chemistry of Polymers	Elective	4

ACH4PR01	Research Project	Core	8

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.

*These courses are offered as open electives for students from other departments also

Core Courses (other than project/dissertation)	:	56
Elective Courses (4x4)	:	16
Project/Dissertation	:	8
Total	**:**	**80**

For more details:

Head of the Department

Department of Chemistry

University of Calicut P.O., 673 635

Kerala

Tel: +91 494 2407413 & +91 494 2407414

Email: chemhod@uoc.ac.in

ACH1C01 - Group Theory and Quantum Chemistry

(3 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.	Understand
C.O.2: apply the postulates of quantum mechanics to simple model systems.	Application
C.O.3: make use of approximation methods to calculate properties of systems of chemical interest.	Analysis
C.O.4: analyse the symmetrical aspects of any given molecule.	Analysis
C.O.5: explain the basic principles of group theory and construction of character tables	Application

UNIT - I Molecular Symmetry (14 Hours)

General introduction, Symmetry elements and symmetry operations, Point Groups and their determination. order of a group. Abelian and Cyclic groups, Group Multiplication table. Rearrangement theorem Sub groups and classes in a group. Similarity 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.

Transformation matrices, Representation of point groups, construction of representations using vectors and atomic orbitals as basis. (H_2O as example). Reducible and irreducible representations. Construction of irreducible representations by block diagonalization of transformation matrices (similarity transformation). Great orthogonality theorem (GOT), General Theorems of representation theory, Reduction formula, Construction of character Tables (C_{2v}, C_{3v}, C_{4v}). Nomenclature of irreducible representations - Mulliken symbols, Reduction of reducible representations (e.g. Γ_{cart}) into Irreducible Representation, Projection formula.

UNIT - II Brief history and Formulation of quantum mechanics (6 Hours)

Origin of quantum mechanics, Explanation of photo electric effect, Electron-diffraction experiments and wave nature of electrons, de Broglie matter waves, Heisenberg's uncertainty principle, Deduction of Schrödinger equation from classical wave equation.

Postulates of Quantum Mechanics: Wave function (Ψ) and the physical significance of Ψ^2, Rules of proper behavior, Normalization of wavefunction and its physical significance, Quantum mechanical operators, their derivation, and properties, Hermitian operators, Commutation of operators and its physical significance, Eigen function and Eigen value, Expectation value, Time-independent and time-dependent Schrödinger Equations, Method of separation of variables.

UNIT – III Particle in a box and Harmonic Oscillator (10 Hours)

Particle in a box Problem: Free particle, The particle in a one-dimensional box, Extension of this model into two- and three- dimensional boxes; Application of Method of separation of variables to solve the problems of multi-dimensional boxes, Degeneracy, Symmetry breaking, Treatment of more than one particle (non-interacting)in a box. Applications. Finite-barrier model and the concept of quantum mechanical tunnelling.

Harmonic Oscillator: Quantum mechanical model for molecular vibrations, Derivation of Schrödinger equation. Wave functions and energies, Hermite equation and Hermite Polynomials, Recursion formula, Application to vibrational spectroscopy. Anharmonic oscillator and its significance in vibrational spectroscopy.

UNIT – IV Rigid Rotor and Hydrogen Atom Models (10 Hours)

Rigid Rotor: Quantum mechanical model for rotational motion. Planar rigid rotator (Particle on a ring), The wave equation in spherical polar coordinates, The Φ-equation and its solution, Nonplanar rigid rotator (particle on a sphere), Separation of the Schrödinger equation into Φ-equation Θ-equation and their solutions, Legendre and Associated Legendre equations, Legendre and Associated Legendre polynomials, Spherical harmonics (**Y**), Polar plots of **Y**, Angular momentum operators L and L^2. Quantization of angular momentum, $\mathbf{L}_x$, $\mathbf{L}_y$, and $\mathbf{L}_z$ and $\mathbf{L}^2$. Commutation relationships of various angular momentum operators and their physical significance. The concept of space quantization of angular momenta.

UNIT – V Quantum Mechanics of Hydrogen-Like atoms (10 Hours)

Hamiltonian operator and Schrödinger equation for Hydrogen-like atoms in spherical polar coordinates. Application of the method of separation of variables to separate the Schrödinger equation into the R-. Θ- and Φ- equations and their solutions. Laguerre and Associate d Laguerre polynomials. Wave functions and energies of hydrogen-like atoms, Orbitals. Radial functions and Radial distribution functions and their plots Angular functions (Spherical harmonics) and their plots. Description of Hamiltonians and Schrödinger equation in atomic units (a.u.).

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 PublishingCo. Pvt. Ltd., New Delhi (1990).
4. D.A McQuarrie, *Quantum Chemistry*, University Sciences Books, 1983.
5. J.P. Lowe, *Quantum Chemistry*, 2nd Edition, Academic Press, Inc. 1993.
6. R.K. Prasad, *Quantum Chemistry,* 2nd Edition, New Age International, 2000.
7. P.W. Atkins, *Molecular quantum mechanics,* 2nd Edition, Oxford University Press, 1983.
8. I.N. Levine, *Quantum Chemistry*, 5th Edition, Pearson Education Inc.2003.
9. A.K. Chandra, Introduction of *Quantum Chemistry*, Tata McGraw Hill, 1994.
10. M.W. Hanna, *Quantum mechanics in Chemistry*, 2nd Edition, W.X. Benjamin Inc. 1969.
11. F.L. Pilar, *Elementary Quantum Chemistry*, McGraw Hill, 1968.
12. G.K. Vemulapally, Physical Chemistry, Prentice Hall of India

ACH1C02 INORGANIC CHEMISTRY I

(3 Credits)

Course Outcome After completion of the full course the student should be able to:	**Cognitive level**
C.O.1: Identify the types of nuclear reactions and their applications in the energy sector	Analysis
C.O.2: Analyze the electronic spectra of lanthanoids and actinoids and their magnetic properties.	Analysis
C.O.3: Describe nanomaterials, synthetic strategies, and application of various nanomaterials.	Application
C.O.4: Analyze the structure, bonding, stability, and reactions of organometallic compounds	Evaluate
C.O.5: Compare the strength of various acids and bases and theirreactivity and explain stereochemistry of coordination compounds and their stability	Application

UNIT – I Chemistry of Lanthanoids and Actinoids (8 h)

Periodic Table. Chemistry of lanthanoides and actinoides. General characteristics of actinoids-difference between 4f and 5f orbitals, oxidation states. The lanthanide- and actinide-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. MRI contrasting agents. Shift reagents.

UNIT – II Chemistry of Nanomaterials (10 h)

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, magnetic nanoparticles, and biomedical applications of magnetic nanoparticles, Template-based synthesis of mesoporous nanomaterials (SiO_2 and TiO_2) and their applications

UNIT – III Acid-Base and Coordination Chemistry (10 h)

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. Symbiosis. Formation constants, stepwise and overall stability constants- factors affecting stability- methods of determination of stability constants- solubility method-chromatographic method and spectrophotometric method. Chelate, macrocyclic and macrobicyclic effects. 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.

UNIT – IV Organometallic Compounds- Synthesis, Structure, and Bonding (12 h)

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 – V Nuclear Chemistry (8 h)

Nuclear stability. Radioactive elements, decay kinetics, α, β, γ decay. Artificial radioactivity. Types of nuclear reactions. Nuclear fission – nuclear reactor, breeder reactor. Nuclear fusion - hydrogen energy. Radioactivity – Isotopic dilution and radiometric titration. Neutron activation analysis. Half-life, life. Caron and rock dating. Applications of radioisotopes in medicine and agriculture.

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, Spectrumacademy 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.
12. H. J. Arnikar, Essentials of Nuclear Chemistry, 4th ed., New Age International, 2011.
13. P. Powell, Principles of Organometallic Chemistry, 2nd edition, Chapman and Hall, London, 1998.
14. S.F.A. Kettle, Concise co-ordination chemistry, Nelson, 1969.
15. Ch. Elschenbroich, A. Salzer, Organometallics – A Concise Introduction, VCH Publishers, 1989.

ACH1C03 – ORGANIC CHEMISTRY I

(3 Credits)

Course Outcome After completion of the full course the students should be able to	Cognitive level
C.O.1: describe the theoretical models that explain delocalised chemical bonding, aromaticity, stability of various conformations, concepts in stereochemistry, reactions of carbonyl compounds, methods of determining reaction mechanism and generation and stability of reactive intermediates	Understand
C.O.2: Categorise various types of bonding interactions including supramolecular forces, different types of reactivity manifestations of carbonyl group and classes of reaction mechanisms and intermediates in reactions	Understand
C.O.3: Qualitatively estimate the relative proportion of possible conformations and their stabilities of a given molecule, propose experiments that will help in determining reaction mechanisms and compare and contrast the reactivity profiles of various types of carbonyl compounds	Application
C.O. 4: Analyse any given molecule based on delocalisation of electrons, steric factors and aromaticity considerations and predict the distribution of electron density; thereby arrive at possible reaction pathways with other molecules	Analysis

Unit I - Delocalised Chemical Bonding

Bonding: Basics of MO theory, delocalised chemical bonding, MO diagrams of conjugated polyenes, allyl and pentadienyl systems, resonance, rules of resonance, effect of resonance on properties and reactivity, cross-conjugation, hyperconjugation, tautomerism.

Aromaticity: Basic concepts, benzenoid, non-benzenoid, charged and heterocyclic aromatic systems. Huckel's rule, Frost circles, criteria for aromaticity, annulenes, anti-aromaticity, homoaromaticity, fullerenes and graphene.

Supramolecular Chemistry: Various types of non-covalent interactions, bonding and applications of addition compounds, crown ethers, cyclodextrins, cryptands, catenanes and rotaxanes.

Unit II - Stereochemistry

Conformational Analysis: Configuration and conformation, conformational analysis, ethane, butane, carbonyl compounds, cycloalkanes, A values, conformational lock, decalins, bridged bicyclic systems, pyranose rings, carbonyl compounds, anomeric effect, effect of conformation on reactivity.

Chirality and Asymmetric Synthesis: Basic concepts, multiple chiral centres, axial chirality, allenes, cumulenes, spiranes, biphenyls, chirality at N, S and P. Prochirality, Si and Re nomenclature, specific rotation and enantiomeric excess, stereospecificity and stereoselectivity, basic principles of asymmetric synthesis, methods of resolution, nature's chiral pool, chiral auxiliaries, asymmetric catalysis, desymmetrisation and kinetic resolution.

Unit III - Reaction Mechanisms and methods of determining them

Acidity and basicity of organic compounds, equilibrium, rate, rate limiting step, intermediates and transition states, reaction profile diagrams, kinetic and thermodynamic control of reactions, Hammond postulate, Curtin-Hammett principle, methods of determining reaction mechanisms- isotopic labelling, kinetic isotopic effects, crossover studies, detection of intermediates, linear Free energy relationships (Hammett and Taft equations).

Unit IV - Chemistry of Carbonyl Compounds

Reactivity of carbonyl groups in aldehydes, ketones, carboxylic acids, esters and acid chlorides with nucleophilic reagents (O, N, C nucleophiles and borohydride). Formation and hydrolysis of acetals, enamines and esters. Nucleophilic addition vs substitution. Acidity of α hydrogen atom- enolate ion formation. Reactivity of enolate ions. Halogenation of enolate ions- haloform reaction. Alkylation of enolate ions. Alkylation using enamine, Use of lithium bases, Aldol and related reactions, Claisen ester condensation, Darzens reaction, Stobbe, Dieckmann, Perkin reactions. Mannich reaction. Michael addition, Robinson annulation. Deprotonation and alkylation of imine anions (metalloenamines).

Unit V - 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 reactions. Rearrangement and fragmentation reactions of free radicals. Applications of free radicals. Benzyne intermediates. Gomberg-Bechmann reaction and Wohl-Zeigler reaction, Hunsdiecker reaction and Reed Reaction, free radical cyclisations. Carbenes and nitrenes: generation, stability, addition, cyclisation, insertion and ring enlargement reactions, Skattebol rearrangement.

REFERENCES

1. March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure, 7th Edition, Michael B. Smith, Wiley, 2013.
2. Advanced Organic Chemistry PART A and PART B., F. A. Carey and R. J. Sundberg, Springer 2007.
3. Organic Chemistry, J. Clayden, N. Geeves and S. Warren, Oxford University Press, 2012.
4. Organic Chemistry, Bruice P. Y. Pearson, 8th Ed, 2020.
5. Organic Chemistry, Morrison, Boyd and Bhattcharjee, 7th Edition, Pearson, 2010.
6. Advanced Organic Chemistry, D. E. Lewis, Oxford University Press, 2016.

7. Organic Chemistry- Structure and Function, P. Vollhardt and N. E. Schore, W. H. Freeman and Co., 7th Ed., 2016.
8. Stereochemistry of Organic Compounds, Second Ed., D. Nasipuri, New Age International, 2005.
9. Stereochemistry of Organic Compounds, E. L. Eliel and S. H. Wilen, Wiley India, 2008.
10. A Guide Book to Mechanism in Organic Chemistry, Peter Sykes, Longman, 1985.
11. Modern Physical Organic Chemistry, A. V. Anslyn and D. A. Dougherty, University Science Books, 2005. 12. D. Feldman and A. Barbalata, Synthetic Polymers, Chapmann and Hall.

ACH1C04 - PHYSICAL CHEMISTRY I

(3 Credits)

Course Outcome After completion of the entire course, the student should be able to:	**CognitiveLevel**
C.O.1: Apply the concepts of thermodynamics to derive relations between molecular properties and to predict spontaneity of processes.	Understand Application
C.O.2: Evaluate dependence of chemical equilibrium on system variables and thermodynamic properties	Evaluation
C.O.3: Understand basics of Ionics in electrochemistry and to describe the theories of ionic conductance and apply the same in solving problems	Understand Application
CO 4: Explain and analyse the relations between thermodynamic functions and electrochemistry	Analysis
C.O.5: Describe and apply the concept of electrodics in explaining and evaluating the electrochemical properties	Evaluation

UNIT I - Thermodynamics I (10 hrs)

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. Physical significance of Chemical potential. Variation of Chemical Potential with temperature and Pressure. Determination of partial molar properties: Direct method, method of intercepts. Gibbs -Duhem equation. Fugacity of gases and its determination. Gibbs-Duhem-Margules equation. Ideal liquid solutions. Raoult's law. Henry's law. Non-ideal solutions. Deviation from Raoult's law. Activity. Thermodynamics of mixing Excess thermodynamic functions. Excess free energy, excess entropy, excess enthalpy and excess volume.

UNIT II - Thermodynamics II (8 hrs)

Thermodynamics of irreversible process: Stationary state concept. Principle of local equilibrium. Simple examples of irreversible processes. Forces and fluxes. The phenomenological relations. Onsager relations: Linear relations Coupled flows. – Direct and Cross coefficients. Domination of direct coefficients– Proof. Onsager reciprocal relation (no derivation). Entropy of production in simple irreversible system (closed systems). Application of reciprocal relation to diffusions. Thermal diffusion. Thermo-osmosis. 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. G.K. Vemulappalli, Physical Chemistry, Prentice Hall of India
6. Rajaram, Kuriacose, Thermodynamics for students of Chemistry, S.L. Nagin Chand&co
7. Gurdeepraj, Advanced Physical Chemistry, Goel Publishing House, Meerut
8. Kulu & Foster Lung, Physical Chemistry

UNIT III - Electrochemistry I (10 hrs)

Equilibrium properties of electrolyte solutions, Types of Electrolytes, Activities, and activity coefficients in electrolytic solutions. Mean ionic activity and ionic strength, Debye – Hückel theory of inter ionic interactions, Charge density near the central ion, Poisson equation, Debye – Hückel limiting law (DHLL) and its various forms. Qualitative and quantitative tests of the Debye – Hückel limiting law. Electrolytic conductance – Kohlrausch's law and its applications, Mechanism of electrolytic conductance - Debye – Hückel – Onsager (DHO) theory of electrolytes. Asymmetry (Relaxation) effect and Electrophoretic effect, Mathematical derivation of DHO equation, Validity of the Debye – Hückel – Onsager equations, Deviations from the Onsager equation. Conductance ratio and Onsager equation. Dispersion of conductance with high frequencies (Debye – Falkenhagen effect) and with high potential gradient (Wien effect).

UNIT IV - Electrochemistry II (8 hrs)

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 junctionpotential and its determination. Fuel cells.

UNIT V - Electrochemistry III (12 hrs)

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.

REFERENCES

1. S. Glasstone, Introduction to Electrochemistry, Van Nonstrand.
2. Bockris and Reddy, Modern Aspects and Electrochemistry Vol. I and IIA and IIB, Academic Press.
3. P.W. Atkins and Julio de Paula, Physical Chemistry (8th and 10th 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.

ACH1C05 - ANALYTICAL CHEMISTRY

(3 Credits)

Course Outcome After completion of the full course the student should be able to	Cognitive level
C.O.1: Explain various sampling methods related to analytical chemistry	Understand
C.O.2:Analyze the experimental data using chemical analysis	Analyze
C.O.3: Demonstrate the application of various electro-analytical techniques	Application
C.O.4: Analyze the applications of various titration methods	Analyze
C.O.5: Evaluate the merits and demerits of various conventional analytical tools	Evaluate

UNIT - I Sampling (6 hrs)

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).

UNIT- II Errors in Chemical Analysis (12 h)

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 - III Conventional Analytical Procedures (12 hrs)

Gravimetry: solubility 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.

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.

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 $KMnO_4$, $K_2Cr_2O_7$, 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.

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, and variamine blue.

UNIT - IV Electro Analytical Methods I (6 h)

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.

UNIT - V Electro Analytical Methods II (12 h)

Polarography and voltammetric techniques: micro electrode and their specialties, 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. Cyclic voltammetry.

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

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4. J.H. Kennedy, Analytical Chemistry: Principles, Saunders College Pub., 1990.
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7. G. D. Christian, Analytical Chemistry, 6th ed., John Wiley & Sons, 2007.
8. R.A. Day, A.L. Underwood, Quantitative Analysis, Prentice Hall, 1967.
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ACH 1P 01 - INORGANIC CHEMISTRY – PRACTICAL I

(2 Credits)

Course Outcome After completion of the full course the student should be able to:	**Cognitive level**
C.O.1: Understand safe laboratory practices and develop basic laboratory skills	Understand
C.O.2: Identify the cations in a mixture of unknown salts.	Application
C.O.3: Estimate binary mixtures of metal ions by volumetry, gravimetry, and colorimetry	Application
C.O.4: Evaluate the merits and demerits of various methods of estimation of bulk and trace metals present in biological significance	Evaluate
C.O.5: Analysis of trace metals using optical methods	Anlaysis

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^{+}, and K^{+} and THREE less familiar metal ions such as Tl, W, Se, Te, Pd, Pt, Au, Mo, Ce, Th, Ti, Zr, V, U and Li. Anions which need elimination not to be given.

(Minimum 5 mixtures to be analyzed and recorded).

Part II

(a) Estimation of calcium using Murexide as indicator

(b) Estimation of copper using pyrocatechol violet as indicator

(c) Estimation of nickel using bromopyrogallol red as indicator

(d) Estimation of Hardness of water using complexometry (Tap water, well water and bore well water)

(e) Estimation of Cr, Ni, & Fe by colorimetric method

REFERENCES

1. A.I. Vogel, A Textbook 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.
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7. R. Srinivasan, Ed. Photochemical Synthesis Vols. I and II.

ACH1P02 - ORGANIC CHEMISTRY – PRACTICAL I

(2 Credits)

Course Outcome **After completion of the full course the students should be able to**	**Cognitive level**
C.O.1: Apply the general laboratory safety, health and environmental hazards of common chemicals and operations, basic lab techniques and fundamentals of qualitative analysis and synthesis.	Understand
C.O.2: Acquire practical skill and theoretical knowledge of isolation, purification and analysis of impure materials. Acquire skill to handle the necessary glassware, equipment, and assembly of required set-ups.	Understand
C.O.3: Develop a systematic approach to handle an unknown sample for determining the number of components, isolating and purifying the individual components in a qualitative manner. Acquire the skill to set up reactions, follow the progress of the reaction, work up, isolate and purify the desired product from the reaction mixture.	Application
C. O. 4: Analyse the obtained products by standard techniques to conform the identity. Estimate the amount and calculate the efficiency of the process. Innovate to minimise the waste.	Analysis

A) Lab Safety training

B) Isolation and Purification Techniques

- Distillation (fractional & vacuum)
- Thin Layer Chromatography (natural samples)
- Solvent extraction (caffeine from teal leaves & b-carotene from carrots)

C) Qualitative Analysis

- Separation of binary mixtures by solvent extraction
- Single step preparations (selected from among borohydride reduction, oxidation, rearrangement, Fischer indole synthesis, aldol, Knoevenagel, von Pechmann, aromatic bromination, nitration, esterification, amidation, drug, dye or polymer synthesis)

  Green and modern protocols to be adopted for synthesis

  Synthesized compounds to be purified by recrystallisation and identified by MP measurement

REFERENCES

1. A Hand book of Organic Analysis-Qualitative and Quantitative by H.T. Clarke, and revised by B. Haynee, Edward Arnold, London 1975.
2. Vogel's Text Book of Practical Organic Chemistry by B.S. Furhen et. al., Longman-Group Ltd.
3. Systematic Qualitative Organic Analysis by H. Middleton, Edward Arnold (Publishers) Limited, London 1959.
4. Elementary Practical Organic Chemistry by Arthur I. Vogel, EX CBS Publishers and Distributors.
5. Experiments in Organic Chemistry by Louis, F.Fieser, D.C. Heath and Company Boston, 1955.
6. Experiments and Techniques in Organic Chemistry, D. Pasto, C. Johnson and M. Miller, Prentice Hall.
7. Macroscale and Microscale Organic Experiments, K.L. Williamson, K.M. Masters, Cengage learning.
8. Systematic Qualitative Organic Analysis, H. Middleton, Adward Arnold.
9. Vogel's Textbook of Practical Organic Chemistry, A.R. Tatchell, John Wiley

ACH1P03 PHYSICAL CHEMISTRY – PRACTICAL I

(2 Credits)

Course Outcome After completion of the full course the student should be able to:	**Cognitive level**
C.O.1: Practice and demonstrate the basic laboratory skills in handling laboratory glassware, equipment, and chemicals.	Application
C.O.2: Illustrate experiments based on various laws of physical chemistry.	Application
C.O.3: Interpret the results obtained from various experiments by constructing ideas to account for results employing recent thoughts.	Evaluation

1. Thermochemical Measurements

Determination of Heat of solution of ammonium oxalate/ succinic acid/ benzoic acid by solubility method

Determination of water equivalent (or heat capacity) of a calorimeter using different volumes of water

Determination of heat of neutralization of HCl and NaOH using thermos flask or beaker as the calorimeter

Solid Liquid Equilibrium

Determination of molal depression constant of naphthalene.

Determination of molecular weight of unknown solute

Phase Diagrams

Phenol – Water System

Determination of mutual solubility curve of Phenol and Water and hence the consulate point

Determination of critical solution temperature (CST) of Phenol and Water in the presence of (i) NaCl (ii) Naphthalene and (iii) Succinic acid

Three component system

Construction of the triangular phase diagram of acetic acid, Chloroform, and water

Construction of the Tie line

Determination of the composition of unknown mixture

Phase diagram of simple eutectic system

Construction of phase diagram of two components (E.g.: - Naphthalene – Biphenyl or Diphenyl amine – Benzophenone) system by cooling curve method

Estimation of eutectic temperature, eutectic composition and composition of unknown composition using phase diagram.

2. Conductometric Measurement

Determination of the strength of given strong acid (HCl) by titrating it conductometric- ally with the given strong base (NaOH).

Determination of the strength of the given weak acid (Acetic acid) by titrating it conductometrically with the strong base (NaOH)

Determination of the strength of the given weak acid (Acetic acid) by titrating it conductometrically with weak base (Ammonium hydroxide)

Estimation of the amount of strong acid (HCl) and weak acid (Acetic acid) present in the given mixture by titrating it conductometrically against strong base (NaOH)

Determination of the solubility and solubility product of sparingly soluble salts (AgCl or $BaSO_4$) conductometrically ($AgNO_3$ vs. KCl or K_2SO_4 vs. $BaCl_2$)

Determination of Equivalent conductance of (i) a strong electrolyte (KCl) and (ii) a weak electrolyte (Acetic Acid) with concentration and to verify Debye – Huckel - Onsager equation.

Determination of equivalent, molar conductance, degree of dissociation and dissociation constant of weak acid (Acetic acid) and to verify of Ostwald's dilution law.

Determination of Activity coefficient of Zn in 0.002 M $ZnSO_4$ using Debye-HuckelLimiting Law (DHLL).

Determination of solubility product of sparingly soluble salts (AgCl, $BaSO_4$).

3. Adsorption and Distribution Measurements

Verification of Freundlich and Langmuir isotherms of adsorption of Acetic acid or Oxalic acid on activated charcoal.

Studies on the distribution of acetic acid between (i) Water and Chloroform and (ii) Water and Cyclohexane.

Determination of distribution coefficient of I_2 between (i) Chloroform and water or (ii) Cyclohexane and water.

To study the equilibrium reaction $KI + I_2 \rightleftharpoons KI_3$ and to determine its equilibrium constant

Determination of concentration of given KI solution using distribution method.

4. Chemical Kinetics – I

To study the kinetics of hydrolysis of methyl acetate (Ester) in the presence of an acid (HCl or H_2SO_4) at room temperature

To study the kinetics of saponification of an ester with sodium acetate.

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

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.
6. A. Anand & R. Kumari, Physical Chemistry Laboratory Manual – An Interdisciplinary Approach – I K International publishing 2019.

ACH1A01 – ABILITY ENHANCEMENT COURSE (AEC)

(2 Credits)

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.

ACH2C06 - CHEMICAL BONDING AND CHEMICAL APPLICATIONS OF GROUP THEORY

(3 credits)

Course Outcome After completion of the entire course, the student should be able to:	Cognitive level
C.O.1: apply approximation methods to calculate properties of many electron systems of chemical interest.	Application
C.O.2: discuss the electron spin of simple chemical systems.	Understand
C.O.3: demonstrate the principles of chemical bonding in diatomic and polyatomic molecules.	Application
C.O.4: apply the principles of Group Theory in chemical bonding and spectroscopy.	Application

UNIT - I Many-electron atoms and approximation methods (10 Hours)

Many-body problem Hamiltonian for many electron systems (example He). Significance of interelectronic repulsion terms.

Approximation methods:

Variation method. Linear variation theorem with proof, illustration of variation theorem using a trial function (e.g. x(a-x) for particle in a 1D-box. Variational treatment of the ground state of Helium atom.

Perturbation method. Time-independent perturbation method (non-degenerate case only). Illustration by application to particle in 1D-box with slanted bottom, Perturbation treatment of the ground state of the helium atom.

Hatree-Fock Self Consistent Method for solving many electron atoms (for He atom), Electron Correlation, Hartee-Fock Limit.

UNIT - II Electron spin and atomic structure (6 Hours)

Concept of electron spin and its origin. Spin quantum numbers, spin eigen functions and spin variable, Spin angular momentum, $\mathbf{S}$, $\mathbf{S}^2$, and $\mathbf{S_z}$ operators, Construction of wave functions including spin for many electron atoms, Symmetric and antisymmetric wave functions, Electron spin and Pauli's exclusion principle, Slater Determinantal wave function, Coupling of angular momenta, LS and JJ-couplings. Spectroscopic Term symbols.

UNIT - III Chemical Bonding (14 Hours)

Schrödinger equation for a molecule, Born-Oppenheimer approximation, Hartree-Fock Self-Consistent Field (HF-SCF) method. Roothan equations. Exchange integrals and Coulomb Integrals. post-Hartree-Fock methods and density functional theory.

Molecular Orbital Theory (MOT) of H_2^+ and H_2; Schrödinger equation, wavefunctions and energy levels, application to diatomic molecules such as, H_2^+, H_2. Concept of σ, σ*, π, π* orbitals and their characteristics; bond order, 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.

Valence Bond approach for Hydrogen Molecule, Schrödinger equation, Wave functions and Energy levels, Comparison between MOT and VBT. Hückel MO (HMO) theory of linear conjugated hydrocarbons (Ethylene, Butadiene, Allylic anion). HMO theory of aromatic hydrocarbons (benzene). Secular determinants, Electron delocalization energy, calculation of charge distribution, bond orders and reactivity. Frost-Hückel circle mnemonic device for cyclic and acyclic polyenes.

UNIT - IV Application of Group theory to Chemical Bonding (10 Hours)

Vanishing and non-varnishing integrals. Overlap integrals and conditions for overlap.

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 ofMOs, Electronic Configuration of H_2O, Symmetries of the ground and excited states.

Group theoretical treatment of hybidization, Construction of hybrid orbital in BF_3 and CH_4, Inverse transformation.

UNIT - V Application of group theory to Molecular Spectroscopy (10 Hours)

Symmetries of the ground and excited states, Transition moment integral and selection rules. Electronic transitions and selection rules (e.g. formaldehyde).

Symmetry of normal modes of vibrations, Construction of Γ_{cart}. Normal coordinates and drawings of normal modes (e.g., H_2O and NH_3), Selection rules for IR and Raman spectroscopy, Complementary nature 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).

REFERENCES

1. J.P. Lowe, *Quantum Chemsitry*, 2nd Edition, Academic Press, Inc. 1993.
2. A.K. Chandra, Introduction of *Quantum Chemsitry*, Tata McGraw Hill, 1994.
3. R.K. Prasad, *Quantum Chemistry,* 2nd Edition, New Age International, 2000.
4. F.A. Cotton, Chemical Applications of Group Theory, John Wiley & Sons, 3rd Ed. (2006).
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8. A McQuarrie, *Quantum Chemistry*, University Sciences Books, 1983.
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13. M.S. Pathania, Quantum Chemistry and Spectroscopy (Problems & Solutions), Vishal Publications, 1984.

ACH2C07 - INORGANIC CHEMISTRY II

(3 Credits)

Course Outcome After completion of the full course the student should be able to:	**Cognitive level**
C.O.1: Analyze and interpret molecular orbital diagram and various transitions taking place in the electronic spectra of coordinationcompounds	Analyze
C.O.2: Analyze the stability of metal complexes and evaluate their reactivity, and the mechanisms of ligand substitution reactions.	Evaluate
C.O.3: Evaluate the mechanism of homogeneous catalytic processes by organometallic complexes	Evaluate
C.O.4: 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.	Analyze
C.O. 5: Evaluate the structure, bonding, and reactions of carbonyl compounds, metal clusters and get an insight into heteropoly and isopoly anions of Mo, W	Evaluation

UNIT - I Molecular Orbital Theory and Electronic Spectra of Coordination Compounds (15 h)

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.

Magnetic properties of transition metal complexes – Types of magnetic properties. Para magnetism - the Curie and Curie – Weiss law. The μ_J, μ_{L+S} and μ spin-only expressions, temperature independent paramagnetism. Antiferromagnetism types and exchange pathways.

UNIT – II Metal Clusters (6 h)

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 (8 h)

Non-metallic clusters - preparation, structure, bonding, and reactions of boron hydrides and borazine, styx numbers, closo, nido, arachno polyhedral strucutures, boron clustercompounds, 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 Reaction Mechanism of Coordination Compounds (12 h)

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. 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 Catalysis by Organometallic Compounds (7 h)

Applications of organometallic compounds in organic synthesis and homogeneous catalysis, Complex formation and activation of H_2, N_2, O_2, 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

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2. K.F. Purcell and J.C. Kotz, Inorganic Chemistry, W.B. Saunders Co.
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6. P. Powell, Principles of Organometallic Chemistry, 2nd edition, Chapman and Hall, London, 1998. 9. S.F.A. Kettle, Concise co-ordination chemistry, Nelson, 1969.
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ACH2C08 – ORGANIC CHEMISTRY II
(3 Credits)

Course Outcome **After completion of the full course the students should be able to**	**Cognitive level**
C.O.1: Describe classification system of organic reactions based on mechanisms. Identify salient features and MO-based explanations of each of these reactions. Describe an overview of various types of natural products, polymers, their classifications and applications	Understand
C.O.2: Provide detailed description of the mechanistic classes of reactions based on changes at MO level and the consequences of these changes on stereochemistry. Explain how MO symmetry and aromaticity control reaction pathways and outcome in pericyclic reactions	Understand
C.O.3: Classify a given reaction into a particular mechanistic class and provide an explanation for observed results based on MO picture. Rationally explain the reactions given by different heterocycles based on delocalisation and aromaticity principles	Application
C. O. 4: Predict possible mechanistic pathways for given combinations of substrates and reagents from the discussed topics, analyse the structure and bonding in polymers and correlate that with the properties.	Analysis

Unit I - Substitution Reactions

Aliphatic Substitutions: The S_N2, S_N1, mixed S_N1 and S_N2, SET and SN prime mechanisms. Stereochemical considerations, common leaving groups and nucleophiles, Mitsunobu reaction. Neighbouring group participation, Classical and nonclassical carbocations, phenonium ions, bridged bicyclic systems, side reactions of carbocations. SNi mechanism. Effects of substrate structure, attacking nucleophile, leaving group and reaction medium, ambident nucleophiles, regioselectivity.

Aromatic Electrophilic Substitutions: Common electrophiles and substitution reactions, arenium ion mechanism, directing, activating and deactivating effects, ipso substitution, regiochemical preferences in common heterocycles, major formylation reactions.

Aromatic nucleophilic Substitutions: General mechanism, Meisenheimer complexes, substitutions of diazonium compounds, benzyne mechanism, vicarious substitution, *von* Richter, Sommelet-Hauser and Smiles rearrangements, Chichibabin reaction.

Unit II - Polar Additions, Eliminations and Synthetic Photochemistry

Addition Reactions: General mechanism and stereochemistry of electrophilic additions to alkenes, halocyclizations, hydroboration, oxymercuration, cyclopropanations, asymmetric epoxidation and dihydroxylation, electrophilic additions to alkynes and allenes. Addition of nucleophiles to alkenes and alkynes, tandem conjugate addition-enolate trapping, nucleophilic epoxidation.

Eliminations: E2, E1 and E1cB mechanisms. Reactivity – effects of substrate structures, base, the leaving group, medium, stereochemical considerations of elimination reactions. Alkyne formation via eliminations.

Photochemistry: Photochemical reactions of alkenes- photocycloaddition, di-pi-methane rearrangement; Photochemical reactions of carbonyl compounds- Paterno-Buchi reaction, Norrish type I and II reactions, oxa-di-pi methane rearrangement. Dienone rearrangement, photo-Fries rearrangement, Photochemistry of diazo compounds.

Unit III - Pericyclic Reactions

Definitions and types of pericyclic reactions (a) Cycloaddition and cycloreversion- antarafacial and suprafacial additions, 4n and 4n+2 systems, 2+2 addition of ketenes, Detailed treatment of Diels-Alder reactions (b) Electrocyclic ring closing and ring opening- conrotatory and disrotatory modes and effect on stereochemistry, 4n, 4n +2, allyl and pentadienyl systems (c) Sigmatropic rearrangements- suprafacial and antarafacial shifts of H and alkyl groups, 1,3, 1,5, 3,3 and 2,3-sigmatropic rearrangements, Valence tautomerism (divinyl cyclopropane and bullvalene) (d) Cheletropic reactions- N_2, SO_2, CO extrusions (e) Group transfers-diimide reduction. Explanations based on FMO and transition state aromaticity methods. Synthetic applications of pericyclic reactions such as Diels-Alder and 1,3-dipolar (nitrones, nitrile oxides, azides) cycloadditions, Nazarov cyclisation, Claisen, Cope and oxy-Cope rearrangements, 2,3-sigmatropic rearrangements and ene reactions.

Unit IV - Heterocycles and Natural Products

Heterocycles: Synthesis, aromaticity, reactions and applications of Pyrrole, Furan, Thiophene, and Indole. Synthesis and reactions of six membered ring compounds. Quinoline, 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.

Natural Products: Terpenes- Classification, nomenclature, occurrence, biosynthesis, isolation, isoprene rule: Steroids- Occurrence, basic skeleton: Alkaloids- Classification based on the Nheterocycle, occurrence and importance, biosynthetic origins, Robinson tropinone synthesis. Lipids- occurrence, structure, and importance.

Unit V - Polymers

Concept of polymers and macromolecules: definition, classification, 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, isotatic, syndiotatic, atatic, illustrated with suitable examples.

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9. Pericyclic reactions- A Textbook, S. Sankararaman, 1st Ed., Wiley-VCH, Weinheim, 2005.
10. Introduction to Organic Photochemistry, J. D. Coyle, 1st Ed., 1986. Heterocyclic Chemistry, J. A. Joule, ELBS.
11. Heterocyclic Chemistry, T. L. Gilchrist, Longman Scientific Technical.
12. An Introduction to Heterocyclic Chemistry, R. M. Acheson, John Wiley.
13. Natural products: Chemistry and Biological Significance, Mann, Davidson, Hobbs, Banthrope and Harborne, Longman, Essex.
14. Organic Chemistry, Vol. 2, I. L. Finar, ELBS.
15. G. Odian, Principles of Polymerisation, McGraw Hill.
16. V.R. Gowarikar and N.V. Vishwanathan, Polymer Science, New Age international 2010 Billmeyer, Textbook of Polymer Science, John Wiley & Sons.

ACH2C09 - 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 apply the basic concepts of statistical mechanics in evaluating the thermodynamic thermodynamic systems.	Analysis
C.O.2: Evaluate the partition function and thermodynamic properties from spectroscopic data and apply the principles of statistical thermodynamics to various systems.	Evaluate
C.O.3: Define the parameters of different crystal systems and elucidate the structure from diffraction patterns.	Analysis
C.O.4: Analyze the electronic structure of solids	Analysis
C.O.5: Understand and apply the properties of solids for developing new materials and devices.	Analysis Applications

UNIT I - Statistical Thermodynamics I

Basic principle, Permutations. Ensembles, Microcanonical, Canonical and Grand Canonical Ensemble. Microstates and macrostates. Statistical weight. Probability distribution of particles in energy states. Most probable distribution. Thermodynamic probability and entropy. Classical statistics, Boltzmann exponential law, 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.

UNIT II - Statistical Thermodynamics II

The perfect gas-ideal monatomic gas – Energy and entropy. Sackur-Tetrode equation. Diatomic gases- Evaluation of energy. Heat capacity of gases. Classical and quantum theories. Diatomic gases. Anomalous heat capacity of hydrogen - Explanation based on ortho and para hydrogen. Heat capacity of solids. Atomic crystals. Einstein theory of atomic crystals, Debye modification.

Need for Quantum statistics-The ideal Fermi Gas. Fermi-Dirac distribution law. Application to electrons in metals. Bose – Bose-Einstein distribution law. The ideal Bose gas. Degenerate gas. 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. Andrews, Equilibrium Statistical Mechanics, John Wiley and Sons
5. O. K. rice, Statistical Mechanics, Thermodynamics and Kinetics, Freeman & Co.
6. M.C. Gupta, Statistical Thermodynamics, Wiley eastern Limited.

UNIT III - Solid State Chemistry I

Crystal symmetry: Symmetry elements and symmetry operations, mathematical proof for the non-existence of 5-fold axis of symmetry, crystal systems, Bravais lattices Allowed combinations of operations leading to 32 crystal classes. Crystallographic point groups - Schönflies& Hermann–Mauguin notations, Stereographic Projections of some simple crystal classes (e.g. 1, 1, 2/m, 222, mmm). Stereographic projections of the 27 axial point groups, translational symmetry elements & symmetry operations - screw axes and glide planes, introduction to space groups.

Bragg's law and applications, lattice planes and Miller indices, reciprocal lattice *d*-spacing formulae, XRD measurements. Laue method. Rotating crystal method. Powder diffraction method.

UNIT IV - Solid State Chemistry II

Theories of solids – Classical and Quantum mechanical free electron theories, Fermi Dirac distribution in solids and calculation of fermi energy.

Zone Theory of solids – Bloch theorem, Kronig – Penney model, Energy spectrum of electrons in solids, Energy bands and Brillouin zones (First and second Brillouin zones of 2 D square lattice), Fermi surfaces, Illustrative representation of electrons in zones, Density of states.

Band Theory of solids – Dispersion relation (E vs. k curve), MO approach (Li metal lattice), Classification of solids into Conductor, Semiconductors, and Insulators.

Defects and Non – Stoichiometry – Point, Line and Plane defects, Intrinsic and Extrinsic defects, Schottky and Frenkel defects, Color centers.

UNIT V - Solid State Chemistry III

Electrical Properties of Solids: Electrical conductivity and Ohm's law, Hall effect, Intrinsic and extrinsic semiconductors, Dielectric properties of solids – Piezoelectricity and Ferroelectricity, Super conductors – Meissner effect, Type I and II superconductors, Basic concepts of BCS theory.

Magnetic Properties of Solids: Classification of magnetic materials, Diamagnetism, Para magnetism, ferro- antiferro- and ferri-magnetism, Super paramagnetism.

Optical Properties of Solids: Optical reflectance, Plasmon Frequency, Photoconduction, Photo and Electroluminescence, Photovoltaic and Photoelectrochemical effects.

Brief Introduction to New Materials: High temperature superconductors, Ionic Conductors, Conducting Polymers, Zeolites, Fullerenes, Molecular Materials etc.

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 and its applications, John Wiley.
7. D K Chakraborthy, 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.,
11. P A Cox, The electronic structure and Chemistry of Solids, Oxford Science Publications
12. G Gottstein, Physical foundation of Material Science, Springer

ACH2C10 - MOLECULAR SPECTROSCOPY & PHOTOCHEMISTRY

(3 Credits)

Course Outcome After completion of the full course the student should be able to:	**Cognitive level**
C.O.1: Understand the interaction of matter with radiation in terms of the relation with the molecular energy levels.	Understand
C.O.2: Explain and apply the selection rules pertaining to various molecular spectral transitions.	Application
C.O.3: Illustrate the rotational, vibrational, and electronic spectra of molecules.	Application
C.O.4: Interpret and analyse the molecular structure from spectral data	Analysis
C.O. 5: Understand and apply the theories of resonance spectroscopy in elucidating the molecular structure.	Application

UNIT I – General Theory of Molecular Spectroscopy

General Theory of Spectra: Electromagnetic radiation and its different regions, Quantization of Energy, Interaction of matter with radiation and its effect on the energy of the molecule. Origin of molecular spectra, Representation of Spectra and elements of practical spectroscopy.

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.

UNIT 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.

UNIT III – Infrared Spectroscopy

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.

Raman Spectroscopy: Principle of Raman spectroscopy, Selection rules, Pure rational, pure vibrational Raman spectra, Vibrational-rotational Raman spectra, Mutual exclusion principle. Raman Spectrophotometer – Instrumentation (brief mention only). Laser Raman spectroscopy and applications.

UNIT IV - Photochemistry & Electronic Spectroscopy

Physical Photochemistry: Laws of Photochemistry, Photophysical and Photochemical processes, Mechanism of absorption and emission of radiation – Electric dipole transitions,

The fate of electronically excited state species - Jablonski diagram, Environmental effects of absorption and emission spectra, Properties of excited state molecules – Excited state dipole moment, Acidity constant, Redox potential etc., Excimers and Exciplexes, Sensitization, Quantum yields, Static and Dynamic quenching, Stern – Volmer equation, Resonance Energy Transfer, Light induced electron transfer. Delayed fluorescence - E-type & P-type, Multi photon excitation and applications, Chemiluminescences.

Electronic Spectroscopy: Beer-Lambert Law, Molar extinction coefficient, Intensity of electronic transitions – Theoretical absorption intensity, Basics of selection rules. Vibrational and rotational structures, Frank – Condon Principle, Photoelectron spectroscopy (Brief mention only), Photodissociation, Predissociation, Lifetimes of excited electronic states, electronic spectra of diatomic molecules, Charge Transfer transitions, electronic spectroscopy of polyatomic molecules.

UNIT V – Resonance Spectroscopy

NMR Spectroscopy: Magnetic properties of nuclie, Theory of nuclear magnetic resonance, measurement techniques, NMR spectrometer -Principles and instrumentation (brief mention only), Solvents used, Chemical shift and factors influencing chemical shift, relaxation effects, 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.

Applications of NMR spectroscopy to structure elucidation of simple organic and inorganic molecules.

ESR Spectroscopy: Theory and measurement techniques, hyperfine interactions, Equivalent and non-equivalent protons, Kramer's theorem.

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, Physical Chemistry, Oxford University Press.
4. Modern Spectroscopy – J.M.Hollas, John Wiley.
5. Applied Electron Specteroscopy for Chemical Analysis Ed.H.Windawi & F.L.Wo.Wiley Interscience.
6. Physical Methods in Chemistry – R.S.Drago, Saunders College.
7. Introduction to molecular Spectroscopy – G.M.Barrow, McGraw Hill.
8. Quantum chemistry & Molecular Spectroscopy, Volume 4, Laxmi Publications – New Delhi.

ACH2P04 INORGANIC CHEMISTRY – PRACTICAL II

(2 Credits)

Course Outcome After completion of the full course the student should be able to:	**Cognitive level**
C.O.1: Synthesis, characterization, and application of metal complexes of macrocycles	Application
C.O.2: Analyze metal ions using volumetric, gravimetric, and colorimetric analysis	Analysis
C.O.3: Green synthesis of nanoparticles, its characterization, and applications	Apply
C.O.4: Synthesis of metal complexes and characterize them by various physicochemical methods.	Evaluate
C.O.5: Interpret electronic spectrum of different metal complexes.	Evaluate

Part I

Estimation of metal ions

(a) Estimation of iron (gravimetric method) and chromium (colorimetric method)

(b) Estimation of iron (gravimetric method) and nickel (colorimetric method)

(c) Estimation of iron (volumetric method) and chromium (colorimetric method)

(d) Estimation of iron (gravimetric method) and calcium (volumetric method)

(e) Estimation of iron (gravimetric method) and chromium (volumetric method)

(f) Estimation of iron (volumetric method) and chromium (volumetric method)

(g) Estimation of iron (volumetric method) and nickel (gravimetric method)

(h) Estimation of copper (gravimetric method) and zinc (volumetric method)

(Minimum 5 experiments to be conducted and recorded)

Part II

Preparation and characterization (IR, NMR, UV-vis, and fluorescence spectroscopy) of nanoparticles and metal complexes

(a) "Green synthesis'' of silver nanoparticles

(b) Bis(dimethylglyoximato)nickel(II)

(c) Hexammine cobalt (III) chloride

(d) Schiff base complexes of various divalent metal ions

(e) Ferrocene

(f) Metal complexes of tetraphenyporphyrin

(Minimum 3 synthesis and characterization is to be performed and recorded)

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.

ACH2P05 ORGANIC CHEMISTRY – PRACTICAL II

(2 Credits)

Course Outcome **After completion of the full course the students should be able to**	**Cognitive level**
C.O.1: Demonstrate the skills required for quantitative analysis. Develop skills for accurate weighing, transfer, measurements and other operations. Awareness about environmental aspects of laboratory practices. Develop knowledge and skill in planning and implementing multistep synthesis and chromatographic separations.	Understand
C.O.2: Acquire practical skill and theoretical knowledge of isolation, purification and analysis of impure materials. Acquire skill to handle the necessary glassware, equipment, and assembly of required set-ups.	Understand
C.O.3: Develop a systematic approach to handle an unknown sample for determining the number of components, isolating and purifying the individual components in a qualitative manner. Acquire the skill to set up reactions, follow the progress of the reaction, work up, isolate and purify the desired product from the reaction mixture.	Application
C. O. 4: Analyse the obtained products by standard techniques to conform the identity. Estimate the amount and calculate the efficiency of the process. Innovate to minimise the waste.	Analysis

A) Quantitative analysis

Estimation of aniline and phenol via bromination method

Determination of saponification value and iodine value of an oil

Estimation of vitamin C content in fruit juice/tablet

B) Green Chemistry

Selected experiments from among the following

Biomass-derived products such as furfural from corn cobs, biodiesel preparation, ionic liquid synthesis and its use in a reaction as solvent, mechanochemical synthesis, synthesis in aqueous medium, multicomponent reactions, sonochemistry.

C) Multistep Organic Synthesis

Any suitable three-step synthesis from the following examples or similar ones

(eg. Banzaldehyde-benzoin- benzil-benzilic acid; Benzaldehyde-cinnamic acid- b-bromostyrene; Benzaldehyde-chalcones-pyrazoline-pyrazole; Hydroquinone-quinone-Diels-Alder reaction; Benzaldehyde-imine-reduction-Mannich etc)

D) Column chromatography

To be integrated to one of the purifications in multi-step organic synthesis (B)

REFERENCES

1. A Hand book of Organic Analysis-Qualitative and Quantitative by H.T. Clarke, and revised by B. Haynee, Edward Arnold, London 1975.
2. Vogel's Text Book of Practical Organic Chemistry by B.S. Furhen et. al., Longman-Group Ltd.
3. Systematic Qualitative Organic Analysis by H. Middleton, Edward Arnold (Publishers) Limited, London 1959.
4. Elementary Practical Organic Chemistry by Arthur I. Vogel, EX CBS Publishers and Distributors.
5. Experiments in Organic Chemistry by Louis, F.Fieser, D.C. Heath and Company Boston, 1955.
6. Experiments and Techniques in Organic Chemistry, D. Pasto, C. Johnson and M. Miller, Prentice Hall.
7. Macroscale and Microscale Organic Experiments, K.L. Williamson, K.M. Masters, Cengage learning.
8. Systematic Qualitative Organic Analysis, H. Middleton, Adward Arnold.
9. Vogel’s Textbook of Practical Organic Chemistry, A.R. Tatchell, John Wiley

ACH2P06 - PHYSICAL CHEMISTRY – PRACTICAL II

(2 Credits)

Course Outcome After completion of the full course the student should be able to	**Cognitive level**
C.O.1: Demonstrate and practice the basic laboratory skills in handling laboratory glassware, equipment, and chemicals.	Application
C.O.2: Illustrate experiments based on various laws of physical chemistry.	Application
C.O.3: Interpret the results obtained from various experiments by constructing ideas to account for results employing recent thoughts.	Evaluation
C.O.4: Perform advance physical chemistry experiments and analyze the results using sophisticated instruments	Create (Synthesis)

1. **Chemical Kinetics – II**
   - To study the kinetics of the interaction of crystal violet with NaOH colorimetric / spectrophotometric method.
   - Kinetics of the reaction between acidified acetone and iodine by using colorimetric or spectrophotometric method.
   - Study of the kinetics of inversion of sugar and mutarotation of glucose by using polarimetry
   - Determination of the individual orders of the reactant (order with respect to KI and H_2O_2) for H_2O_2 – KI clock reaction
2. **pH measurements**
   - To prepare the following buffer solutions and to measure the pH of each of the solution using pH meter (Acidic buffer: Sodium Acetate – Acetic acid; Basic buffer: Ammonium chloride – Ammonium hydroxide)
   - Determination of the dissociation Constant (Ka) of a given acid by using pH titration, method

3.Potentiometric Measurements

- To study the titration curve for an acid with alkali potentiometrically and to determine the normality of the given acid solution.
- To find out the strength of the given potassium dichromate solution by titrating it potentiometrically with standard Mohr's salt solution.
- Determination of the thermodynamic parameters, ΔG, ΔH, ΔS and the equilibrium constant K_c of the Daniel Cell from emf measurements.

9. Viscosity Measurement

- Determination of absolute and relative viscosities of the given liquid taking waster as the reference.
- Studies on the variation of viscosity with different concentrations of sugar solutions.
- Studies on the variation of coefficient of viscosity with different concentrations of poly vinyl alcohol (PVA) in water and to determine the molar mass of PVA.\

10. Refractometry

- Analysis of a binary mixture and determination of molar refraction of a solid and thecomposition of chloroform and acetone in its azeotropic mixture by refractometry
- Determine the refractive index of a given liquid by Abbe Refractometer and find thespecific and molar refractions.

11. Cyclic Voltammetry

- Determination of the diffusion coefficient of $[Fe(CN)_6]^{3-}$ in 0.1 M KCl by using Cyclic voltammogram (CV) under different scan rate.
- Determination of the electrochemically active surface area (ECSA) of the electrode from CV measurements.

12. Spectrophotometric Measurements

- Determination of the dissociation constant of Phenolphthalein indicator by colorimetric method.
- To study the absorption spectra of $KMnO_4$ (in water) and $K_2Cr_2O_7$ (in 0.1 M H_2SO_4) in the range of 200 – 500 nm and determine the λ_{max} values (Calculate the energies of these transitions in different units, kJ.mol^{-1}, eV etc.)

- Record UV spectra (180 – 400 nm) of given compounds (Acetone, Acetaldehyde, 2- propanol, Acetic acid etc.) in Cyclohexane and water and calculate the energies of electronic transitions involved in it.

13. Photochemistry

- Construction of simple Jablonski diagram of a polyaromatic compound.
- Estimation of the Quantum yield of Perylene and Pyrene excimer formation.
- Determine the quenching constant for the fluorescence quenching of fluorescein by iodide ion in basic solution.

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.
6. A. Anand and R. Kumari Physical Chemistry Laboratory Manual – An Interdisciplinary Approach

ACH2A02 – PROFESSIONAL COMPETANCY COURSE (PCC)

(Credits: 2)

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
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, drugs and cosmetics manufacturing, 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 software.

ACH3C11 - INORGANIC CHEMSITRY III

(3 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	Analyze
C.O.2: Discuss the photochemical reactions of coordination compounds and its mechanisms	Analyze
C.O.3: Evaluate the structure of metal complexes using IR and NMR	Evaluate
C.O.4: Identify the role of metals in biological systems and the natural process taking place with the aid of metal ions in biological systems	Application
C.O.5: Analyze the ESR spectra of any given transition metal complex and Mossbauer spectra of iron, and tin complexes.	Application

UNIT – I Photochemistry of Coordination Compounds (10 h)

Photochemical reactions of metal complexes. Prompt and delayed reactions. Excited states of metal complexes – intra ligand, ligand field, charge transfer and delocalized states. Charge transfer 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 (7 h)

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 (7 h)

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 (12 h)

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. 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 O_2 binding site, nature of heme-dioxygen binding, cooperativity. Hemerythrin and hemocyanin.

UNIT – V Bioinorganic Chemistry-II (12 h)

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 B_{12} 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.

ACH3C12 – ORGANIC CHEMISTRY III

(3 Credits)

Course Outcome After completion of the full course the students should be able to	Cognitive level
C.O.1: Give accounts on various spectroscopic methods including basic principles, and specific applications for structure determination of organic molecules. Describe the various reagents that are used in classical and modern organic synthesis. Describe the structure, classification and uses of biopolymers and synthetic industrial polymers	Understand
C.O.2: Categorise the structural information available from different spectroscopic techniques, describe the measurement techniques, estimate quantitatively by using appropriate mathematical relationships, explain various levels of selectivity of different reagents and reactions, explain migratory aptitudes and stereochemistry of migrations in rearrangement reactions.	Understand
C.O.3: Apply spectroscopic techniques to detect presence of functional groups, bonds, molecular mass and symmetry elements in given unknown compounds. Predict suitable reagents and conditions for specific transformations, correlate structure and function in biopolymers and industrial polymers.	Application
C. O. 4: Analyse given spectroscopic data and arrive at complete structure of unknown compounds, Design reactions and reagents for specific synthetic tasks, compare and contrast biopolymers with synthetic polymers and design new polymeric materials.	Analysis

UNIT – I IR and UV-Spectroscopy and Mass Spectrometry

Applications of UV, IR and MS in the structural elucidation of organic compounds (structure identification 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.

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, molecular ion peak, metastable peak, McLafferty rearrangement. Nitrogen rule, patterns given by chloro and bromo compounds.

UNIT – II NMR Spectroscopy

^{1}H NMR - The chemical shift and shielding, local diamagnetic shielding, Magnetic anisotropy, Spin-spin coupling, coupling constants, the mechanism of coupling (One bond and two bonds coupling only), spin systems, Pople notation, Karplus curve-variation of coupling constant with dihedral angle, chemical and magnetic equivalence, 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, effect of hindered rotation, nOe.

^{13}C NMR - ^{13}C chemical shifts, correlation charts, proton decoupled spectra, off-resonance decoupling.

UNIT – III Reagents, Reactions and synthesis

Oxidations: Alcohols- Cr-based, DMSO-based (Kornblum, Mofftatt, Swern), hypervalent iodine-based and TEMPO-based oxidants. Alkenes- DMDO, OsO_4-NMO (UpJohn), $NaIO_4$, ozonolysis, Sharpless asymmetric epoxidation and dihydroxylation.

Reductions: Hydride reducing agents- sodium borohydride, Luche reduction, cyano and acetoxy borohydrides, LAH, DIBAL-H. Asymmetric CBS reduction. Birch reduction. Catalytic (Pd-C and RaNi) and transfer hydrogenations, dimide reduction.

Olefinations: Wittig, Peterson, Julia, McMurry and Tebbe olefinations. Shapiro reaction

Reagents: N-Bromosuccinimide (NBS), Diazomethane, Dicyclohexylcarbodiimide (DCC), Selenium dioxide, *m*-chloroperbenzoic acid, Dichloro-dicyano-benzoquinone (DDQ), sulfonium and sulfoxonium ylides, allyl silanes.

Synthesis: Concept of retrosynthesis, disconnection approach, synthons and synthetic equivalents. Umpolung (acyl anion equivalent- cyanide and dithiaacetal), overall yield, linear and convergent synthesis.

UNIT - IV Rearrangement Reactions

Rearrangement to electron deficient Carbon: Wagner-Meerwin rearrangement, Pinacol-Pinacolone rearrangement, Tiffeneau-Demjanov, Dienol-Phenol. Rearrangement to electron deficient Nitrogen: Beckmann, Lossen, Hofmann, Curtius. Rearrangement to electron deficient Oxygen: Baeyer-Villiger, Dakin reaction. Acyl carbene rearrangements: Wolff, Arndt-Eistert synthesis. Anionic rearrangements: Favorskii, Benzilic acid, Brook, Stevens. Other-Achmatowicz, Baker-Venkataraman rearrangements, Eschenmoser fragmentation.

UNIT – V Industrial and Biopolymers

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. Biodegradable polymers. Fundamentals of structure and function of biopolymers (carbohydrates, nucleic acids, proteins)

REFERENCES

1. Spectrometric Identification of Organic Compounds, Silverstein, Bassler and T Morrill, John Wiley.
2. Application of Spectroscopy of Organic Compounds, J. R. Dyer, Prentice Hall.
3. Spectroscopic Methods in Organic Chemistry, D.H. Williams, I. Fleming, Tata McGraw-Hill.
4. Organic Spectroscopy, William Kemp, Mac publsihers, 3rd Edition, 2011.
5. D. L. Pavia, G.M. Lampman, G.S. Kriz and J. R. Vyvyan; Introduction to Spectroscopy, 5th ed. Cengage India, 2015.
6. Modern Synthetic Reactions, H.O. House, W.A. Benjamin.
7. Some Modern Methods of Organic Synthesis, W. Carruthers, Foundation Books.
8. Principles of Organic Synthesis, R.O.C. Norman and J.M. Coxon, Blackie Academic & Professional.
9. Advanced Organic Chemistry Part B, F.A. Carey and R.J. Sandburg, Plenum Press.
10. Reagents in Organic Synthesis, Fieser and Fieser, Wiley.
11. D. Feldman and A. Barbalata, Synthetic Polymers, Chapmann and Hall.
12. G. Odian, Principles of Polymerisation, McGraw Hill.
13. V.R. Gowarikar and N.V. Vishwanathan, Polymer Science, New Age international
14. Billmeyer, Textbook of Polymer Science, John Wiley & Sons.

ACH3C13 - PHYSICAL CHEMISTRY III
(3 Credits)

Course Outcome After completion of the full course the student should be able to	**Cognitive level**
C.O.1: Explain and apply the concepts of chemical kinetics of gas and solution phase reactions and solving problems.	Analysis
C.O.2: Illustrate the power of photochemistry and radiation chemistry as individual technique and have a notion about their complementarity	Application
C.O.3: Explain photochemical, radiochemical, and fast reaction kinetics and techniques employed for their studies.	Application
C.O.4: Describe various adsorption phenomena and apply the properties of colloidal systems and their applications	Application
C.O.5: Describe the concepts of catalysis and apply their potential for industrial processes.	Application
C.O.6: Describe the basic principles and concepts related to the application of computers in chemistry	Understand

UNIT I - Chemical Kinetics - I

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). Potential energy surface (brief treatment). Comparison between Collision theory and Transition state theory. Thermodynamic treatment of reaction rates.

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. Linear free energy relationships. Hammett and Taft Equations.

UNIT II – Chemical Kinetics II

Study of fast reactions: Flash photolysis, Flow techniques and Relaxation methods.

Kinetics of Photochemical Reactions: Kinetics of chain reactions (H_2 – Cl_2 and H_2 – Br_2 reactions, Photolysis of HI, Ammonia etc.) Techniques for studying kinetics of photochemical reactions: Rotating sector techniques, Laser photochemistry – Principles of light amplifications, Types of lasers, Conditions of laser actions, laser cavities and laser radiation, Laser spectroscopy – Ultrafast (Pump-probe) and multi-photon spectroscopy.

Radiation Chemical Reactions: Primary processes, Pulse radiolysis, Radiation chemistry of water and aqueous ferrous sulphate solution. Radiation dosimetry – Frick's dosimeter - Calculation of absorbed dose. Szilard - Chalmers effect and their applications.

REFERENCES

1. Fundamental Chemical Kinetics, Margaret Robson Wright. Horwood publishing Limited.
2. K. J. Laidler, Chemical Kinetics, McGraw Hill, New York
3. Kinetic and Mechanism, A.A. Frost and R. G. Pearson, John Wiley.
4. Steinsfeld, Francisco and Hase, Chemical Kinetics and Dynamics, 2nd Edition, Prentice Hall International Inc.
5. Physical Chemistry, F Daniels and R.A. Alberty, Wiley. Hall International Inc.

UNIT III - Surface Chemistry

Structure and chemical nature of surfaces, Adsorption at surfaces – Adsorption isotherms, The Langmuir isotherm its kinetic and statistical derivation. Freundlich equation, BET equation, derivation, Determination of surface area and pore structure of adsorbents, Heat of adsorption and its determination.

Colloids, their preparation and purification, stability of colloids, Zeta potential and its determination- electrokinetic phenomena Electrophoresis, Electroosmosis, Sedimentation and streaming potential. Colloidal Surfactants, Micelles, HLB number. Stabilising action of surfactants, Practical importance of surfactants. Langmuir- Blodget films.

UNIT IV - Catalysis

Homogeneous catalysis, Theories of homogeneous catalysis. Acid base catalysis, Bronsted catalysis law. Enzyme catalysis: features, Michaelis Menten Mechanism. Auto catalysis. Oscillating reactions. – mechanisms of oscillating reactions (Lotko -Volterra, brusselator, and oregonator). Catalytic inhibitors and poisons, Heterogeneous catalysis: Adsorption and catalysis. Kinetics and mechanism of surface catalyzed reactions. Unimolecular surface reaction: Bimolecular reactions: Eley – Rideal Mechanism. Langmuir – Hinshelwood Mechanism- illustration using the reaction $2CO + O_2 \rightarrow 2CO_2$. Industrial Applications (brief mention only). Methods of preparation of heterogeneous catalysts - precipitation and coprecipitation methods, sol-gel methods, hydrothermal method, flame hydrolysis. Preparation of Zeolites and silica supports. Introduction to Phase transfer catalysis, biocatalysis, nanocatalysis, and polymer supported catalysis.

REFERENCES

1. Keith J. Laidler, Chemical Kinetics 3rd edn., Pearson Education, 1987 (Indian reprint 2008).
2. E. K Rideal, Concepts in catalysis, academic press.
3. A. Clark, theory of adsorption and catalysis, Academic press.
4. R. Opearce and Patterson (Ed.) Catalysis and Chemical process, Blackie and sons Ltd (1981).
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. Richard I. Masel, Chemical Kinetics and Catalysis, Wiley Interscience, 2001.
9. A.W. Adamson, Physical Chemistry of surfaces, 4th edition, Interscience, New York, 1982.
10. Dipak Kumar Chakrabarty, Adsorption and Catalysis by Solids, New Age.2007.
11. Kurt K. Kolasinski, Surface Science: Foundations of Catalysis and Nanoscience, 3rd Edn, Wiley U. K., 2012.

UNIT V – Introduction to Computational Chemistry

Application of computational quantum chemistry to molecules, specification of molecular geometry using a) cartesian coordinates b) internal coordinates, The Z matrix. Z-matrix of simple molecules (example: H_2O, formaldehyde). Basis sets. Slater and Gaussian functions, classification of basis sets - minimal, double zeta, triple zeta, split valence, polarization and diffuse basis sets, contracted basis sets, Pople style basis sets and their nomenclature, correlation consistent basis sets. Geometry optimization, stationery point, potential energy surface - local minima, global minima, saddle point and transition states, electron density, energy levels, molecular orbitals, vibrational frequency, NMR parameters.

References

1. F. Jensen, Introduction to Computational Chemistry, 2nd ed., Wiley, New York, 2009.
2. Cramer C.J., Essentials of Computational Chemistry – John Wiley
3. D. Young, Computational Chemistry: A Practical Guide to Real World Problems, Wiley, New York, 2001.

ACH3C14 - 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: Understand the theory, instrumentation, and application of various optical methods of analysis	Understand
C.O.2: Analyze the properties of materials using surface characterization techniques	Application
C.O.3: Understand the theory of thermal, and radiochemical methods and its applications	Application
C.O.4: Apply the use of various chromatographic techniques in analytical chemistry	Application
C.O.5: Understand new trends and techniques in analytical chemistry and its probable applications and design of new materials.	Create

UNIT – I Molecular Spectral Analysis (10 h)

Introduction to instrumental methods, selection of instrumental methods: precision, sensitivity, selectivity, and detection limit. Sources of noise and S/N ratio. Fundamental law of spectrophotometry, nephelometry and turbidometry and Fluorimetry. UV-visible and IR spectrophotometry – instrumentation, single and double beam instruments, Spectrophotometric titrations. Introduction to NMR spectroscopy: magnets, shim coils, sample spinning, sample probes (^{1}H, ^{13}C, ^{31}P).

UNIT – II Atomic and Surface Techniques (12 h)

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. Instrumentation of X-ray methods: X-ray absorption and X-ray diffraction. Photoelectron spectroscopy. XPS, UPS. Auger, ESCA. SEM, TEM, AFM, STM.

UNIT – III Thermal and Radiochemical Methods (10 h)

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. Radiation dosimetry – Fricks dosimetry-calculation of absorbed dose.

UNIT – IV Chromatography (10 h)

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, TCD, FID, ECD, and NPD, 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 – instrumentation, pumps, sample injection, columns, solvent selection, and detectors. Partition chromatography - bonded phase. Ion exchange chromatography - ion exchange equilibria, packings, detectors, and 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.

UNIT – V Modern Techniques in Analytical Chemistry (6 h)

Hyphenated techniques – Gas Chromatography – Mass Spectrometry (GC-MS), Liquid Chromatography – Mass Spectrometry (LC-MS), Gas Chromatography/Liquid Chromatography-Infrared Spectroscopy (GC/LC-IR), Liquid Chromatography-Nuclear Magnetic Resonance Spectroscopy (LC-NMR), Tandem Mass Spectrometry (MS/MS) techniques, Flow injection analysis (FIA).

REFERENCES

1. D. A. Skoog, D. M. West, F.J. Holler, S.R. Crouch, Fundamentals of Analytical Chemistry, 8th Edn., Saunders College Pub., 2007.
2. J.H. Kennedy, Analytical Chemistry: Principles, Saunders College Pub. 1990.
3. G.H. Jeffery, J. Bassett, J. Mendham, R.C. Denney, Vogel's Textbook of Quantitative Chemical Analysis, 5th Edn., John Wiley& sons,1989.
4. G. D. Christian, Analytical Chemistry, 6th ed., John Wiley & Sons, 2007.
5. R.A. Day, A.L. Underwood, Quantitative Analysis, Prentice Hall, 1967.
6. A.I. Vogel, A Textbook of Practical Organic Chemistry, Longman,1974.

7. H.A. Laitinen, W.E. Harris, Chemical Analysis, McGraw Hill,1975.
8. V.K. Ahluwalia, Green Chemistry: Environmentally Benign Reactions, CRC,2008.
9. F.W. Fifield, D. Kealey, Principles and Practice of Analytical Chemistry, BlackwellScience, 2000.

ACH3P07 – INSTRUMENTAL METHODS OF ANALYSIS – PRACTICAL

(2 Credits)

Course Outcome After completion of the full course the student should be able to:	**Cognitive level**
C.O.1: Analyze various samples using optical and electrochemical techniques	Analysis
C.O.2: Evaluate the structural and physical properties of metal complexes	Evaluate
C.O.3: Perform the separation and analysis of various materials using solvent extraction, and chromatography	Analysis
C.O.4: Analyze the composition of pharmaceutical samples by spectroscopic methods	Analysis
C.O.5: Perform the computational modeling of simple organic and inorganic molecules - Geometry optimization, electron density, molecular orbitals, IR, UV-vis, NMR parameters.	Analysis

Section A

Determination of organic, inorganic, and environmentally hazardous materials using (i) fluorimetry, (ii) flame photometry, (iii) nephelometry, (iv) turbidimetry, (v) elemental analysis, (vi) electrogravimetry, (vii) atomic absorption spectroscopy (AAS), (viii) inductively coupled plasma –mass spectrometry (ICP-MS), and (ix) polarimetry.

(Minimum 6 experiments to be conducted and recorded)

Section B

(a) Determination of stoichiometry of complexes using (i) mole ratio method, and (ii) continuous variation method (Job's plot), (b) determination of binding constant using Benesi-Hildebrand equation (UV-vis and fluorescence spectroscopy), (c) determination of quantum yield, (d) time-resolved fluorescence lifetime measurements, (e) determination of dehydration kinetics of simple oxalate hydrates by TGA and DSC (f) synthesis of semiconductor particles (ZnO or TiO_2) and determination of band gap using Tauc plot method, and (g) spectral analysis of organic compounds (IR, NMR, Mass Spectrometry)

(Minimum 4 experiments to be conducted and recorded)

Section C

Separation techniques using (i) solvent extraction, (ii) ion-exchange, (iii) paper chromatography, (iv) thin layer chromatography, and (v) column chromatography.

Estimation of pharmaceutical samples (i) paracetamol, and (ii) aspirin

(Minimum 3 experiments to be conducted and recorded)

Section D

Computational modeling of simple organic and inorganic molecules - Geometry optimization, electron density, molecular orbitals, IR, UV-vis, NMR parameters.

REFERENCES

1. A.I. Vogel, A Textbook 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.

ACH3E01 - ORGANOMETALLIC CHEMISTRY

(4 Credits)

Course Outcome After completion of the full course the student should be able to:	**Cognitive Level**
C.O.1: Analyze the synthesis, structure, reactivity, and applications of main group organometallic compounds.	Analyze
C.O.2: IIlustrate the structure and properties of organometallic π complexes – metal-alkene complexes, and metal-alkyne complexes	Analyze
C.O.3: Analyze organometallic reaction in homogeneous Catalysis	Analyze
C.O.4: Evaluation of various types of metal ligand interactions	Evaluate
C.O.5: Evaluate the structure, bonding, and reactions of organometallic compounds and metal clusters and its applications	Application

UNIT I

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, and microwave assisted substitution.

UNIT II

General aspects of synthesis, structure, reactivity and applications of main group organometallic compounds. Metal complexes of NO, H_2, 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 III

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, C_5H_5 (ferrocene structure, bonding, and reactions), C_6H_6, C_7H_7 and C_8H_8, Polyalkyls, polyhydrides and f-block organometallic complexes, Fluxional organometallics.

UNIT IV

Organometallic reactions – Oxidative addition, Reductive elimination and Insertion reaction -Concerted Additions, SN_2 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 V

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, hydrocyanation of alkenes.

REFERENCES

1. B. D. Gupta, A. J. Elias, Basic Organometallic Chemistry - Concepts, Synthesis and Applications, 2nd, University Press, 2013.
2. R. H. Crabtree, The Organometallic Chemistry of the Transition Metals, 4th 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. 5th edition, John and Wiley, 1999.
5. R.S. Drago. Physical Methods in Inorganic Chemistry, 2nd edition, East Westpress, 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.
8. S. F. A. Kettle, Physical Inorganic Chemistry-A Co-ordination chemistry Approach, Spectrum Academy Publishers, 1996.
9. Purcell and Kotz, Inorganic Chemistry.
10. D. J. Shriver, P. W. Atkins, Inorganic Chemistry, 5th edition, Oxford university press,2010.

ACH3E02 - NANOMATERIALS & NANOTECHNOLOGY

(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 behavior.	Understand
C.O.2: Discuss the chemistry of various synthetic approach for the development of nano structures.	Understand
C.O.3: Understand the theory of analytical tools in nanoscience and apply them in the investigation of structure and physical properties of nanomaterials	Understand Application
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, energy, drug delivery and environmental applications.	Application

UNIT – I Introduction to Various Nanomaterials

Historical introduction, Bulk vs. nano size dependence on material properties, quantum mechanical explanation for the nanoscale behavior. Examples for nanoscale systems: metal nanoparticles, semiconductor quantum dots, nanowires and nanotubes, magnetic nanoparticles, Carbon nanostructures: fullerenes, carbon nanotubes, graphene etc., Nanoporous materials (meso and micro-porous materials), nanocomposites, gas phase clusters (water etc). micelles, bilayers, bio-inspired materials. Organic nanomaterials – examples – Rotaxanes and Catenanes

UNIT – II Nanomaterial Synthesis

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

UNIT – III Analytical Tools of Nanoscience

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 – IV Properties of Nanomaterials

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 – V Major Applications of Nanomaterials

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

REFERENCES

1. C.P. Poole Jr. & F.J. Owens; Introduction to Nanotechnology; Wiley India, New Delhi (2003).
2. T. Pradeep; NANO: The Essentials; Tata McGraw Hill, New Delhi (2007).
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: An Introduction to synthesis, properties and applications; WILEY VCH (2008).
7. K.K. Cathopadhyay & A.N. Banerjee; Introduction to Nanoscience and Technology; PHl Learning Pvt. Ltd. (2009).
8. G.A. Ozin, A. Arsenault and L. Cademartiri; Nanochemistry: A Chemical Approach to Nanomaterials; RSC Publishing (2008).
9. H. Gleiter; Nanostructured Materials: Basic Concepts, Microstructure and Properties; Elsevier, Acta Materialia (2000).
10. P. Sheng and Z. Tang (Ed); Nano Science and Technology Novel Structures and Phenomena; Routledge Taylor & Francis, New York (2003).
11. A. Nabok; Organic and Inorganic Nanostructures; Artech House, Boston (2005).
12. Edward A. Rietman; Molecular engineering of Nanosystems; Springer- Verlag, New York (2001).

ACH3E03 – ADVANCED ORGANIC CHEMISTRY

(4 Credits)

Course Outcome **After completion of the full course the students should be able to**	**Cognitive level**
C.O.1: Describe the various modern reactions in the toolset of synthetic chemists, understand unique features of the main group elements in various reactions, describe the vocabulary of retrosynthetic analysis, need and practice of total synthesis, structure and function of discussed biomolecules.	Understand
C.O.2: Classify important reactions and reagents based on their salient features, stereochemical models, describe advantages of new techniques, importance of environmental and economic considerations in synthesis, relevance of biological chemistry and applications of modern biochemical tools.	Understand
C.O.3: Predict the outcome including stereochemistry of given conversions, predict the suitable reagents and conditions for a given outcome, plan a total synthesis via stepwise disconnection of a complex target, identify compatible protection and deprotections in synthetic sequences.	Application
C. O. 4: Analyse and compare more than one synthetic approaches to the same target, contrast the environmental and economic aspects of different approaches, contrast synthetic chemistry with chemistry in living systems, attempt to design biomimetic methods for specific applications.	Analysis

UNIT – I Modern methods in organic synthesis

CH-functionalisation, Cascade and multicomponent reactions (Strecker, Mannich, Passerini and Ugi reactions), Click Chemistry, flow chemistry, boron-based aldol reactions (stereoselectivity, Zimmerman-Traxler TS), Modern organocatalysis (proline aldol and NHC-catalysis), chiral auxiliary (exemplified by Evans aldol), enzymatic resolution method.

UNIT – II B, S and Si in Organic Synthesis

Boron: Allyl and crotyl borons, Suzuki-Miyaura coupling. Sulfur: Sulfur stabilised anions, dithiaacetals, sulfur ylides, sulfoxide elimination and rearrangements, Pummerer rearrangement. Silicon: Uses of allyl, vinyl, aryl and alkynyl silanes. Formation and uses of silyl enol ethers. Fleming-Kumada oxidation.

UNIT – III Synthetic planning and strategy

Concept of retrosynthesis, disconnection approach, introduction to synthons and synthetic equivalent, types of transforms, functional group inter-conversions, classification of disconnections, reversal of polarity (umpolung of carbonyl- acyl anion equivalents), common building blocks, the importance of the order of events in organic synthesis.

UNIT – IV Protecting groups and total synthesis

Necessity and essential features of protecting groups. Methods of introducing and removing protecting groups for alcohols (benzyl, PMB, TMS, TBDMS and THP ethers), diols (acetonide), amino (Ac, Boc, Fmoc, Cbz), carboxyl (Me and t-butyl ester) and carbonyl (dimethyl acetal and 1,3-dithianes).

Total synthesis, semi and formal synthesis, overall yield, linear and convergent synthesis, biomimetic synthesis.

UNIT – V Proteins and Nucleic acids

Proteins: Primary, secondary and tertiary structure and function. Theories of enzyme activity. Active site and enzyme inhibition. Function and importance of receptors. **Nucleic acids**: Nucleosides, nucleotides and nitrogen bases. Structure and function of DNA and RNA. Ploymerase chain reaction and its uses.

REFERENCES

1. Organic Chemistry, J. Clayden, N. Geeves and S. Warren, Oxford University Press, 2012.
2. Organic Chemistry, Morrison, Boyd and Bhattcharjee, 7th Edition, Pearson, 2010.
3. Advanced Organic Chemistry, D. E. Lewis, Oxford University Press, 2016.
4. Organic Chemistry- Structure and Function, P. Vollhardt and N. E. Schore, W. H. Freeman and Co., 7th Ed., 2016.
5. Advanced Organic Chemistry, Part A and Part B: Reaction and Synthesis, Francis A. Carey, Richard
6. J. Sundberg, 5thed. Springer Verlag, **2012**.
7. Modern Methods of Organic Chemistry, W. Carruthers and Iain Coldham, 4th ed. Cambridge University Press, **2004**.
8. Advanced Organic Chemistry, Reactions, Mechanisms and Structure, J. March, 4th ed. John-wiley, 1999.
9. Organic Synthesis, Warren, S. Wiley, 1982.
10. Modern Organic Synthesis, House, H. O. Benjamin, W. A. Inc., New York, 1965.
11. The Logic of Chemical Synthesis, E. J. Corey and X.-M. Cheng, Wiley, 1995.
12. Natural products: Chemistry and Biological Significance, Mann, Davidson, Hobbs, Banthrope and Harborne, Longman, Essex.
13. Organic Chemistry, Vol. 2, I. L. Finar, ELBS

ACH3E04 - ADVANCED ELECTROCHEMISTRY

(4 Credits)

Course Outcome After completion of the full course the student should be able to	**Cognitive level**
C.O.1: Apply the concepts of ionics in electrochemistry in explaining the ionic interactions and properties of electrolytes.	Analysis
C.O.2: Explain electrode kinetics and apply the Nernst, Butler-Volmer and Tafel equations in describing the properties of electrochemical systems.	Application
C.O.3: Describe and apply various electrochemical methods such as: chronoamperometry, cyclic voltammetry, chronopotentiometry and coulometry, and describe how ac impedance and spectroelectrochemistry can be used to obtain information about electrochemical systems	Application
C.O.4: Describe various adsorption phenomena and apply the properties of colloidal systems and their applications	Application
C.O.5: Compare, contrast and evaluate the properties various electrochemical energy storage materials and systems such as super capacitors, batteries, fuel cells, etc.	Application
C.O.6: Explain the concept of electro catalysis and evaluate the properties of electro catalysts and photo electrochemical systems	Application

UNIT I – Ionics (14 hr)

Characteristics of ionics and electrodics, properties of materials and surfaces, Ionics: Ion-solvent interaction, structure of water, ion- dipole model and ion -solvent interaction, dielectric effects and dielectric constants of solution, ion- dipole model and ion-solvent interaction, Dielectric effects and dielectric constants of solution, ion -quadrupole model of ion – solvent interaction, Ion – ion interaction, Debye-Huckel ion cloud theory, Linearized Poisson – Boltzmann equation and its solution, Activity coefficient and ion – ion interaction, ion cloud and chemical potential change, activity, activity coefficient and ion -ion interaction, and ion -

solvent interaction, merits and demerits of Debye- Huckel theory of activity coefficient, Debye- Huckel Limiting Law.

Ionic diffusion under chemical potential gradient, Fick's law, diffusion coefficient, random walking model, Einstein- Smoluchowski's equation, ionic drift under electric field, quantitative link between electron flow and ion flow in electrolytes – Faraday's law, electric field and current density,, ionic migration, Einstein relation between absolute mobility and diffusion coefficient,, Nernst- Einstein relation, stoke's - Einstein relation, Interdependence of ionic drift, diffusion potential, Onsagar phenomenological equation, Debye – Huckel -Onsagar equation, Changes to Debye – Huckel – Onsagar equation.

UNIT II - Electrodics (14 hr)

Overview of reversible electrode processes, electrochemical cells and reactions, Faradaic and non - Faradaic processes, Nature of electrode - solution interface, ideal polarized electrode, capacitance and charge of an electrode, Electrical Double Layer and theories of EDL, thermodynamics of double layer, surface excess and electro capillary equation, Double layer capacitance and charging current, Faradaic process and factors affecting rates of electrode reaction, mass transfer controlled reactions – modes of mass transfer, Kinetics of electrode reaction, relation between reaction rate, current and potential, current - potential diagram, Butler -Volmer model of electrode kinetics, Polarization phenomena and over potential, Over potentials in electrolysis, Dependence of the Electrochemical Reaction Rate on Overpotential, Butler Volmer Equation & Tafel equation and Tafel plot. Solid state electrochemistry-Ion conducting polymers, electronically conducting polymers and redox polymers.

UNIT – III Electrochemical Techniques (12 hrs)

Electrochemical Techniques: Basic Potential step and potential sweep methods, Potentiometry, Voltammetry : Polarography, Pulse Voltammetry, Cyclic Voltammetry (detailed description), Anode Stripping Voltammetry, Hydrodynamic Voltammetry, Chronopotentiometry, Amperometry, Chrono amperometry , Coulommetry, Chrono coulometry, Spectroelectrochemistry. Electrochemical impedance and its application.

References

1. Bockris and Reddy - Modern Aspects and Electrochemistry vol. I and II, Academic Press. P.W. Atkins - Physical Chemistry, ELBS Oxford University Press.
2. Allen J Bard and Larry R Faijlkner, Electrochemical Methods – Fundamentals & Applications.
3. S. Glasstone - Introduction to Electrochemistry, Van Nonstrand
4. Skoog and West - Fundamentals of Analytical Chemistry.
5. Joseph Wang - Analytical Electrochemistry.

UNIT – IV Application of Electrochemical Science & Technology (12 hrs)

Super capacitors, Fuel cells, Sensors and Actuators:. Performance parameters of electrochemical sensors including selectivity, sensitivity, linearity, detection limit, repeatability, reproducibility, stability and variations Instrumentation used for electrochemical sensing including laboratory bench-top potentiostat and highly-integrated electrochemical sensing systems, Detailed description on supercapacitors: Similarities and differences between supercapacitors and batteries, ragone plot, Energetics, Double layer electrostatic capacitor, Pseudocapacitance, origin, kinetic theory, Classification of supercapacitors, Graphene as a material for electrochemical capacitors, electrolyte factor, energy density and power density, Impedance of a pseudocapacitance, Cyclic voltammetry of electrochemical double layer capacitors and pseudocapactors, Charge Discharge studies,Technology development, various oxides and conducting polymers as pseudocapacitors, electrochemo mechanical systems.

UNIT – V Electrocatalysis & Photo-electrochemistry (12 hrs)

Electro catalysis – Homogeneous & Heterogeneous electrocatalysts, Electro catalysis in simple redox reactions involving adsorbed species, Electronic and geometric factors in electrocatalysts, Discussion on the mechanisms of simple electrocatalytic reactions - Hydrogen evolution, Oxygen evolution and Oxygen reduction reactions .Photo electrochemistry – Photoelectrodes and charge transfer Processes, Photoreactions at Semiconductor electrodes, Electron transfer dynamics between excited molecules and semiconductor electrodes, Materials engineering of semiconductor electrodes: General considerations, Redox catalysis in photoelectrochemical solar energy conversion systems, Photoelectrochemical cells: Overview on the water splitting, CO_2 reduction and dinitrogen reduction reactions.

REFERENCES

1. Bard & Faulkner, Electrochemical Methods: Fundamentals and Applications 2 nd Ed
2. Brett & Brett, Electrochemistry: Principles, Methods and Applications, 1993,
3. V. S. Bagotsky, Fundamental of Electrochemistry, 2 nd Ed.
4. C. H. Hamann, A. Hamnett & W. Vielstich, Electrochemistry 2 nd Ed.
5. Semiconductor electrochemistry, Rudiger Memming, Wiley publishers, Germany
6. Photoelectrochemisry, photocatalysis and photoreactors, Mario Schiavello, Springer Science,Germany.
7. Semiconductor photoelectrochemistry, Yuri Pleskov & Yuri Gurevich, Consultants Bureau,NewYork.
8. Wolfgang Kaim & Axel Klein – Spectroelectrochemistry.
9. Robert James Gale – Spectroelectrochemistry.
10.Allen J Bard and Larry R Faulkner, Electrochemical Methods – Fundamentals &Applications.

ACH3E05 – ORBITAL INTERACTIONS IN CHEMISTRY

(4 Credits)

Course Outcome After completion of the full course the student should be able to	**Cognitive level**
C.O.1: examine the physical properties associated with molecules and the pathways taken by chemical reactions.	Analysis
C.O.2: qualitatively corelate the shape and energy of orbitals and the chemical reaction exhibited by any molecule.	Application
C.O.3: explore the effects of symmetry, overlap, and electronegativity in the molecular orbital in case of chemical reaction.	Analysis
C.O. 4: explore the structures and reactivity relationships associated with any molecule.	Application

UNIT - I **(12 hrs.)**

Atomic and Molecular Orbitals, Concepts of Bonding and Orbital Interaction, Orbital Interaction Energy, Molecular Orbital Coefficients, Electron Density Distribution, Perturbational Molecular Orbital Theory, Linear H_3, HF, and the Three-Orbital Problem.

UNIT – II **(12 hrs.)**

Molecular Orbital Construction from Fragment Orbitals, Triangular H3, Rectangular and Square Planar H4, Tetrahedral and Linear H4, Pentagonal H5 and Hexagonal H6, Molecular Orbitals of Diatomic Molecules and Electronegativity Perturbation, Geometrical Perturbation of Molecular orbitals, Molecular Orbitals of AH2, Walsh Diagrams, Jahn–Teller Distortions.

UNIT – III **(12 hrs.)**

Molecular Orbitals of Small Building Blocks, AH System, AH3 Systems, pi-Bonding Effects of Ligands, AH4 System, Molecules with Two Heavy Atoms, A2H6 Systems, Orbital Interactions through Space and through Bonds.

UNIT – IV **(12 hrs.)**

Polyenes and Conjugated Systems, Acyclic Polyenes, Hückel Theory, Cyclic Systems, Conjugation in Three Dimensions, Solids, Energy Bands, Hypervalent Molecules.

UNIT – V **(12 hrs.)**

Transition Metal Complexes. Octahedral ML_6, π-Effects in an Octahedron, Distortions from an Octahedral Geometry, Square Planar, Tetrahedral ML_4 Complexes, Five

Coordination, Square Pyramidal ML_5 Fragment, ML_3 Fragment, ML_2 and ML_4 Fragments, M_2L_8 Dimers, CpM and Cp_2M, Isolobal Analogy.

REFERENCES

1. T. A. Albright, J. K. Burdett, M.-H. Whangbo, Orbital Interactions in Chemistry, 2nd ed., John Wiley and Sons, Inc., Hoboken, New Jersey, 2013.
2. I. Flemming, Molecular Orbitals and Organic Chemical Reactions, Students ed., Wiley, 2009.
3. A. Rauk, Orbital Interaction Theory of Organic Chemistry, 2nd ed., Wiley-Blackwell, 2000.
4. W. L. Jorgensen, L. Salem, The Organic Chemist's Book of Orbitals, Academic Press, 1973.
5. Haaland, A. Molecules and Models: The Molecular Structures of Main Group Element Compounds, Oxford University Press, Oxford, New York, 2008.

ACH4PR01 - RESEARCH PROJECT

(8 Credits)

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

ACH4E06 - BIOORGANIC AND BIOCOORDINATION CHEMISTRY

(4 Credits)

Course Outcome **After completion of the full course the students should be able to**	**Cognitive level**
C.O.1: Give accounts of bonding models, stereochemistry, and reactions of coordination compounds, role of various metals and metal ions in biological processes, structure and function of biomolecules involved in metal-mediated processes, role of electron transfer reactions, chemical basis of life	Understand
C.O.2: Classify the key biological processes on the basis of type of chemistry involved, explain the formation of biomacromolecules from simple building blocks, role of enzymes and co-enzymes, biogenesis of natural secondary metabolites, chemical methods of structure determination of proteins.	Understand
C.O.3: Explain and rationalize biological processes in terms of the fundamental chemical transformations, compare and contrast reactivity of involved biomolecules by applying fundamental principles of structure and bonding in chemistry.	Application
C. O. 4: Analyse the transformations involved in life sustaining process, compare and contrast biochemical processes with lab reactions and regents, develop biomimetic process design capabilities, predict and design structural features that can interact effectively with biological targets.	Analysis

UNIT – 1 STABILITY AND REACTIVITY OF COORDINATION COMPOUNDS

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. Lability and inertness of the complexes, VB and MO explanations. Trans-effect, theories and applications of trans effect, the cis effect. Reactions of coordinated ligands: hydrolysis, acid dissociation, aldol condensation, transamination. Template effect and macrocyclization. Inner-sphere and outer-sphere electron transfer processes, significance in biological systems, effect of the nature of metal and ligand, bridging group effects. Metal-ligand redox reactions. Two electron transfer processes.

UNIT – II METALS IN BIOLOGICAL SYSTEM

Occurrence of metals in biological systems, crustal abundance and biological distribution, emergence of bioinorganic chemistry. Bulk-and trace metal ions. Co-ordination sites in biologically important ligands- water- proteins -nucleic acids. Metal protein interactions. Role of metal ions in biological functions. Biomineralization. Nonmetals in biological systems, biological role of some trace nonmetals. (B, Si, S, Se, As, CI, Br, I). Biological importance of nitric oxide. Biological metal ion complexation, transport of ions across biological membranes, active and passive transport, metal transport and metallochaperons, Na+/K+ pump, transport and structural role of Ca, electron transport in biology.

UNIT – III OXYGEN / METAL/ELECTRON MANAGEMENT PROTEINS

Porphyrins, oxygen transport by haeme proteins. Myoglobin and haemoglobin. Structure of the O2 binding site, nature of haeme-dioxygen binding, cooperativity. Hill plot. CO binding modes of haemoglobin, role of carbonic anhydrase. Hemerythrin, hemocyanin and hemovanadin. Storage and transport of metal ions-ferritin, transferring and siderophores. A brief idea on structure and function of cytochromes, iron-sulphur proteins, superoxide, dismutase. A brief idea on structure and function of copper proteins in electron transport process, tyrosinase. Lewis acid role of Zn(II) and Mn (II) containing enzymes, carbonic anhydrase, carboxy peptidase. Vitamin B12 and coenzymes. Chlorophyll, structural features, photo systems I and II. Nitrogen fixation – Nitrogenase, structure and functions.

UNIT – IV MOLECULES OF LIFE

Prebiotic chemistry, chemical origins of life, HCN and formaldehydes as building blocks of molecules of life, formation of purines and pyrimidines from HCN, formose reaction. Miller-Urey experiment, nucleic acids, structure, genetic information in DNA, Proteins, primary, secondary, tertiary and quaternary structures of peptides, Sanger's method and Edman degradation for peptide sequencing, enzymes, mechanism of peptide hydrolysis by chymotrypsin, fundamental aspects of structure and function of carbohydrates and lipids, phospholipid membranes.

UNIT – V REACTIONS IN LIVING SYSTEMS

Reduction and oxidation in biological systems, mechanism of NAD+ and NADH, pyridoxamine and pyridoxal in amino transfer and decarboxylation reactions, acetyl co-enzyme A and its enol-type chemistry in citric acid synthesis, polyketide synthesis, thiamine pyrophosphate and its reaction with pyruvic acid, biotin and its role in CO_2 transport.

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. 34 Page 35 of 66
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.
9. D. van Vranken, G. Weiss, Introduction to Bioorganic Chemistry and Chemical Biology, Garland Science, New York, 2013.
10. An Introduction to Medicinal Chemistry, 5th Edition, G. L. Patrick, Oxford University Press, 2013.
11. Organic Chemistry, J. Clayden, N. Geeves and S. Warren, Oxford University Press, 2012.
12. General Organic and Biological Chemistry: An integrated Approach, K. W. Raymond, Wiley, 2016.
13. Biochemistry- An Organic Chemistry based Approach, M. B. Smith, CRC Press, New York, 2020.

ACH4E07 – ESSENTIALS OF COMPUTATIONAL CHEMISTRY

(4 Credits)

Course Outcome After completion of the full course the students should be able to	**Cognitive level**
C.O.1: describe the basic concepts of the various theoretical models and methods.	Understand
C.O.2: classify the different basis sets used in the computational calculations.	Understand
C.O.3: calculate the geometry of a molecule, its IR and UV spectra, its thermodynamic and kinetic stability, and other information needed for the prediction of the reactivity.	Application
C. O. 4: analyse the results from molecular dynamics simulations	Analysis

UNIT – I **(12 hrs.)**

Scope of computational chemistry, Introduction to molecular mechanics and force fields, various potential energy terms, parameterization, potential energy surface universal force fields; comparison of popular force fields; performance of molecular mechanics, Molecular dynamics, - Fundamental molecular forces-the dynamic equation, the fundamental concepts of quantum mechanics - Schrödinger equation, Born-Oppenheimer approximation, potential energy surfaces, local and global minima, transition states, variational method, LCAO, Hartree-Fock theory, restricted HF calculations; open shell systems, ROHF and UHF calculations, Roothan–Hall equations, Koopmans theorem, HF limit and electron correlation,

UNIT – II **(12 hrs.)**

Basis sets, basis set approximation, Slater and Gaussian functions, contractions, polarization and diffuse functions, split-valence sets, classification of basis sets – minimal, double zeta, triple zeta, correlation-consistent sets, core-valence sets, general contractions, EMSL basis set exchange, Semi empirical methods, post Hartree-Fock Method, Configuration interaction, Many-body perturbation theory, Coupled-cluster theory, Nondynamical correlation and multiconfigurational self-consistent-field (MCSCF) theory, Density Functional Theory, Comparing the performance of electronic structure theories, Modeling of surface chemistry, Hybrid QM/MM

UNIT – III **(14 hrs.)**

Input of molecular structure, Z-matrix construction, single point energy calculations, geometry optimizations, Electronic Energy, Vibrational frequency analysis, symmetry analysis, zero-point vibrational energies (ZPVE's), distinguishing minima from transition states, Intrinsic reaction coordinate (IRC) analysis, transition barrier and activation energy, conformational energetics, reaction energetics, enthalpy of formation, bond dissociation energy, ionization energy, isomerization energy and barrier, potential energy surface, reaction mechanism, enthalpy, entropy and free energy changes for reactions, isodesmic reactions.

UNIT – IV **(14 hrs.)**

Analysis of gaussian output files, dipole moment, multipole moments, polarizability, hyperpolarizability, and molecular electrostatic potential, partial atomic charges, thermodynamic properties, atomic spin, ionization potentials, electron affinities, infrared spectra and NMR spectra, use of graphics programs like Chemcraft, Molden in analyzing Gaussian output data, identification and visualization of normal modes of vibration, calculation and interpretation molecular orbitals

UNIT – V **(12 hrs.)**

Molecular dynamics simulations, basic principles, ensembles, periodic boundary conditions, structure of input file, extracting information from simulations, free energy calculations, band gap, DOS for materials

REFERENCES

1. Cramer, C. J. Essentials of computational Chemistry: Theories and models, 2nd Ed., John Wiley & Sons, 2004.
2. Jensen, F. Introduction to Computational Chemistry, 3rd Ed., Wiley, New York, 2017.
3. Leach, A. R. Molecular Modelling Principles and Applications, 2nd Ed., Pearson Education Limited, 2001
4. Szabo, A. and Ostlund, N. S. Modern Quantum Chemistry, Introduction to Advanced Electronic 5. Structure Theory, 2nd Ed., Dover, 1996.
5. Mc Quarrie, D. A. Quantum Chemistry, 2nd Ed., University Science Books, 2007.
6. Levine, I. N. Quantum Chemistry, 7th Ed., Pearson, 2013.
7. Cotton, F. A. Chemical Applications of Group Theory, 3rd Ed., Wiley, New York, 1990.
8. Wilson, E. B., Decius, J. C. and Cross, P. C. Molecular Vibrations: The Theory of Infrared and Raman Vibrational Spectra, Dover, New York, 1980.

ACH4E08 – MEDICINAL CHEMISTRY

(4 Credits)

Course Outcome **After completion of the full course the students should be able to**	**Cognitive level**
C.O.1: Explain the basic principles of drug action, biological targets, drug binding, importance of design in drug development, classification and regulatory processes in drug marketing.	Understand
C.O.2: Describe in detail the importance of structure including conformation of biomolecules involved in drug binding, understand the non-covalent interactions involved in drug binding, various modes of drug action, theories of drug action, modern techniques in industry.	Understand
C.O.3: Rationalise the mechanism of drug binding and action in terms of fundamental chemical principles of involved molecules, analyse drug structures and correlate it with the activity, rationalise pharmacokinetic phenomena in terms of physical chemistry principles.	Application
C. O. 4: Analyse and predict suitable structures for binding to a given target, suggest potential modifications to improve desirable properties, identify targets suitable for given diseases, and foresee issues in physical properties, toxicity and regulatory affairs of drugs.	Analysis

UNIT - I Drug Targets

Introduction to medicinal chemistry, intermolecular binding forces, Introduction to various drug targets; **Proteins**- primary, secondary and tertiary structure, protein function, proteomics; **Enzymes**- catalytic role, active site, allosteric binding, feedback control, binding interactions, isozymes, co-factors; **Receptors**- types of receptors, their roles, neurotransmitters, hormones, receptor activation and regulation; **Nucleic acids**- DNA, primary and secondary structure of DNA, function of DNA, molecular biology and genetic engineering.

UNIT – II Drug-target binding

Introduction to Pharmacodynamics and pharmacokinetics (ADME), Enzymes as drug targets- types of enzyme inhibitors, medicinal use of enzyme inhibitors with examples; Receptors as drug targets- agonists, antagonists, allosteric modulators, partial agonists, inverse agonists, desensitization, tolerance and dependence, affinity and efficacy; Nucleic acids as drug targets-

Intercalating agents, topoisomersae poisons, alkylating/metallating agents, chain cutters, chain terminators, examples of medicinal use. Miscellaneous drug targets (tubulin)

UNIT – III Drug design and development

Development of new drugs, structure-activity relationship (SAR), factors affecting bioactivity, resonance, inductive effect, isosterism, bio-isosterism. Theories of drug activity, Quantitative structure activity relationship, Physico-chemical parameters: lipophilicity, partition coefficient, electronic ionization constants, steric factors, blood brain barrier (BBB) and its significance.

UNIT – IV Drug discovery

Choosing disease and target, hits and leads, sources and ideal features of lead compounds, importance of natural ligand of the target, in vitro and in vivo tests, high-throughput screening, libraries of synthetic compounds, combinatorial and parallel synthesis, computer-aided drug design (CADD), in silico methods, repurposing existing drugs, pro-drug approach and targeted drug delivery

UNIT – V Drug action and classification

Various types of drugs, systems of classification. Antibacterials- penicillins, cephalosporins and sulfonamides. Antiviral agents: RNA viruses DNA viruses, principle of vaccination. Anticancer agents: apoptosis and anti-oncogenes, angiogenesis, metastasis, antibodies, antibody-drug conjugates, photodynamic therapy. Drug abuse. Basics of regulatory processes.

REFERENCES

1. An Introduction to Medicinal Chemistry, 5th Edition, G. L. Patrick, Oxford University Press, 2013.
2. Wilson and Gisvold's Textbook of Organic Medicinal and Pharmaceutical Chemistry, Ed Robert F Dorge, 12th Edition, 2010.
3. An Introduction to Drug Design, 1st Edition, S. S. Pandeya and J. R. Dmmock, New Age International, 1999.
4. Burger's Medicinal Chemistry and Drug Discovery, Vol. 1, 7th Edition, Ed. M E Wolff, John Wiley, 2010.
5. Principles of Medicinal Chemistry by William Foye, 7th Edition, Ippincott Williams & Wilkins, Woltess Kluwer (India) Pvt.Ltd, New Delhi.

ACH4E09 - 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 diagramfor each one	Understand Analysis
C.O.4: Illustrate the crystal defects and predict the consequences	Application
C.O.3: Understand and apply the electrical, magnetic, optical, thermal, and mechanical properties of solids for developing new materials and devices.	Application
C.O.4: Design novel materials based by interpreting the kinetics and mechanism of solid-state reactions	Application
C.O.5: Understand and apply the knowledge on structure, preparation, and properties of new materials for their applications in energy, sensing and gas storage etc.	Application

UNIT – I Solid State - Structure & Theories (12 hrs)

Solid state structure: Types of solids, Symmetry in crystals, X-ray diffraction, common crystal structure motifs, quasi crystals.

Theories of Solid State: Overview of Free electron, Zone and Band Theories, MO approach of Band Theory. Classification of solids into Conductor, Semiconductors, and Insulators.

UNIT – II Defects and Non-Stoichiometry in Solids (12 hrs)

Point, Line and Plane defects; Intrinsic and extrinsic defects – Vacancies, Schottky and Frenkel defects – Charge compensation, non-stoichiometry, and defects – thermodynamic and Structural defects. Thermodynamics of Schottky and Frenkel defects formation, Edge and screw dislocation, Burgers vector, Plane defects, Large angle and small angle boundaries, Stalking fault.

UNIT – III Properties of Solids (12 hrs)

Electrical Properties: Electrical conductivity and Ohm's law, Conductivity in pure metals, Hall effect, Intrinsic and Extrinsic semiconductors, Hopping semiconductors, p-n juctions.
Dielectric properties of solids: Piezoelectricity and Ferroelectricity and their applications.
Superconductivity: Meissner effect – Type I and II superconductors, Basic concepts of BCS Theory, Josephson devices.

Magnetic Properties: Classification of magnetic materials, Langevin diamagnetism, Paramagnetism, Cooperative phenomena Ferro-, Antiferro-, and Ferri-magnetism, Magnetic domains and hysteresis, super paramagnetism.

Optical Properties: Optical reflectance, Plasmon Frequency, Photoconduction, Photo and Electroluminescence, Photovoltaic and Photoelectrochemical effects.
Thermal Properties: Thermal conductivity and Specific Heat
Mechanical Properties: Strength of real crystals as compared with an ideal crystal, different strengthening mechanisms.

UNIT – IV Materials: Growth & Synthesis (12 hrs)

Decomposition reactions of the typeA (solid) → B (solid) + C (gas). Process limiting the rate of solid-state reactions. Nucleation, Nucleus growth (brief discussion). Isothermal and non-isothermal decomposition reactions, kinetics analysis and elucidation of the mechanism of decomposition reactions (brief discussion).

Crystal growth: Mechanism of growth, Twinning, Recrystallization, Martensite transformation. Crystal growth techniques, and Zone refining

Transformations in Solids: Thermodynamic consideration, First order and Second order transitions, Order-disorder transitions, Phase rule – Iron – Carbon system, Kinetics of transformations: Homogeneous and Heterogeneous nucleation

UNIT – V New Materials and their Applications (12 hrs)

Microporous and Mesoporous Materials: Zeolites, metallosilicates, silicalites and related microporous materials: synthesis of Metallo phosphates/phosphonates, incorporation of heteroelements in microporous inorganic frameworks and their potential utilities. Mesoporous silica, metal oxides and related functionalized mesoporous materials: synthesis, characterizations and applications.

Covalent organic frameworks, porous organic polymers and related organic porous materials: sensing, adsorption and gas storage applications. Organic-Inorganic hybrid materials - metal organic frameworks.

Carbon Nanostructures: Fullerenes - Structure and Bonding- Nomenclature, Production and Purification, Properties, Hydrogenation and Halogenation, Nucleophilic Addition to Fullerenes. Carbon Nano Tubes: Structure, Nomenclature, Single-Walled and Multiwalled Carbon Nanotubes -Structure and properties. Spectroscopic Properties and applications of Carbon Nanotubes. Graphene: Structure and Preparation, graphene, Electronic Properties - Band Structure of Graphene, Spectroscopic Properties of graphene.

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 1964.
8. B.S. Skoog and D.M. West, Principles of Instrumental Analysis, Sanndes College, Philadelphia (1980).
9. Anke Krueger, Carbon Materials and Nanotechnology, Wiley-VCH , 2010.
10. Yury Gogotsi, Carbon Nanomaterials", Taylor and Francis, 2006.

ACH4E10 - 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 catalyst synthesis, zeolites, catalyst characterization and activity studies.	Analysis
C.O.3: Review industrial catalysis, new catalysts and different catalyst deactivation processes and catalyst regeneration	Comprehension
C.O. 4: Understand and Evaluate biocatalysis and phase transfer catalysis	Evaluation
C.O.5: Apply catalysts in various industrial processes	Application

UNIT – I Adsorption and Catalysis: Theories

Adsorption and catalysis – adsorption and reaction rate – strength of adsorption bond and catalysis – adsorption-physical, chemical activated and non activated chemisoroption, adsorption equilibrium and catalysis, potential energy level diagrams, Adsorption isotherms, Langmuir, BET and Freundlich.-applications, kinetics of heterogeneous catalysis: diffusion steps neglected – unimolecular reactions – bimolecular reactions – Langmuir-Hinshelwood and Eley-Rideal mechanism, kinetics of heterogeneous catalysis: diffusion controlling – mechanism of diffusion – diffusion and reaction in pores – selectivity and diffusion, electronic factors in catalysis by metals, electronic factors in catalysis by semiconductors, geometric factors and catalysis. Hysteresis and shapes of capillaries.

UNIT – II Catalyst: Preparation and physico-chemical characterization methods

Support materials. Preparation and structure of supports. Surface properties. Preparation of catalysts. Introduction of precursor compound. Pre-activation treatment. Activation process. Catalyst preparation methods such as precipitation, impregnation, sol gel, hydrothermal, pechini method etc. General methods of synthesis of zeolites. structures of some selected zeolites – zeolites A, X and Y, pentasils – ZSM-5, ZSM-11, shape selective catalysis by zeolites.

Surface area and porosity measurement – acid base property studies – Hammett indicator method and temperature programmed desorption of probe molecules.

X-ray diffraction study and FTIR spectral analysis of catalysts, Structure of surfaces-techniques for the study of surfaces-low energy electron diffraction, photoelectron spectroscopy-ESCA, Electron diffraction, scanning tunneling microscopy (STM), high resolution transmission electron microscopy (HRTEM),

UNIT – III Industrial catalysis, new catalysts, and catalyst deactivation

Development of Industrial catalysts – brief history. Catalytic performance, activity, turn over number, selectivity, catalyst life, stability, accessibility, mechanical strength.

Mesoporous materials, nanoparticles, super acid catalysts, metal oxides redox catalyst systems, nanocarbon catalysts, Metal organic frame works (MOF), Graphene, MXenes, Electrocatalysts and photocatalysts.

Deactivation of catalysts, classification of catalyst deactivation processes, poisoning of catalysts, coke formation on catalysts, metal deposition on catalysts, sintering of catalysts, Regeneration of deactivated catalysts, feasibility of regeneration, description of coke deposit and kinetics of regeneration.

UNIT – IV Biocatalysts and Phase Transfer Catalysts

Enzymes – an introduction to enzymes – enzymes as proteins – classification and nomenclature of enzymes – structure of enzymes – how enzymes work – effect on reaction rate – thermodynamic definitions – catalytic power and specificity of enzymes – optimization of weak interactions between enzyme and substrate in the transition state – binding energy, reaction specificity and catalysis

Basic concepts in phase transfer catalysis – phase transfer catalyzed reactions – basic steps of phase transfer catalysis – effect of reaction variables on transfer and intrinsic rates – outline of compounds used as phase transfer catalysts Use of quaternary salts. Macrocyclic and macrobicyclic ligands. PEG’s and related compounds. Use of dual phase transfer catalyst or co-catalyst in phase transfer systems. Separation and recovery of phase transfer catalysts. Insoluble phase transfer catalysts.

UNIT – V Industrial Catalysis and some relevant catalytic processes

Oil based chemistry; catalytic reforming; catalytic cracking; paraffin cracking; naphthenic cracking; aromatic hydrocarbon cracking; isomerization; hydrotreatment; hydrodesulphurization; hydrocracking; steam cracking; hydrocarbons from synthesis gas; Fisher-Tropsch process, Mobil process for conversion of methanol to gasoline hydrocarbons. Catalysis for environmental protection, removal of pollutants from exhausts, mobile and static sources.

Catalysis by organaometallics – Monsanto process, Oxo process, Ziegler Natta reaction, Oxidation and ammoxidation catalysts, alkylation catalysts.

REFERENCES

1. R.J. Farrauto and C.H. Bartholomew, Fundamentals of Industrial Catalytic Processes, Blackie Academic and Professional – Chapman and Hall, 1997.
2. R. Pearce and W.R. Patterson, Catalysis and chemical processes, Academic press, Leonard Hill, London, 1981.
3. Clark, Theory of adsorption and catalysis, Academic Press, 1970.
4. J.M. Thomas & W.J. Thomas, Introduction to principles of heterogeneous catalysis, Academic Press, New York, 1967.
5. R.H.P. Gasser, An introduction to chemisorption and catalysis by metals, Oxford, 1985.
6.D.K Chakraborthy, Adsorption and catalysis by solids, Wiley Eastern Ltd.1990.
7. J.R. Anderson and M. Boudart (Eds), Catalysis, Science and Technology, Vol 6, Springer-Verlag, Berlin Heildberg, 1984.
8.R. Szostak, Molecular sieves: principles of synthesis and identification, Van Nostrand, NY, 1989.
9.R. Hughes, Deactivation of catalysts, Academic press, London, 1984.
10. C.M. Starks, C.L. Liotta and M. Halpern, Phase Transfer Catalysis – fundamentals, applications and industrial perspectives, Chapman & Hall, New York, 1994.
11. A.L. Lehninger, Principles of Biochemistry, Worth Publishers, USA, 1987.

ACH4E11 – 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

UNIT – I Structure, Properties and Characterization 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, 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 - 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, gel point-experimental, observation, Ring opening 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 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 – V 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.

QUESTION PAPER PATTERN

Duration : 3 hrs

Max. Marks : 50

SECTION A

Answer all questions. Each question carries 1 mark (10 ×1 = 10 marks)

SECTION B

Answer all questions. Each question carries 2 marks (5 ×2= 10 marks)

SECTION C (5 out of 8)

Answer any five questions. Each question carries 3 marks (5 ×3= 15 marks)

SECTION D (3 out of 5)

Answer any three questions. Each question carries 5 marks (3 ×5= 15 marks)

FIRST SEMESTER P.G. EXAMINATION NOVEMBER 2022
M.Sc. APPLIED CHEMISTRY (CCSS)

(2022 Admission)

ACH1C04 PHYSICAL CHEMISTRY I

SECTION A

*Answer **all** questions. Each question carries 1 mark*

Time: 3 Hours   Maximum Marks: 50 Marks

1. The two parameters that do not change while mixing two ideal gases are ……..
2. Onsager reciprocal relation states that ……….
3. The parameters that influence fugacity coefficient are ………
4. Write the linear phenomenological relation in matter flow, and specify the terms
5. Mean ionic activity of a 1:1 electrolyte is………..
6. What is the physical significance of Debye length
7. How does the free energy and electrode potential are related?
8. Concentration dependence of electrode potential is given by:
   a) Nernst equation   b) Tafel equation   c) Gibbs-Duhem equation   d) None of the above
9. Which of the following is the diffuse model of electrical double layer:
   a) Helmholtz model b) Stern model c) Gouy-Chapman model d) None of the above
10. What is E° for the following balanced reaction?
    Zn(s) + Pb2+(aq) → Zn2+(aq) + Pb(s)
    Zn2+(aq) + 2e– → Zn(s) –0.763
    Pb2+(aq) + 2e– → Pb(s) –0.126

(10 ×1 = 10 marks)

SECTION B

*Answer **all** questions.*

Each question carries 2 marks

11. Give the significance of Duhem Margule’s equation.
12. How does the concept of local equilibrium fit in non-equilibrium systems?
13. Evaluate the ionic strength of the electrolyte solution containing 0.1M Aluminium sulphate in 1M sulphuric acid?
14. Differentiate outer potential, inner potential and surface potential.

15. Exemplify concentration polarization? Give its significance?

(5 ×2= 10 marks)

SECTION C

*Answer **any five** questions.*

Each question carries 3 marks

16. Predict how temperature and pressure influence chemical potential.
17. Illustrate that if the solvent obeys Raoult's law, solute will obey Henry's law.
18. Prove the positive entropy production in a closed system with heat flow.
19. Explain how Lewis Randall rule is used to determine the fugacity of a gas in a mixture?
20. Evaluate the thickness of ion atmosphere of 0.01M $CaCl_2$ in water at 25 ^oC. Dielectric constant of water is 78.5
21. Illustrate DHL expression? - Construct the qualitative and quantitative test for DHL?
22. Explain concentration cells? – Derive the expression for the EMF of concentration cells without transference
23. Explain what is meant by electrical double layer ? Explain different models of electrical double layer.

(5 ×3= 15 marks)

SECTION D

*Answer any **three** questions.*

Each question carries 5 marks

24. Demonstrate the Jacobians method of relating thermodynamic partial derivatives.
25. Discuss how Onsager reciprocal law relates electrokinetic properties. electroosmosis.
26. (a) Figure out the mechanism of electrolytic conductance?

    (b)Compare the dispersion of conductance at high frequencies and potential gradient?

27. Discuss theory and applications of polarography.

28. Outline the working of $H_2 - O_2$ fuel cell - Explain the two most significant challenges of Fuel Cells

(3 ×5= 15 marks)

FIRST SEMESTER P.G. EXAMINATION NOVEMBER 2022
M.Sc. APPLIED CHEMISTRY (CCSS)

(2022 Admission)

ACH1C01 GROUP THEORY & QUANTUM CHEMISTRY

Time 3 Hours **Marks 50**

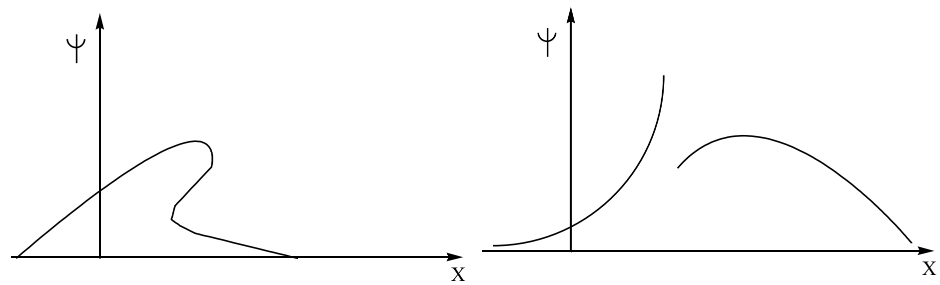
SECTION A

Answer ALL questions. Each question carries 1 mark

1. Evaluate $d/dx[\sin(ax)]$.

2. Show that $\hat{L}_x$ satisfy those characteristics of a quantum mechanical operators.

3. Identify the acceptable and not acceptable wave functions in the below plot.



4. Find the ground state term of C.

5. The wave function of a rigid rotor is $\Psi(\varphi) = Ae^{im\varphi}$, where m is a quantum number. Evaluate A.

6. The correct point group of 1,1-dichloroethylene is
(A) C_{2h} (B) D_{2h} (C) C_{2V} (D) D_{2d}

7. The transition that belongs to the Lyman series in the hydrogen–atom spectrum is ______________________

8. Point group of allene is ________________

9. Improper rotation is rotation about a C_n axis followed by
(A) Rotation about a vertical plane (B) reflection about a horizontal plane (C) inversion (D) inversion and reflection

10. The total number of irreducible representations is equal to
(A) number of classes (B) order of the group (C) 3N-6 (D) 3N-5

(1 × 10 = 10)

SECTION B

Answer ALL questions. Each question carries 2 marks

11. Describe an infinite group with an example.

12. Calculate the probability that a particle in a one-dimensional box of length L is found to be between 0 and L/2.

13. An electron confined in an infinite square well of width 10×10^{-15} m. Calculate the wavelength of the emission when it undergoes a transition from the first excited to the ground state.

14. Write down the various symmetry elements for the T_d point group.

15. Polynomial is the only acceptable solution for the simple harmonic oscillator and not infinite series. Explain.

(2 × 5 = 10)

SECTION C

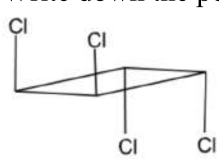
Answer ANY FIVE questions. Each question carries 3 marks

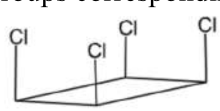
16. The ionization energy of hydrogen atom is 13.59 eV. What will be the ionization energy of Be^{3+} ?

17. Find the degeneracy of the sixth energy level, E_6, for a particle in a cubic box.

18. Show that for a nondegenerate system, the eigenfunctions of Hermitian operators are orthogonal.

19. Write down the point groups corresponding to the following molecules



and


20. Treating the π-electrons in butadiene as particles moving in a one-dimensional box, calculate the lowest absorption frequency (in cm-1) and the wavelength (in nm) of absorbed light. What is the total ground state energy of the molecule? Given, C–C single and C=C double bond length are 1.54 and 1.35 Å respectively.

21. What is a Group Multiplication Table. Write down the Group Multiplication Table for a C_{2V} group.

22. Prove that the three σ_v planes in C_{3V} point group belong to a class.

23. Discuss how can you find out the translational energies of H^+-ion.

(3 × 5 = 15)

SECTION D

Answer ANY THREE questions. Each question carries 5 marks

24. Identify the atomic orbital of H-atom associated with the function $\frac{\sqrt{2}}{81\sqrt{\pi}}\left(\frac{Z}{a_0}\right)^{3/2}\left(\frac{6Z}{a_0}r - \frac{Z^2}{a_0^2}r^2\right)e^{-\frac{Z}{3a_0}r}\cos\theta$. Identify number of nodes and draw the plots of radial distribution function and angular probability distribution function of the same.

25. Evaluate the energy expression for a particle in a square well, in which the particle is confined to a rectangular surface with dimensions L_1 and L_2.

26. Prove that $[\hat{L}_x, \hat{L}_y] = i\hbar\hat{L}_z$.

27. Show that the spherical harmonics for $l = 1$, $m = 0$ is eigenfunction of $\hat{H}$ and $\widehat{L_z}$.

28. State and explain Great Orthogonality Theorem. Write down some of the important rules that originates from this theory.

(5 × 3 = 15)

Syllabus 2022 Admission onwards
M.Sc. APPLIED CHEMISTRY (Choice based credit semester system)
CO and PSO Mapping

		P.S.O. 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	P.S.O. 2: Explain and correlate the structure -property relationship of materials based on principles of Chemistry	P.S.O. 3: Design and perform the chemical synthesis and characterise the products, execute experimental routines for detection and quantification of chemical entities	P.S.O. 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	P.S.O. 5: Demonstrate the basic principles of instrumental methods of analysis and the operation of advanced instruments to execute in-depth analysis of chemical problems	P.S.O. 6: Employ the acquired time management skills in planning and executing experiments and to recognize importance of ethical and cultural values	P.S.O. 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
Semester – I	ACH1C01 Quantum Chemistry and Group Theory	**5**	**5**					**5**
	ACH1C02 Inorganic Chemistry I	**5**	**5**					**5**
	ACH1C03 Organic Chemistry I	**4**	**4**					**4**
	ACH1C04 Physical Chemistry I	**5**	**5**					**5**
	ACH1C05 Analytical Chemistry	**5**	**5**	**5**		**5**	**1**	**5**
	ACH1P01 Inorganic Chemistry – Practical I			**5**	**5**			**5**
	ACH1P02 Organic Chemistry – Practical I			**4**	**4**			**4**
	ACH1P03 Physical Chemistry – Practical I			**3**	**3**			**3**
	ACH1A01 Ability Enhancement Course	**1**				**4**		**4**
Semester – II	ACH2C06 Chemical Bonding and Chemical Application of Group Theory	**4**	**4**					**4**
	ACH2C07 Inorganic Chemistry II	**5**	**5**				**1**	**5**
	ACH2C08 Organic Chemistry II	**4**	**4**					**4**
	ACH2C09 Physical Chemistry II	**5**	**5**					**5**
	ACH2C10 Molecular Spectroscopy & Photochemistry	**5**	**5**					**5**
	ACH2P04 Inorganic Chemistry – Practical II			**5**	**5**	**2**	**5**	**5**
	ACH2P05 Organic Chemistry – Practical II			**4**	**2**	**3**	**4**	**4**
	ACH2P06 Physical Chemistry – Practical II			**4**	**3**	**3**	**4**	**4**
	ACH2A02 Professional Competancy Course (PCC)	**4**				**1**	**7**	**7**
Semester – III	ACH3C11 Inorganic Chemistry III	**5**	**5**			**2**		**5**
	ACH3C12 Organic Chemistry III	**4**	**4**			**2**		**4**
	ACH3C13 Physical Chemistry III	**6**	**6**					**6**
	ACH3C14 Instrumental Methods - Theory and Instrumentation	**5**	**5**			**5**		**5**
	ACH3P07 Instrumental methods of Chemical Analysis – Practical			**5**	**5**	**5**		**5**
	ACH3E01 Organometallic Chemistry	**5**	**5**					**5**
	ACH3E02 Nanomaterials & Nanotechnology	**5**	**5**					**5**
	ACH3E03 Advanced Organic Chemistry	**4**	**4**			**1**		**5**
	ACH3E04 Advanced Electrochemistry	**6**	**6**			**1**		**6**
	ACH3E05 Orbital Interactions in Chemistry	**4**	**4**					**4**
Semester – IV	ACH4PR01 Research Project						**2**	**2**
	ACH4E06 Bioorganic and Biocoordination Chemistry	**4**	**4**					**4**
	ACH4E07 Essentials of Computational Chemistry	**4**	**4**					**4**
	ACH4E08 Medicinal Chemistry	**4**	**4**					**4**
	ACH4E09 Solid State Chemistry	**5**	**5**					**5**
	ACH4E10 Industrial Catalysis	**5**	**5**					**5**
	ACH4E11 Chemistry of Polymers	**5**	**5**		**4**			**5**