Semester Syllabus
for
M. Sc. in Applied Chemistry

(with effect from the session 2017-18)

SCHOOL OF CHEMISTRY (AUTONOMOUS)
SAMBALPUR UNIVERSITY
Jyoti Vihar, Burla - 768 019

Semester Syllabus for M. Sc. in Applied Chemistry
(With effect from the session 2017-18)

FIRST SEMESTER

Course No	Course Title	Credit	Mark
ACH-401	GROUP THEORY AND SOLID STATE CHEMISTRY	03	50
ACH -402	TRANSITION METAL CHEMISTRY	03	50
ACH -403	STRUCTURE AND REACTIVITY	03	50
ACH -404	STEREOCHEMISTRY	03	50
ACH -405	THERMODYNAMICS	03	50
ACH -406	DYNAMICS	03	50
ACH -407	INORGANIC PRACTICAL	02	50
ACH -408	PHYSICAL PRACTICAL	02	50
	Total	**22**	**400**

SECOND SEMESTER

Course No	Course Title	Credit	Mark
ACH -411	METAL π-COMPLEXES AND CLUSTERS	03	50
ACH -412	BIOINORGANIC CHEMISTRY	03	50
ACH -413	ORGANIC REACTION MECHANISM - I	03	50
ACH -414	ORGANIC REACTION MECHANISM - II	03	50
ACH -415	STATISTICAL THERMODYNAMICS & HMO THEORY	03	50
ACH -416	SURFACE CHEMISTRY	03	50
ACH -417	ORGANIC PRACTICAL	02	50
ACH -418	ANALYTICAL PRACTICAL	02	50
	Total	**22**	**400**

THIRD SEMESTER

Course No	Course Title	Credit	Mark
ACH -501	INSTRUMENTAL METHODS OF ANALYSIS	03	50
ACH -502	INDUSTRIAL POLLUTION & ITS MANAGEMENT	02	50
ACH -503	INDUSTRIAL POLICY & ENTREPRENEURSHIP	02	50
ACH -504	PROJECT	16	100
	Total	**23**	**250**

FOURTH SEMESTER

Course No	Course Title	Credit	Mark
ACH -511	COMPUTER APPLICATION IN CHEMISTRY	02	50
ACH -512	ENERGY & MATERIAL BALANCE AND NANOMATERIALS	03	50
ACH -513	INDUSTRIAL PROCESSES	03	50
ACH -514	MEDICINAL CHEMISTRY	03	50
ACH -515	SURFACTANTS AND DETERGENTS	03	50
ACH -516	PRACTICAL ON COMPUTER IN CHEMISTRY	03	50
ACH -517	INDUSTRIAL PRACTICAL	02	50
ACH -518	REVIEW	02	50
ACH -519	SEMINAR	02	50
	Total	**23**	**450**

FIRST SEMESTER

ACH-401: GROUP THEORY & SOLID STATE CHEMISTRY 3 credits

UNIT-I: Symmetry and Group Theory

Symmetry operation, symmetry element, classification of symmetry elements, definition of group, subgroup, cyclic groups, molecular point groups, platonic solids, group multiplication table, group generators, conjugacy relation and classes, matrix representation of symmetry elements, character of a representation, reducible and irreducible representation, the great orthogonality theorem (without proof) and its explanation, properties of irreducible representation.

UNIT-II: Symmetry and Spectroscopy

Character table (explanation and significance), construction of character tables for C_{2v}, C_{3v}, C_{4v} and D_4 point groups, direct product, the standard reduction formula, Applications of group theoretical methods for selection rules in Infrared, Raman and electronic spectroscopy.

UNIT-III: Solid State Chemistry

General idea of crystal lattice, unit cell, classification of crystals, crystal planes, Miller indices, Bragg's law and applications, determination of cubic crystal structure from systematic absences in diffraction pattern, perfect and imperfect crystals, point defects, Schottky defects and Frenkel defects, thermodynamics of Schottky and Frenkel defects, bonding in ionic solids, colour centers, non-stoichiometry defects, general idea of band theory of solids.

BOOKS:

1. *Chemical Applications of Group Theory by F. A. Cotton, Wiley India (P) Ltd., 3rd edn, 2009, New Delhi.*
2. *Symmetry and Spectroscopy of Molecules by K. V. Ready, New Age International Ltd. 2nd edn, 2009, New Delhi.*
3. *Symmetry and Group Theory in Chemistry by R. Ameta, New Age International Ltd., 1st edn, 2013, New Delhi.*
4. *Solid State Chemistry by D. K. Chakravarty, New Age International Limited, 1996, New Delhi.*
5. *Solid State Chemistry and its Applications by A.R. West, Wiley, 1989, 2nd edition, Singapore.*
6. *Principles of the Solid State by H.V. Keer, Wiley Eastern. Limited, 1993, New Delhi.*

ACH-402: TRANSTION METAL CHEMISTRY 3 credits

UNIT-I Theories of Metal-Ligand Bonding

Crystal field theory (CFT): Splitting of d-orbital under the influence of octahedral, tetrahedral, tetragonal, square planar, trigonal bipyramidal and square pyramidal fields, Streochemical and thermodynamic effect of CF splitting, CFSE and Jahn-Teller effect.

Molecular orbital theory (MOT): Sigma bonding in octahedral complexes: Classification of metal valence orbitals into sigma symmetry, formation of ligand group orbitals (LGOs) of sigma symmetry, Formation of molecular orbitals of sigma symmetry, construction of molecular orbital energy level diagram involving only sigma bond contribution from ligands, pi bonding in octahedral complexes, Classification of metal valence orbital into pi symmetry, Formation of LGOs of pi symmetry. Formation of pi MOs and construction of molecular orbital energy level diagram involving sigma and pi contribution from pi donor ligands, Sigma and pi bonding in tetrahedral complexes.

Ligand field theory (LFT) and adjusted crystal field theory (ACFT).

UNIT-II ***Complex Equilibria and Term Diagram***

Complex Equilibria: Types of complex equilibria in solution and types of complex equilibrium constant (stability constant), The complex formation functions, Determination of stability constant by spectrophotometric method and pH titration method, Stabilization of unusual oxidation state.

Term Diagram: Russell-Saunders or L-S coupling scheme, Term symbols and their derivation by Pigeon-Hole diagram especially for p^n and d^n configuration, Inter-electron repulsion parameters and spin-orbit coupling parameters, The effect of weak crystal field on S, P, D, F, G, H and I terms, Orgel diagram for d^1 to d^9 configuration, Term interaction and the energies of the levels.

Correlation diagram: Strong field configuration of O_h symmetry, the method of descending symmetry, correlation diagram for d^2 and d^3-confuguration, Tanabe-Sugano diagram (qualitative explanation and significance).

Unit-III ***Electronic Spectral and Magnetic Properties of Metal Complexes***

Electronic spectral properties of metal complexes: Introduction, types of experimental recording of the spectra, selection rules (mechanism of electronic transition, orbital selection rule, Laporte rule or purity selection rules, spin selection rule), Relaxation of selection rules (departure from cubic symmetry d-p mixing vibronic coupling), Nature of electronic spectral bands with respect to band intensity and bandwidth, Classification of electronic spectra. Ligand field spectra of octahedral and tetrahedral complexes and evaluation of Dq, B' and beta(β) parameters for the complex with T_1 ground state and A_2 ground state, Spectrochemical and nephlelauxetic series, charge transfer spectra.

Magnetic properties of metal complexes: Origin of magnetic behavior, concept of magnetic susceptibility, dia, para, ferro and antiferro magnetism, magnetic moments from multiple width cases, quenching of orbital magnetic moment by crystal field, spin-orbit coupling and anomalies magnetic moments, Spin-crossover in coordination compounds.

BOOKS:

1. *Theoretical Inorganic Chemistry by M. C. Day and J. Selbin*
2. *Advanced Inorganic Chemistry by F. A. Cotton and G. Wilkinson*
3. *Introduction to Ligand Field by B. N. Figgs*

ACH-403: STRUCTURE AND REACTIVITY 3 credits

UNIT-I: ***Nature of Bonding in Organic Molecules***

Delocalized chemical bonding, Conjugation, Cross conjugation, Resonance, Hyperconjugation, Bonding in fullerenes, Tautomerism. Aromaticity in benzenoid and non-benzenoid compounds, Alternant and non-alternant hydrocarbons, Huckel's rule, energy levels of pi-molecular orbitals of simple systems, Annulenes, Anti-aromaticity, Homo-aromaticity, Bonds weaker than covalent-addition compounds.

UNIT-II: ***Reaction Mechanism: Structure and Reactivity***

Types of mechanisms, Types of reactions, Thermodynamic and kinetic requirements, Kinetic and thermodynamic control, Hammond's postulate, Potential energy diagrams, Transition states and intermediates, Methods of determining mechanisms, Hard and soft acids and bases,

Effect of structure on reactivity: Resonance and field effects, Steric effect, Quantitative treatment, The Hammett equation and linear free energy relationship, Substituent and reaction constants, Taft equation.

UNIT-III: Reagents in Organic Synthesis

Gilman's reagent, Lithium dimethyl cuprate, Lithium diisopropyl amide, DCC, 1,3-Dithiane, Trimethyl sillyl iodide, Tri-n-butyl tin hydride, Osmium tetroxide, Selenium dioxide, Phase transfer catalysis (Crown ether, Merrifield resin, Wilkinson's catalyst), Dichloro dicyano benzoquinone (DDQ).

BOOKS:

1. *Advanced Organic Chemistry: Reaction Mechanism and Structure by Jerry March (Wiley Eastern Limited)*
2. *Physical Basis of Organic Chemistry by N. Isaac (Wiley Eastern Limited)*
3. *Mechanism and Theory in Organic Chemistry by Lowry and Richardson (Harper Row Publishers, New York)*
4. *Organic Chemistry by Morrison and Boyd*

ACH-404: STEREOCHEMISTRY 3 credits

UNIT-I: Chirality, Fischer projection and R and S notations, Threo and erythro nomenclature, E and Z nomenclature, Optical isomerism in biphenyls and allenes, Concept of Pro-stereoisomerism and Asymmetric synthesis (including enzymatic and catalytic nexus), Conformation of a few acyclic molecules (alkanes, haloalkanes), Conformation of cyclic systems having one and two sp2 carbon atoms.

UNIT-II: Dynamic stereochemistry: Conformation and reactivity, Selection of substrates, Quantitative correlation between conformation and reactivity, (Weinstein-Eliel equations and Curtin-Hammett principles), Conformational effects on stability and reactivity in acyclic compounds (ionic elimination, intramolecular rearrangements, NGP) and in cyclic systems, (Nucleophilic substitution reaction at ring carbon, Formation and Cleavage of epoxide rings, Addition reactions to double bonds, Elimination reactions).

UNIT-III: Molecular dissymmetry and chiroptical properties, Linearly and circularly polarised lights, Circular birefringence and circular dicroism, ORD, Plane curves, Cotton effect, Rotatory Dispersion of ketones, Axial haloketone rule, the Octane rule. Helicity rule.

BOOKS:

1. *Stereochemistry of Organic Compounds by D. Nashipuri.*
2. *Stereochemistry by Kalsi*
3. *Stereochemistry by Elliel*

ACHP-405 THERMODYNAMICS 3 credits

UNIT-I: Classical Thermodynamics

Brief resume of the concepts of laws of thermodynamics, Free energy, chemical potential and entropy, Third law of thermodynamics and determination of entropy, Entropy and probability, Boltzmann-Planck equation, Partial molar properties (partial free energy, molar volume and molar heat content), Their significance and determination. Concept of fugacity and its determination.

UNIT-II Thermodynamics of Living Systems

Bioenergetics and thermodynamics, Phosphate group transfer and ATP, Biological oxidation-reduction reactions.

UNIT-III Non-Equilibrium Thermodynamics

Microscopic reversibility, Entropy productions and irreversible process, Different types of forces and fluxes, Steady states & Cross phenomena, Phenomenological equations, Onsager reciprocity theorem, Chemical Reactions.

BOOKS:

1. *Text Book of Physical Chemistry (Vol-1-4) by K.L. Kapoor*
2. *Physical Chemistry by D.N. Bajpai*
3. *Principles of Physical Chemistry by Puri, Sharma & Pathania*
4. *Physical Chemistry by Atkins*
5. *Physical Chemistry Through Problems by Dogra & Dogra*
6. *Chemical Thermodynamics by Rastogi & Mishra*
7. *Thermodynamics for Chemists by S. Glasstone*

8. *Molecular Thermodynamics by McQuarrir & Simon*
9. *Principle of Biochemistry by A.L. Lehninger*

ACH-406: DYNAMICS 3 credits

UNIT-I: Chemical Kinetics

Theories of reaction rates, Collision theory, Transition state theory, Arrehenius equation and the activated complex theory, Reaction between ions, Salt effect, Steady-State Kinetics, Kinetic and Thermodynamic concept of Reactions, Treatment of unimolecular reaction (Lindemann-Hinshelwood and Rice-Ramspeger-Kassel-Marcus (RRKM) theories), Dynamic chain (H_2 + Br_2 reaction, pyrolysis of CH_3CHO, Decomposition of ethane).

UNIT-II: Catalytic & Fast Reaction

Kinetics of Catalytic Reactions: Acid-base Catalysis, Enzyme Catalysis, Homogeneous & Heterogeneous Catalysis.

Fast reactions: General feature, Study of Fast reactions by relaxation, Stopped flow and Flash photolysis.

UNIT-III: Electrochemistry

Interionic attraction theory and Debye-Huckel treatment, Derivation of Onsager limiting law and its verification and modification, Activities, activity coefficients, Debye-Huckel treatment, Debye-Huckel-Bronsted equation, Salt effect, Determination of activity coefficients from solubility method, Ion association, Determination of thermodynamic dissociation constant of weak electrolytes by Shedlovsky method and by EMF method, Nernst equation, redox systems, electrochemical cells.

BOOKS:

1. *Text Book of Physical Chemistry (Vol-1-4) by K.L. Kapoor*
2. *Physical Chemistry by D.N. Bajpai*
3. *Principles of Physical Chemistry by Puri, Sharma & Pathania*
4. *Physical Chemistry by Atkins*
5. *Physical Chemistry Through Problems by Dogra & Dogra*
6. *Electrochemistry by S. Glasstone*
7. *Modern Electrochemistry (Vol-I) by Bookris & Reddy*
8. *Chemical Kinetics by K.J. Laidler*
9. *Reaction Kinetics by Pilling & Seakins*

ACH-407: INORGANIC PRACTICAL 2 credits

1. Inorganic salt mixture analysis

   Inorganic salt mixture analysis containing not more than four radicals. The mixture will include rare earth metal anions like Tungstate, Vanadate and Molybdate. Insoluble matters and other interfering radicals will also be included. Organic radicals are excluded
2. Estimation metal ions via volumetric analysis
   a) Estimation of Ca and Mg ions in a given a sample of cement by EDTA method.
   b) Estimation of Cu ion in a given a sample of brass by iodometry method.

BOOKS:

1. *Vogel's Qualitative Inorganic Analysis, 7th edition; Revised by G. Svehla.*
2. *Vogel's Text Book of Quantitative Chemical Analysis, 5th Revised by G. H. Jeffery, J. Bassett, J. Mendham and R. C. Denny.*
3. *Advanced Practical Inorganic Chemistry, 22nd edition; By Gurdeep Raj*

ACH-408: PHYSICAL PRACTICAL **2 credits**

1. Determination of ionization constants of weak acids and verification of Oswald's Dilution law.
2. Conductometric titration of Strong/Weak acid with Stron/Weak base
3. Conductometric titration of a mixture of $HCl+CH_3COOH$ with NaOH
4. Potentiometric titration of strong acid with strong base.
5. Verification of Beer's Lambert Law and unknown concentration determination.
6. Verification of additivity rule spectrophotometrically.
7. Determination of temperature coefficient and energy of activation of hydrolysis of ethyl acetate.
8. To study the complex formation between ammonia and Cu^{+2}.
9. Determination of unknown dextrose solution by polarimetry
10. Study of inversion of cane sugar in acid medium by polarimetry.

BOOKS:

1. *Experimental Physical Chemistry by Das and Behera*
2. *Practical Physical Chemistry by B. Vishwanathan & P.S. Raghavan*
3. *Experimental Physical Chemistry by V.D. Athawale*

SECOND SEMESTER

ACH-411: METAL π-COMPLEXES AND CLUSTERS 3 credit

UNIT-I ***Carbon Monooxide Complexes***

Metal carbonyls, structure and bonding, vibrational spectra of metal carbonyls for bonding and structural elucidation, important reaction of metal carbonyls, carbonylate anions and carbonylate hydride, carbonyl halides and related compounds. Nature of M-C bond in carbonyls.

UNIT-II ***Complex of Carbon Monoxide Analogs***

Preparation, bonding and important reaction of transition metal complexes with isocyanide, cyanide, dinitrogen, carbon disulphide and nitrogen monoxides.

Transition metal to carbon multiple bonded: Compounds chemistry of carbenes, carbynes.

UNIT-III ***Metal Cluster and Polyacids***

Metal cluster: Occurrence of metal-metal bonds in metal complexes, Bonding in metal cluster. Metal carbonyl type clusters. Anionic and hydride cluster. Method of synthesis, super large cluster, electron counting in medium size cluster (Wade's rule, Capping rule), Isolable relationship, cluster of Fe, Ru, Os groups. Cluster of Co, Rh, Ir groups. Cluster of Ni, Pd, Pt groups. Catalysis by cluster.

Isopoly and heteroply acids and salts.

BOOKS:

1. *Advance Inorganic Chemistry by F.A. Cotton, G. Wilkinson & C. Murillo (6^{th} edition)*
2. *Inorganic Chemistry by J.E. Helay, Harper and Row*
3. *Comprehensive Coordination Chemistry, Eds. by Wilkinson, Gillarsand*
4. *Modern Aspect of Inorganic Chemistry by Emelius and Sharpe*

ACH-412: BIOINORGANIC CHEMISTRY 3 credits

UNIT-I ***Biomolecules and their Roles in Metal Ions Storage and Transportation***

Amino acids, peptides and proteins, structures of proteins, Ramachandran's plot, lipids, lipid bilayer, biological membranes, chemistry of biologically relevant molecules like ADP, ATP, FAD, NADP, nucleotides. Biologically important metal ions (Na, K, Mg, Ca, Cu, Fe, Zn, Co and Mo) and their functions, mechanism of transport of metal ions through biological fluids and membranes, different types of passive and active transport processes and their mechanism, Na^+/K^+ pump, calcium pump, and ionophores. Storage and transport of iron, copper and zinc, siderophores, structure and function of ferritin, transferrin in regard to Fe-storage and transportation,

UNIT-II ***Role of Proteins as Oxygen and Electron Carriers***

Chemistry of porphyrin, Iron porphyrins (Heme proteins): Hemoglobin (Hb), Myoglobin (Mb) and their behavior as oxygen carrier, O_2 affinity, cooperativity and Bohr's effect, Heme protein as electron carrier with particular reference to cytochrome-c and cytochrome-450, and cytochrome oxidase. Catalases and peroxidases. Non-heme oxygen uptake protein (hemerythrin and hemocyanin). Magnesium porphyrins (Chlorophyll): Photosynthesis, the light and dark reaction (Calvin cycle). Non-heme iron-sulphur protein as electron carrier, rubredoxins and ferredoxins.

UNIT-III ***Biomolecular Catalysis***

Preliminary idea about enzyme, cofactor, co-enzyme, apoenzyme, prosthetic group, metal-activated enzyme and metalloenzyme. Enzyme-substrate binding problem, carboxypeptidase, carbonic anhydrase and their biological significance, Interchangeability of zinc and cobalt enzyme. Blue-oxidases (ascorbate oxidase, cerulloplasmin, laccase) and non-blue Oxidases (amine oxidase, galactose oxidase, lysyl oxidase, cytochrome c oxidase), structure and biological functions of molybdenum nitrogenase, superoxide dismutase.

BOOKS:

1. *Bio-Inorganic Chemistry by Asim K Das.*
2. *Bio-Inorganic Chemistry by E. Ochia.*
3. *Bioorganic, BioInorganic and Supramolecular Chemistry by P. S. Kalsi and J. P. Kalsi.*
4. *Inorganic Chemistry (4^{th} Edn) by Huheey, Keiter, Keiter and Medhi.*
5. *Bioinorganic and Suparmolecular Chemistry by A. Bhagi and G. R. Chatwal.*

ACH-413: ORGANIC REACTION MECHANISM - I 3 credits

UNIT-I The S_N2, S_N1, mixed S_N1 and S_N2 and SET mechanisms. The neighboring group mechanism, Neighboring group participations by sigma and pi bonds, anchimeric assistance. Classical and non-classical carbocations, phenonium ions, norbornyl system, common carbocation rearrangements, application of NMR spectroscopy in the detection of carbocations. The S_NI mechanism. Nucleophilic substitution at an allylic, aliphatic trigonal and a vinylic carbon. Reactivity effects of substrate structure, attacking nucleophile, leaving group and reaction medium, phase transfer catalysis, ambident nucleophile, regioselectivity.

UNIT-II Alipahatic Electrophilic Substitution mechanism: S_E1, S_E2 and S_E^I mechanisms, Effect of substrate, leaving group and solvent, Reactions (hydrogen exchange, migration of double bonds, keto-enol tautomerism, halogenation, aliphatic diazonium coupling, Stork-enamine reaction).

Aromatic electrophilic substitution mechanism: Structure reactivity relationship in mono-substituted benzene, ring isomer proportions, orientation in benzene ring with one or more than one substituent, Orientation in other ring systems, Vilsmeir - Haack reaction, Pechmann reaction.

UNIT-III Aromatic Nucleophilic Substitution mechanism: Introduction to different mechanisms, Aromatic nucleophilic substitutions (S_NAr, S_N1 aryne), Effect of substrates, leaving groups, and nucleophile, Reactions: Nucleophilic displacement in areno-diazonium salts by different nucleophiles, Chichibabin reaction.

Free radical Substitution: Intermediates, Reaction at sp^2 carbon, Reactivity in aliphatic substrates, Reactivity at bridge head position, Reactivity in aromatic substrates.

BOOKS:

1. *Advanced Organic Chemistry: Reaction Mechanism and Structure by Jerry March (Willey Eastern Limited)*
2. *Organic Reaction Mechanism by Kalsi*

ACH-414: ORGANIC REACTION MECHANISM – II 3 credits

UNIT-I Addition to carbon-carbon multiple bonds, Electrophilic, Nucleophilic and Free radical addition, Orientation and Reactivity, Addition to cyclopropanes, Reactions: Hydroboration, Michael reaction, Sharpless Asymmetric epoxidation.

Addition to carbon-heteroatom multiple bonds: Mechanism and reactivity, Reactions: Mannich reaction, $LiAlH_4$ reduction of carbonyl compounds, acids, esters, nitriles, addition of Grignard reagents - Reformatsky reaction, Aldol condensation, Knoevenagel condensation, Perkin reaction, Tollens reaction, Wittig reaction, Prins reaction, Benzoin condensation.

UNIT-II Elimination mechanism: E_1, E_2, E_1CB and E_2CB mechanisms, Orientation, Effect of substrate, base, leaving group and medium, Orientation of double bond, Sayetzeff and Hoffman rules, Pyrolytic elimination reaction, Oxidative elimination (oxidaton of alcohol by chromium, Moffatt oxidation). Reactions: Cleavage of quaternary ammonium hydroxides, Chugaev reaction, Shapiro reaction.

UNIT-III General mechanistic considerations – nature of migration, migratory aptitude, memory effects.

A detailed study of the following rearrangements, Wagner-Meerwein, Favorskii, Carbene intermediate, Arndt-Eistert synthesis, Neber, Nitrene intermediates (Beckmann, Hofmann, Schmidt, Lossen, Curtius), Baeyer-Villiger, Shapiro reaction, Von-Richter, Sommelet-Hauser rearrangement.

BOOKS:

1. *Advanced Organic Chemistry: Reaction Mechanism and Structure by Jerry March (Willey Eastern Limited),*
2. *Organic Reaction Mechanism by Kalsi*
3. *Physical Basis of Organic Chemistry by N. Isaac (Willey Eastern Limited),*

ACH-415: STATISTICAL THERMODYNAMICS & HMO THEORY 3 credits

UNIT-I Classical and Quantum Statistical Mechanics

Concept of probability, Starling approximations, Most probable distribution, System, Phase Space, μ-Space, ϒ-Space, Liouville's Theorem, Statistical Equilibrium, Brief Concepts on Ensembles, Canonical, Grand Canonical and Micro-canonical ensembles. Bose-Einstien statistics, Fermi-Dirac statistics and Maxwell-Boltzmann statistics

UNIT-II Partition Functions & Statistical Thermodynamic Properties of Solids

Significance of partition function, Calculation of thermodynamic properties and equilibrium constant in terms of partition functions, Evaluation of transnational, vibrational and rotational partition function for monoatomic and polyatomic ideal gases, electronic partition function.

Some thermal characteristics of crystalline solids, Classical treatment of solids, Einstein Model, Debye Modification, Limitation and modification of Debye theory.

UNIT-III Huckel Molecular Orbital Theory

Huckel molecular orbital theory of conjugated systems (Ethylene, Allyl systems, butadiene, cyclopropenyl, cyclobutadiene, bicyclobutadiene, H_3^+, H_3 and H_3^-), Calculation of bond order, charge density, free valence index, Application of group theory for the simplification of MO determinants of 1,4- butadiene and naphthalene.

BOOKS

1. *Physical Chemistry by D.N. Bajpai*
2. *Statistical Thermodynamics by M. C. Gupta*
3. *Introduction to Quantum Chemistry by A.K. Chandra*
4. *Notes on Molecular Orbital Calculations by J.D. Roberts*

ACH-416: SURFACE CHEMISTRY 3 credits

UNIT-I Phase Rule

Concept of Equilibrium between phases, Derivation of phase rule, Ideal Solution, Liver Rule, Brief concept on one and two component system, Application of phase rule to three component systems of both solids and liquids.

UNIT-II Adsorption

Surface tension, Capillary action, Adsorption, types of adsorption, Gibbs adsorption isotherm, Freundlich's adsorption isotherm, Langmuir's adsorption isotherm and its limitations, BET adsorption isotherm and its applications, Heat of adsorption, estimation of surface areas of solids from solution adsorption studies.

UNIT-III Macromolecules

Polymer-definition, Classification of polymer, Polymer structure, Number average and molecular weight average, Step growth & chain growth polymerization, Kinetics of polymerization, Stereochemistry of polymerization.

BOOKS:

1. *Text Book of Physical Chemistry Vol-1-4 by K.L. Kapoor*
2. *Physical Chemistry by D.N. Bajpai*
3. *Physical Chemistry by A.W. Atkins*
4. *Introductory Quantum Chemistry by A.K. Chandra*
5. *Polymer Science by Gowariker, Viswanathan & Sreedhar*
6. *Polymer Science & Technology by J. R. Fried*

ACH-417: ORGANIC PRACTICAL **2 credits**

1. Isolation and identification of multi-functional compounds in a mixture of two organic compounds.
2. Preparation of;
   a) Benzoin, benzil and benzillic acid from benzaldehyde.
   b) p-idotoluene from p-toluidene.
   c) Ethyl acetoacetate from ethyl acetate.
3. Estimation of;
   a) Nitrogen by Kjeldahl method.
   b) keto group by gravimetric method.

BOOK: *Advanced Practical Organic Chemistry, 3/e by N K Vishnoi*

ACH-418: ANALYATICAL PRACTICAL **2 credits**

1. Determine the pK value of an acid-base indicator.
2. To estimate metal ions by spectrophotometric titration.
3. To determine the pH of a given solution by spectrphotometrically.
4. Adsorption of CH_3COOH on activated charcoal and verification of Freundlich's & Langumir's adsorption isotherm.
5. Simultaneous estimation of Mn and Cr in a solution of $KMnO_4$ and $K_2Cr_2O_7$.
6. Determination of hydrolysis constant of aniline hydrochloride.
7. Determination of ionisation constants of multibasic acid potentiometrically.
8. Determination of association constants of CH_3COOH by distribution method between water and toluene.
9. To study the rate of acid catalysed iodination of acetone in presence of excess acid and acetone.
10. To study the stability constant of a metal complex.
11. Estimation of Fe ion in a solution of Mhor's salt.

BOOKS:
1. *Experimental Physical Chemistry by Das and Behera*
2. *Practical Physical Chemistry by B. Vishwanathan & P.S. Raghavan*
3. *Experimental Physical Chemistry by V.D. Athawale*

THIRD SEMESTER

ACH-501: INSTRUMENTAL METHODS OF ANALYSIS 3 credits

UNIT-I: ***Chromatography & Imaging Analysis***

Introduction to chromatography, Basic principles, instrumentation and Applications of different chromatography (TLC, HPTLC, column chromatography, paper chromatography, Gas chromatography and HPLC).

Principle & applications of Optical Microscopy, Scanning Electron Microscope, Transmission Electron Microscope and X-ray Diffraction Analysis.

UNIT-II ***NMR and Mass Spectrometry***

NMR: Magnetic properties of Nuclei, Theory of Nuclear Magnetic Resonance with special reference to proton, NMR Instrumentation, Chemical shift, Shielding and de-shielding Effects, Diamagnetic anisotropy, simple spin-spin interaction, NOE.

Mass spectrometry: Introduction to mass spectrum, Determination parent peak and base peak, Use of molecular fragmentation, Mass spectra of some classes of compounds such as hydrocarbons, alcohols, phenols, ketones, aldehydes, acids and esters, McLafferty rearrangement.

UNIT-III ***Electroanalytical Method***

Polargraphy: Basic principle, instrumentation, theory of current-voltage curve, Theory of diffusion current, Ilkovic equation, polarography wave and half wave potential. Application of polarography.

Cyclic voltametry anodic stripping voltametry, amperometry, conductometry and ion selective electrodes.

BOOKS:

1. *A Guide to Materials Characterization and Chemical Analysis by John P. Sibilia*
2. *X-Ray Diffraction by C. Suryanarayana, C., Norton, M. Grant*
3. *Electron Microscopy and Analysis by Peter Goodhew*
4. *Analytical Chemistry (Theory and Practical), U.N. Dash*
5. *Spectroscopic Identification of Organic Compounds, Silverstein & Basselr*
6. *Organic Spectroscopy by V.K. Ahluwalia*
7. *Spectroscopy by Donald L. Pavia, Gary M. Lampman, and George S. Kriz*

ACH-502: INDUSTRIAL POLLUTION AND ITS MANAGEMENT 3 credits

UNIT-I Concept and definition of Industrial pollution, History of major industrial air pollution episodes. Types and classification of Industrial air pollutants. Characterization of gaseous effluents of major industries (thermal power plant, steel, cement, aluminum, paper, fertiliser) and their health effects. Permissible limit and ambient air quality, Methods for control of gaseous air pollutants (Combustion, Absorption and Adsorption). Methods for control of particulate air pollutants (Mechanical device, Filtration, Dry scrubber, Electrostatic precipitator)

UNIT-II History of major industrial water pollution episodes, Classification and types of Industrial water pollutants, Characterization of some liquid effluents of major polluting industries (Paper Mills, Sugar industry, Iron and steel and Textile) and their health effects, Water quality standard : Drinking water quality standard, Irrigation water standard and effluent standard, methods of treatment of industrial waste water: Preliminary treatment, primary treatment, (Sedimentation, equalization and neutralization etc.), secondary treatment (Activated sludge technique and Trickling filter) tertiary treatment methods for waste water treatment (Evaporation, Ion exchange, Adsorption, Electrodialysis, Electrolytic recovery, reverse osmosis).

UNIT-III Classifications and types of Industrial solid wastes, Generation, disposal and management of industrial solid wastes with special reference to fly ash, red mud, heavy metals (Mercury, Lead, Arsenic, Cadmium), other organic solid wastes and radio-active wastes. Industrial sources of noise, Loudness on Decibel scale, noise levels in decibel scale, effect of noise on human health, prevention and control of industrial noise pollution.

BOOKS:

1. *Industrial Pollution and Management by Arvind Kumar*
2. *Industrial Pollution and its Management by P.C. Trivedi*

ACH-503: INDUSTRIAL POLICY AND ENTREPRENEURSHIP **2 credits**

UNIT-I

a) Orissa Industrial Policy
b) Industries development & Regulation Act-1951
c) Micro & small scale Industries development Act-2006

UNIT-II The Explosive Act-1884, Insecticide Act-1981, Petroleum Act-1976, Gas Cylinder Rule-2004, Employer's liability Act-1938

UNIT-III

a) Water Act
b) Air Act
c) Environmental Protection Act

ACH-504: PROJECT **16 credits**

FOURTH SEMESTER

ACH-511: COMPUTER APPLICATION IN CHEMISTRY 2 credits

UNIT-I: ***Introduction to Computers***

Basic structure of a computer: The CPU, the I/O devices, the internal memory, commonly used secondary storage media. Data representation: Overview of binary, octal and hexadecimal number system. The software: Concept of low level and high level languages, Compiler interpreter, editor, operating system concepts, salient features of MS-DOS. Windows operating systems.

UNIT-II: ***Programme Development Process***

Algorithm, Flowchart, Decision-table, elements of high level programming languages. Input-output statements, conditional statements, control structure, concept of data file, file operations like searching, storing, with reference to C Programming.

BOOKS:

1. *Computational Chemistry, A.C. Norris*
2. *Microcomputer Quantum Mechanics, J.P. Killngbeck*
3. *C Programming Language, Brian W. Kernighan and Dennis M. Ritchie*
4. *An Introduction to Digital Computer design, V. Rajaraman & T. Radhakrishnan*
5. *Computer Aids to Chemistry, Ed. G. Vernin & M. Chanon*

ACH-512: ENERGY & MATERIAL BALANCE AND NANOMATERIALS 3 credits

UNIT-I: ***Energy and Material Balance***

Energy and Thermo-Chemistry, Energy Balances, Heat Capacity of Gaseous Mixtures, Latent Heats, Enthalpy Changes During Phase Transfers Accompanied by Sensible Heat Changes, Enthalpy Changes accompanying Chemical Reactions.

Material Balances Without Chemical Reactions: Process Flow-Sheet, Material Balances, Recycling Operations, Material Balances of Unsteady State Operations.

Material Balances Involving Chemical Reactions, Definition of Terms, Electrochemical Reactions, Recycling, Parallel and Bypassing Operations, Metallurgical Applications

UNIT-II: ***Nanomaterials and Applications***

Nanomaterials for Solar Energy Conversion Systems. Principles of photovoltaic energy conversion (PV), Structural characteristics and concepts. Types of photovoltics Cells, Physical concept of photovoltaic cells, Organic solar cells, Dye-Sensitized Solar Cells, Organic-Inorganic Hybrid solar cells. Current status and future trends.
Conducting and ferroelectric materials, structure and features of ferroelectric materials, ceramic materials, organic/inorganic hybrid materials and their applications.

UNIT-III: ***Structural Properties of Polymers and Applications***

(a) Structure-property relationship, stress-strain behavior, crystalline melting point, effect of chain flexibility and other steric factors, entropy and heat of fusion, glass transition temperature, relationship between Tm and Tg. Effect of molecular weight, property requirements and its utilization.

(b) Synthetic procedure commercial polymers (polycarbonate, polyurethane, polymethylmethacrylate, polyethyethyleneterpthalate, Nylon, polystyrene), Fire retarding and biomedical polymers

BOOKS:

1. *Stochiometry by B I Bhatt and S. M. Vora (Tata McGraw Hill, New Delhi)*
2. *Semiconductor for Solar Cells by H J Moller, Artech House Inc, MA, USA, 1993.*
3. *Solis State Electronic Device by Ben G Streetman, Prentice Hall of India Pvt Ltd., New Delhi 1995.*
4. *Organic Photovoltaics – Materials, Device Physics and Manufacturing Technologies, (eds. by C. Brabec, V. Dyakonov, U. Scherf), 2nd Ed., Wiley-VCH, Germany, 2014.*
5. *Text Book of Polymer Science by F.W. Billmeyer Jr, Wiley.*
6. *Polymer Science by V.R. Gowariker, N.V. Viswanathan and J. Sreedhar, Wiley-Eastern.*

ACH-513: INDUSTRIAL PROCESSES 3 credits

UNIT-I: Petroleum and coal based chemicals: Composition of petroleum, cracking processes, Commercial production of ethylene, acetylene, polymerization mechanisms, Addition, condensation, step growth, chain growth, method of polymerization, Distillation of coal.

UNIT-II: Oil based Industries: Oils and fats: Solvent extraction of oils, hydrogenation of oil, use of oil in the manufacturing of soap, paints and varnishes.

Surface active agents: classification and manufacturing of detergents used for cleansing purpose.

Fermentation Industries: A general discussion on fermentation conditions, manufacturing of penicillin.

UNIT-III: Pesticides and Pharmaceutical industries: DDT manufacture, BHC manufacture, 2,4-D manufacture, parathion manufacture, Pharmaceutical industry

BOOKS:

1. *Outlines of Chemical Technology by M. Gopala Rao and Marshall Sittig, Affiliated East-West Press Pvt. Ltd.*
2. *Industrial Chemistry by B. K. Sharma*

ACH-514: MEDICINAL CHEMISTRY 3 credits

UNIT-I: ***Advanced Medicinal Chemistry***

Drug discovery and development, Definition, outline, achievements in the field of medicinal, parameters involved in drug design physicochemical ionization , H-bonding, chelation, surface active agents, redox potentials. Drug receptor interactions isosterism, steric features of drug concept of drug receptor, Receptors, their types, location, isolation transdunction mechanism.

UNIT-II: ***Strategies for Synthesis of Candidate Drug***

1. Target selection
2. Retro synthesis (the disconnection approach consecutive versus conversion synthesis including LHASA, strategic bond approach, strategic bond in ring approach, degradation of techniques in, synthetic design of venalflaxin, doxopicomine, clobutinol, nisoxetine, bropirimine.

UNIT-III: ***Drug and their Applications***

Chemotherapy of cancer: veincristine and vinblastine and taxol, drug related hormones insulin, vasopressin and oxitosin, prostaglandin, histamine, antiparkinosin agents antialzehimer agents, antirheumatics and antigout agents.

BOOKS

1. *Medicinal Chemistry by Alfred Burger.*
2. *Introduction to the Principles of Drug Design by Smith and Williams.*
3. *Strategy of Drug Design by Purcell.*
4. *Principle of Biochemistry by A.L. Lehninger, D.L. Nelson & Michael M Cox.*
5. *Organic Chemistry by J. Clayden, N. Greeves, S Warrens, P.Wothers.*

ACH-515: SURFACTANTS & DETERGENTS 3 credits

UNIT-I: ***Structural Aspects of Surfactants***

Surfactants, Classification(Anionic surfactants, Cationic head surfactant, Zwitterionic surfactants, Nonionic surfactant, Biosurfactants, Gemini surfactant, double tailed surfactant, Bolaform), Synthesis of Surfactant, Behaviour of Surfactants in aqueous and nonaqueous solution, Different types of interactions, Surface activity, Surface tension, Factors for organization of surfactants and types of organized assemblies, Hydrophobic interactions, electrostatic interactions, Critical micellar concentration (CMC), Factors affecting CMC, Methods of CMC determination. Aggregation number, Shape and Size of micelle.

UNIT-II: ***Characterization and Application of Surfactant Assemblies***

Spectroscopic investigation and analytical methods, determination of polarity of micelle, structures of micelle, Determination of aggregation number, Industrial Applications of surfactants, Beneficiation of minerals, micellar catalysis, Drug delivery, Wetting, Dispersion and foaming.

UNIT-III: ***Characterization and Application of Detergents***

Detergents, Principal groups of synthetic detergents, Anionic detergents, Cationic detergents, Non-ionic detergents, Amphoteric detergents, Industrial methods of preparation of Detergents, Concept of hard and soft water, Removal of hardness of water, Oil and fat, General idea of Suds regulators, builders, additives, Manufacture of Shampoos. theories of glyceride structure, Hydrolysis of glycerides, Use of oil in the manufacturing of soap, Principle of soap cleaning, Analysis of soaps as per BIS standards The use of enzymes in detergents, Catalytic hydrogenation of oil, Recovery of Nickel from hydrogenated oil product.

BOOKS:

1. *Industrial Chemistry by B. K. Sharma, 9th Edn.*
2. *The Manufacture of Soaps other Detergents and Glycerin Edited by Edgar Woollatt.*
3. *Synthetic Detergent Edited by Milwidsky.*
4. *Bailey's Industrial Oil and Fat Products Vol-1 (4th Edition) Edited by Daniel Swern.*
5. *Soaps & Detergent Edited by K.S. Parasuram.*
6. *Surfactants and Interfacial Phenomenon by M.J. Rosen*
7. *Catalysis in Micellar and Macromolecular Systems BY E.J. Fendler and J.H. Fendler*

ACH-516: PRACTICAL ON COMPUTER IN CHEMISTRY **2 credits**

1. Use of computer programmes like EXCEL, Chemdraw.
2. Execution of the Software to solve problems.
3. Development of small programmes for solving chemical problems.

ACH-517: INDUSTRIAL PRACTICAL **2 credits**

1. Determination of percentage of purity of commercially available different N, P and K fertilizer.
2. Water analysis: (a) Residual chlorine in town supply water (b) Ammonia content of sewage water
3. Determination of acid value, saponification value and iodine value of different oils
4. Preparation of indigo from anthranilic acid.
5. Preparation of cinnamic acid from benzaldehyde.
6. Preparation from flavone from o-hydroxy acetophenone.
7. Estimation of sulfur in isothiouronium chloride prepared from thiourea.
8. Separation of components from a mixture by TLC and column chromatography.

ACH-518: REVIEW **2 credits**

ACH-519: SEMINAR **2 credits**