Model Curriculum for Three/Four Year Degree Course (With Multiple Entry/Exit Option)

Based on NEP-2020

Chemistry

Odisha State Higher Education Council, Bhubaneswar

Government of Odisha

Semester	Subjects
I	Core I - Atomic Structure, Periodicity of Elements and Chemical Bonding
	Core II- FundamentalOrganicChemistry
II	Core III- Statesofmatter,andIonic equilibrium
	Core IV - Chemicalthermodynamics,equilibrium,andColligativeproperty
III	Core V- AcidsandBases,Metallurgy,Chemistryofmaingroupelements
	Core VI- Chemistryofhalogen,oxygenandsulphur containingorganiccompounds
	Core VII- Phaseequilibrium,Chemicaldynamics, catalysisandsurfacechemistry
IV	Core VIII- Coordination Chemistry, Chemistry of d- and f-block elements,InorganicReactionMechanismandelectron transfer reactions
	Core IX- NaturalProducts,HeterocyclicCompounds,NitrogencontainingcompoundsandPolynuclear Hydrocarbons
	Core X- Conductance,electrochemistry,electricalpropertiesofatomsandmolecules
V	Core XI- Organic Spectroscopy
	Core XII- Basicquantumchemistry,Molecular&electronicspectroscopy,andphotochemistry
	Core XIII- ChemistryofOrganometallicCompounds
VI	Core XIV- AnalyticalMethodsofChemistry
	Core XV- Solidandporousmaterials,andmagneto chemistryandpowercells
VII	Core XVI- ChemistryofBiomolecules
	Core XVII- PolymerChemistry
	Core XVIII- GreenChemistry
	Core XIX- Oxidation,Reduction,Reagents,RearrangementsandName Reactions
VIII	Core XX- Quantumchemistry&StatisticalThermodynamics
	Core XXI- Chemicalgrouptheory,electronicspectraofmetal complexes, and nuclear chemistry
	Core XXII- Pericyclicreactions,Photochemistryand Retrosynthesis
	Core XXIII- ResearchMethodologyforChemistry

Programme Outcomes

- To prepare the students for a career in Chemistry.
- To prepare the students for Higher Education and Research inChemistry.
- To develop a conceptual understanding of the subject and to develop an inquisitiveness in the subject.
- To enable the student to acquire basic skills necessary to understand the subject and to master the skills to handle equipment's utilized to learn the subject.
- To generally promote wider reading on the subject and allied inter disciplinary subject.

Core ISemester -I

Atomic Structure, Periodicity of Elements and Chemical Bonding

Course Outcomes:

- Solvetheconceptual questions usingthe knowledgegained bystudyingthequantummechanicalmodelof theatom.
- Learnthevariousatomic propertiesof atomsand theirvariationsintheperiodic table.
- Gaintheideaofdifferenttypesofbondingandtheirassociatedproperties.
- Understandthetheoryandapplicationsofvariousacid-basetitrations.

Unit–I: Atomicstructure

Rutherford's nuclear model of atom, Bohr's theory and the origin of hydrogen spectrum, Sommerfeld's extension of Bohr's theory, de-Broglie equation, Heisenberg's Uncertainty Principle and its significance. Postulates of wave mechanics, Derivation of Schrödinger's wave equation for hydrogen atom, significance of ψ and ψ^2. Radial and angular wave functions, Radial function plots, radial probability distribution plots, angular distribution curves. Shapes of s-, p-, d- and f-orbitals, Relative energies of orbitals. Slater's rule and its limitations,Quantumnumbersandtheirsignificance.Pauli'sExclusionPrinciple,Hund'srule of maximum spin multiplicity and Aufbau principle.

Unit– II:Periodicityof elements:

Introductiontolongformperiodictable,Causeofperiodicity,Divisionofelementsintos-,p-, d-andf-blocks.Atomicradius,ionicradius,covalentradiusandVanderWallsradius.Periodic trends in ionic and covalent radii. Ionization energy, electron affinity, electronegativity, and their variations in the periodic table. Applications of electronegativities. Pauling's/Mulliken's scale of electronegativity, Sanderson's electron density ratio.

Unit– III:Chemicalbonding

Ionic bond-General characteristics, types of ions, size effects, radius ratio rule and its limitations. Packing of ions in crystals. Lattice energy, Born-Haber cycle and its application, Born-Lande equation, Madelung constant, importance of Kapustinskii equation for lattice energy. Solvation energy, Covalent character in ionic compounds, polarizing power and polarizability. Fajan's rules and consequences of polarization.

Unit– IV:Chemicalbonding

Covalentbond-Valenceshellelectronpairrepulsion(VSEPR)theory,shapesofthefollowing simple molecules and ions containing lone pairs and bond pairs of electrons: CH_4, H_2O, NH_3, PCl_3, PCl_5,

SF_6, ClF_3, I_3^-, BrF_2^+, PCl_6^-, ICl_2^-, ICl_4^-, NH_4^+, PO_4^{3-} and SO_4^{2-}. Valence Bond theory (Heitler-London approach). Hybridization, equivalent and non-equivalent hybrid orbitals. Ionic character in covalent compounds: Dipole moment. Percentage ionic character from dipole moment and electronegativity difference, Molecular orbital diagrams of homo- & hetero-diatomic molecules (N_2, O_2, C_2, B_2, F_2, CO, NO) and their ions. Calculation of bond order. Concept of bent rule.

Metallicbond:

Conceptofmetallicbond,Thefreeelectronmodel,Thevalencebondmodel,Thebandmodel(molecular orbital approach), semiconductor and insulators.

Hydrogenbond:

Conceptofhydrogenbond,natureofhydrogenbonding,consequencesofhydrogenbondingandits importance.

List ofexperiments

1. Calibrationanduseofapparatus
2. PreparationofsolutionsofdifferentMolarity/Normality.
3. EstimationofoxalicacidusingstandardNaOHsolution
4. EstimationofsodiumcarbonateusingstandardHCl.
5. Estimationofcarbonateand hydroxidepresenttogetherinamixture.
6. Estimationofcarbonateandbicarbonatepresenttogetherinamixture.

Text Books:

- ✓ *B.R.Puri,L.R.Sharma,K.C.Kalia,PrinciplesofInorganicChemistry,VishalPublishing Co., 33rd Ed., 2017.*
- ✓ *A.J.Elias,TheChemistryofthep-BlockElements-Syntheses,ReactionsandApplications, University Press (India) Pvt Ltd., 2009.*
- ✓ *G.H.Jeffery, J.Bassett, J.Mendham,R.C. Denney,Vogel's Textbookof Quantitative Chemical Analysis, John Wiley and Sons, 1989.*

ReferenceBooks:

- ✓ *J.D.Lee,ConciseInorganicChemistry,WileyIndia, 2010.*
- ✓ *B.E.Douglas,D.H.McDaniel,J.J.Alexander,ConceptsandModelsof InorganicChemistry, John Wiley & Sons, 1994.*
- ✓ *P. W.Atkins, T. L. Overton,J. P. Rourke,M. T. Weller,F. A. Armstrong, Shriver and Atkins Inorganic Chemistry, 5th Edition, Oxford UniversityPress, 2010.*
- ✓ *P.Chndra,C.Gupta,ChemicalDynamicsandCoordinationchemistry,1st Ed.,2022.*
- ✓ *A.K.Das,M.Das,FundamentalConceptsofInorganicChemistry,1stEdition,Volume CBS Publishers & Distributors Pvt. Ltd., 2014.*
- ✓ *J.E. Huheey, E.A.Keiter, R. L.Keiter, O.K. Medhi,Inorganic Chemistry-Principles of Structure and Reactivity, Pearson Education, 2009.*
- ✓ *D.C.Harris,C.A.Lucy,QuantitativeChemicalAnalysis,9th Ed,Freemanand Company,2016.*

Core IIFundamentalOrganicChemistry

CourseObjectives:

To provide the fundamental knowledge on organic chemistryin order to comprehend other organic chemistry courses in comingsemesters with greaterdepth. Thepurposeofthis corepaperis to reviewthebasicconcepts of electron displacement and the chemistry of aliphatic and aromatic hydrocarbons. Stereochemistry is also introduced to help to student to visualize the organic molecules and their spatial arrangement in three dimensional spaces and hands on experience on detection of organic molecules.

CourseOutcomes:

1. Understandingthebasicconceptsofelectronicdisplacementphenomenainorganicmolecules,variousbond breaking processes and types of organic reactions.
2. Fundamentalknowledgeonsymmetryandasymmetryaspectoforganicmoleculesandtheirspatial arrangements in two-dimension and three-dimension with their stereochemistry.
3. Learning the synthesis, structure and stability of unsaturated hydrocarbons, understanding the concept of aromaticity and chemical reactions of unsaturated hydrocarbons and aromatic hydrocarbons.
4. Knowledgeonselectionofsuitablesolventforpurificationandseparationoforganiccompoundsand detection of various elements present in it.

Unit–I:BasicsofOrganicChemistry

Electronic Displacements: Inductive, electromeric, resonance and mesomeric effects, hyperconjugation and theirapplicationsindipolemoment;organicacidsandbases;theirrelativestrength.Homolyticandheterolytic fission with suitable examples. Curly arrow rules; Electrophiles and Nucleophiles; Nucleophilicity and basicity; Types, shape and relative stability of carbocations, carbanions, free radicals and carbenes.
Introduction to types of organic reactions with suitable examples: Addition, Elimination, Substitution, Rearrangement and Pericyclic reactions.
Carbon-carbon sigma bonds, chemistry of alkanes: Formation of alkanes, Wurtz Reaction, Corey-House Reactions, Free radical substitutions: Halogenation –relative reactivity and selectivity.

Unit–II:Stereochemistry

Concept of Chirality/Asymmetry, Geometrical isomerism and Optical Isomerism: Optical Activity, Specific Rotation. Determination of Relative and absolute configuration in chiral molecules usingD/L, R/S, cis/trans, Syn/AntiandE/ZdescriptorsusingC.I.Prules.RepresentationbyFischerProjection,NewmannandSawhorse Projectionformulaeinmoleculescontainingoneandtwochiral-centres.Enantiomers,Distereoisomers,meso-structures, Racemic mixture and their resolution.
Stabilityand Conformational analysis: types of cycloalkanes and theirrelativestability, Baeyerstrain theory, Conformational analysis of alkanes (ethane and n-butane): Relative stability with energy diagrams. Energy diagrams of cyclohexane: Chair, Half chair, boat and twist boat forms.

Unit–III:**ChemistryofUnsaturatedHydrocarbons**

Carbon-CarbonPi Bonds: Formation ofalkenes and alkynes byelimination reactions, Mechanism ofE1,E2, E1cb reactions. Saytzeff and Hofmann eliminations.
Reactions of alkenes: Electrophilic additions their mechanisms (Markownikoff/AntiMarkownikoff addition), mechanism of oxymercuration-demercuration, hydroboration-oxidation, ozonolysis, syn and anti-hydroxylation (oxidation).1,2- and 1,4-addition reactions in conjugated dienes and Diels-Alder reaction; Reactions of alkynes: Acidity, Electrophilic and Nucleophilic additions. Hydration to form carbonyl compounds, Alkylation of terminal alkynes.

Unit–IV:ChemistryofAromaticHydrocarbons

Aromaticity: Hückel's rule, aromaticity in benzenoid and non-benzenoid compounds, cyclic carbocations/carbanions and heterocyclic compounds with suitable examples.
Electrophilicaromaticsubstitutionwithmechanism:halogenation,nitration,sulphonationandFriedel-Craft's alkylation/acylation with their mechanism. Directing effects of the functional groups.

List ofExperiments

1. Detectionofextraelements (N,Cl,Br, IandS)inorganiccompoundsbyLassaigne'stest.
2. Functional group tests for alcohols, phenols, carbonyl and carboxylic acid groups in known organic compounds.
3. Separation and purification of any one component of following binary solid mixture (Benzoic acid/*p*-Toluidine; *p*-Nitrobenzoic acid/*p*-Aminobenzoic acid; *p*-Nitrotolune/*p*- Anisidine) based on the solubility in common laboratory reagents/solvents like water (cold, hot), ethanol (cold, hot), dil. HCl, dil. NaOH, dil.$NaHCO_3$ etc.
4. Determinationofmeltingpoint andboilingpoint ofdifferentorganic compounds

TextBooks:

- ✓ *R.T.Morrison,R.N.Boyd,S.K.Bhattacharjee,OrganicChemistry,7th Ed.,PearsonEducationIndia, 2010.*
- ✓ *A.Bahl,B.S.Bahl,Advanced OrganicChemistry,5th Ed.,S.Chand,2012.*
- ✓ *B.S.Furniss,A.J.Hannaford,P.W.G.Smith,A.R.Tatchell,Vogel'sTextbookofPracticalOrganic Chemistry, 5th Ed., Pearson Education India, 2003.*

ReferenceBooks:

- ✓ *T. W. Graham Solomons,C. G. Fryhle,S. A. Snyder, Solomons' Organic Chemistry,Global Ed.,Wiley, 2024.*
- ✓ *J.Clayden,N.Greeves,S.Warren,OrganicChemistry,2nd Ed.,OxfordPublisher, 2012.*
- ✓ *R.K.Bansal,OrganicReactionMechanism,3rd Ed.,TataMcGraw-HillPublications, 1998.*
- ✓ *D.Nasipuri,StereochemistryofOrganiccompounds, 4th Ed.,NewAgeInternationalPublisher,2020.*
- ✓ *P.Sykes,AGuidebooktoMechanisminOrganicChemistry, 6thEd.,PearsonEducation,2003.*
- ✓ *F.A.Carey,R.J.Sundberg,AdvancedOrganicChemistry,Part-AandPart-B,5thEd.,Springer2007.*
- ✓ *N.K.Vishnoi,AdvancedPracticalOrganicChemistry,3rd Ed.,VikasPublishingHouse, 2009.*
- ✓ *O.P.Agarwal,AdvancedPracticalOrganicChemistry, KrishnaPrakashan,2014.*
- ✓ *V. K. Ahluwalia, R. Aggarwal, Comprehensive Practical Organic Chemistry: Preparation and Quantitative Analysis, Universities Press, 2004.*
- ✓ *H.T.Clarke,AHandbookofOrganicAnalysis:QualitativeandQuantitative,4thEd.,CBSPublishers, 2021.*

CoreIIISemester II

Statesofmatter,andIonic equilibrium

CourseObjectives:

The objective of this course is to develop basic and advance concepts regarding gases and liquids. It aims to study the similarity and differences between the two states of matter and reasons responsible for these. The objective of the practical is to develop skills for working in physical chemistry laboratory. The student will perform experiments based on the concepts learnt in Physical chemistry-I course.

CourseOutcomes:

1. Derivemathematicalexpressionsfordifferentpropertiesofgasandliquidandunderstandtheirphysical significance.
2. Apply the concepts of gas equations and liquids while studying other chemistry courses and understand the importance of pH in every-day life.
3. UnderstanddifferentlatticesystemsandapplyworkingprinciplesofXRD forunderstandingcrystal structure by powder and single crystal method.
4. HandlestalagmometerandOstwaldviscometerproperlyanddeterminethedensityofaqueoussolutions.Data reduction, interpretation using numerical and graphical methods.

Unit-I:Gaseousstate

Kinetic molecular model of a gas, Collision frequency, Collision diameter, Collision cross section, Mean free path and viscosityof gases, includingtheirtemperature and pressuredependence, Relation between mean free path and coefficient of viscosity, Maxwell distribution of molecular velocities (no derivation); average, root mean square and most probable velocities and average kinetic energy, Law of equipartition of energy, Behaviourofrealgases:Deviationsfromidealgasbehavior,Causesofdeviationfromidealbehavior,Vander Wall equation and its application, Compressibility factor Z, and its variation with pressure for different gases, Critical Phenomenon and critical constant derivation.

Unit-II:**Liquidstate**

Qualitativetreatmentofthestructureoftheliquidstate;physicalpropertiesofliquids;vapourpressure,surface tension and coefficient of viscosity, and their determination. Effect of addition of various solutes on surface tension and viscosity. Capillary action in relation to cohesive and adhesive forces, Explanation of cleansing action of detergents. Temperature variation of viscosity of liquids and comparison with that of gases. Qualitative discussion of structure of water.

Unit-III:Solid state

Nature of the solid state, law of constancy of interfacial angles, law of rational indices, Miller indices, elementaryideasofsymmetry,symmetryelementsandsymmetryoperations,sevencrystalsystemsandfourteen Bravaislattices; X-raydiffraction,Bragg'slaw,asimpleaccount ofrotatingcrystalmethodandpowderpattern method.Analysesofpowderdiffractionpatternsof NaCl,CsClandKCl.Defectsincrystals(stoichiometricand non-stoichiometric).

Unit-IV:Ionicequilibria

Strong, moderate and weak electrolytes, degree of ionization, factors affecting degree of ionization, ionization constant and ionic product of water. Ionization of weak acids and bases, pH scale, common ion effect; dissociation constantsofmono-anddiproticacids. calculation ofhydrolysis constant, degreeofhydrolysis and pH for different salts. Buffer solutions; derivation of Henderson equation and its applications. Solubility and solubility product of sparingly soluble salts and its application.

Listofexperiments:

1. Determinethesurfacetension by(i)dropnumber(ii)dropweightmethod.
2. Study the variation of surface tension of detergent solutions withconcentration and determination ofCMC
3. Determinationofviscosityofaqueoussolutionsof(i)polymer(ii)ethanoland(iii)sugaratroom temperature.

4. Studythevariationofviscosityofsucrosesolutionwith theconcentrationofsolute.
5. pHmetrictitrationof(i)strongacidvs.strongbase,(ii)weakacid vs.strongbase.
6. PreparationofbuffersolutionsofdifferentpH(i)Sodiumacetate-aceticacid(ii)
7. Ammoniumchloride-ammonium hydroxide
8. Determinationofdissociationconstantofaweakacid.
9. DeterminationofsolubilityproductofPbI2bytitrimetricmethod.

TextBooks:

- ✓ *P.W.Atkins,J.dePaula, ElementsofPhysical Chemistry,OxfordUniversityPress,6th Ed., 2006.*
- ✓ *G.W.CastellanPhysical Chemistry4thEdn.Narosa2004.*
- ✓ *Khosla,B.D.;Garg,V.C.&Gulati,A.SeniorPracticalPhysicalChemistry,R.Chand&Co.,NewDelhi 2011.*

Referencebooks:

- ✓ *Puri,Sharma&Pathania,PrinciplesofPhysical Chemistry,VishalPublishingCo,47th Edn., 2017.*
- ✓ *R.G.,MortimerPhysical Chemistry,Elsevier(AcademicPress),3rdEd,2008.*
- ✓ *T.Engel&P.ReidPhysicalChemistry,3rdEd.Pearson2013*
- ✓ *KapoorK.L.,TextBookofPhysicalChemistry,McGrawHill,3rdEdn.2017*
- ✓ *HrishikeshChatterjee,UnderstandingPHYSICALCHEMISTRYThroughTheoriesandProblems,Nonlinear insights (opc) pvt. ltd. Publication division, 1st Ed., 2023.*

Core IV

Chemicalthermodynamics,equilibrium,andColligativeproperty

CourseObjectives:

The learners should be able to apply principles and laws of thermodynamics to reversible and irreversible systems. In addition, they should be able to use spectroscopic data to calculate thermodynamic properties of ideal &real mixtures. In addition, understand the change in thermodynamic properties, equilibrium constants, partial molar quantities, chemical potential. Also able to identify factors affecting equilibrium constant using the principles and techniques of statistical thermodynamics.

CourseOutcomes:

Bytheend ofthecourse,the students will beableto:

- Discussthelawsofthermodynamicsandapplicationsto naturalphenomena.
- Acquireastrongfoundationofpartialmolarproperties,itsvariationwithtempandpressurefor different systems and able to apply on the thermodynamics of simple mixtures.
- Inculcatefirmfoundationsinthefundamentalsandapplicationofchemical equilibrium,andΔGderive the relationship between different equilibrium constants.
- UnderstandthebasicconceptofSolutionsofnon-volatilesolutes,colligativeproperties.Calculate various thermodynamic properties (ΔHneutralization, ΔHhydration & Cv) for chemical reactions using calorimeter.

Unit-I:Chemicalthermodynamics

Intensive and extensive variables; state and path functions; isolated, closed and open systems; zeroth law of thermodynamics.Firstlaw:Conceptofheat,q,work,w,internalenergy,U,andstatementof**firstlaw**;enthalpy, H,relationbetweenheatcapacities,calculationsofq,w,UandHforreversible,irreversibleandfreeexpansion of gases (ideal and van der Waals) under isothermal and adiabatic conditions. Thermochemistry: Heats of reactions: standard states; enthalpy of formation of molecules and ions and enthalpy of combustion and its applications;calculation ofbondenergy,bonddissociationenergyandresonanceenergyfromthermochemical data, effect of temperature (Kirchhoff's equations) and pressure on enthalpy of reactions.

Unit-II

Carnot cycle, efficiency of heat engine, Carnot theorem; **Second Law:** Concept of entropy; thermodynamic scaleoftemperature,statementofthesecondlawofthermodynamics;molecularandstatisticalinterpretationof entropy.Calculationofentropychangeforreversibleandirreversibleprocesses.**ThirdLaw:**Statementofthird law, concept of residual entropy, calculation of absolute entropy of molecules. Free Energy Functions: Gibbs andHelmholtzenergy;variationofS,G,AwithT,V,P;Freeenergychangeandspontaneity.Relationbetween Joule-Thomson coefficient and other thermodynamic parameters, inversion temperature, Gibbs-Helmholtz equation, Maxwell relations, thermodynamic equation of state.

Unit-III:Systemsofvariablecomposition

Partial molar quantities, dependence of thermodynamic parameters on composition; Gibbs Duhem equation, chemical potential of ideal mixtures, change in thermodynamic functions in mixing of ideal gases. **Chemical equilibrium**: Criteria of thermodynamic equilibrium, degree of advancement of reaction, chemical equilibria inidealgases,conceptoffugacity.ThermodynamicderivationofrelationbetweenGibbsfreeenergyofreaction and reaction quotient (vant Hoff's reaction). Equilibrium constants and their quantitative dependence on temperature,pressureandconcentration.Freeenergyofmixingand spontaneity;thermodynamicderivationof relations between the various equilibrium constants K_p, K_c and K_x. Le Chatelier principle (quantitative treatment) and its applications.

Unit-IV:SolutionsandColligativeProperties

Dilute solutions; lowering of vapour pressure, Raoult's and Henry's Laws and their applications. Thermodynamicderivationusingchemicalpotentialtoderiverelationsbetweenthefourcolligativeproperties:
(i) relative lowering of vapour pressure, (ii) elevation of boiling point, (iii) Depression of freezing point, (iv) osmotic pressure and amount of solute. Applications in calculating molar masses of normal, dissociated and associated solutes in solution.

Listofexperiments

1. Determination of heat capacity of a calorimeter for different volumes using change of enthalpy data of a known system (method of back calculation of heat capacity of calorimeter from known enthalpy of solution or enthalpy of neutralization).
2. Determination of heat capacity of the calorimeter and enthalpy of neutralization of hydrochloric acid with sodium hydroxide.
3. Calculation ofthe enthalpyofionization ofethanoicacid.
4. Determination of heat capacity of the calorimeter and integral enthalpy (endothermic and exothermic) solution of salts.
5. Determination of basicity/proticity of a polyprotic acid by the thermochemical method in terms of the changes of temperatures observed in the graph of temperature versus time for different additions of a base. Also calculate the enthalpy of neutralization of the firststep.
6. Determinationofenthalpyofhydrationofcoppersulphate.
7. Determinationofheatof solution (ΔH)ofoxalicacid/benzoic acidfrom solubilitymeasurement.

TextBooks:

- ✓ *P.W.Atkins&J.dePaula,ElementsofPhysicalChemistry, Oxford UniversityPress, 6th Ed., 2006.*
- ✓ *D.A.McQuarrie,&J.DSimon.MolecularThermodynamics VivaBooksPvt. Ltd.:NewDelhi 2004.*
- ✓ *K. L.Kapoor,TextBook ofPhysicalChemistry, Mac GrowHill,3rd Edn.2017*
- ✓ *B.D.Khosla,V.C.Garg,&A.Gulati,SeniorPracticalPhysicalChemistry,R.Chand&Co.:NewDelhi 2011.*

ReferenceBooks:

- ✓ *T.Engel&P.Reid,PhysicalChemistry3rd Ed.Pearson2013.*
- ✓ *S.C.KheterpalPradeep'sPhysicalChemistry,Vol.I&II,PradeepPublications 2011.*
- ✓ *Puri,Sharma&Pathania,PrinciplesofPhysical Chemistry,Vishal PublishingCo,47th Edn.,2017.*

Core V Semester III

AcidsandBases,Metallurgy,Chemistryofmaingroupelements

CourseObjectives:

To provide the basic knowledge on general principles of acids and bases, principle of metallurgy and chemistryofs-and p-block elements. Students can learnabout chronological developments ofthe concepts of acids and bases. It will help students to get aware of the pH scale and classify a substance as acidic, basic, or neutral based on their pH or hydrogen ion concentration. Students can achieve the knowledge regarding volumetric analysis and preparation of metal complex.

CourseOutcomes:

1. Know howthevarioustheoriesofacidandbase,and understandtheoccurrence andpurificationof metals
2. Learnthedifferentproperties ofs-andp-block elements
3. Understandthepreparationandpropertiesofinorganicpolymers.
4. Achieveknowledgeonhow tostandardize,estimateand prepareinorganiccompounds/metalions.

Unit–I:AcidsandBases

Different concepts of acids and bases: Arrhenius theory, Bronsted-Lowry theory, Lewis theory, The Lux-Flood definition, The Usanovich definition, acids and bases in proton solvents, Concept of conjugate acid and conjugate base, Concept of pH, Pearson's classification of Lewis acid and Lewis bases into Hard and Soft Acids and Bases (HSAB), HSAB principle, application of HSAB principle.

Principleof metallurgy

Chief modes of occurrence of metals, Ellingham diagrams for reduction of metal oxides using carbon and carbon monoxide as reducing agent, electrolytic reduction, hydrometallurgy. Methods of purification of metals:electrolyticprocess,partingprocess,VanArkel-deBoerprocess,Mond'sprocessandZonerefining.

Unit– II:Chemistryof*s*-BlockElements

Generalcharacteristics: meltingpoint,flamecolour,reducingnature,diagonalrelationshipsandanomalous behavioroffirstmemberofeachgroup.Reactionsofalkaliandalkalineearthmetalswithoxygen,hydrogen, nitrogen and water. Common features such as ease of formation, thermal stability and solubility of the followingalkali and alkaline earth metal compounds: hydrides, oxides, peroxides, superoxides, carbonates, nitrates, and sulphates. Complex formation tendency of s-block elements; structure of the following complexes: crown ethers and cryptates of Group I; Hydride and their classifications: ionic, covalent and interstitial, EDTA complexes of calcium and magnesium. Solutions of alkali metals in liquid ammonia and their properties.

Unit– III: Chemistryof*p*-BlockElements

Electronic configuration, atomic and ionic size, metallic/non-metallic character, melting point, ionization enthalpy,electrongainenthalpy,electronegativity,catenation,allotropyofC,P,S;inertpaireffect,diagonal relationship between B and Si and anomalous behavior of first member of each group. interhalogen and pseudo halogen compounds, Structure, bonding and properties (acidic/basic nature, stability, ionic/covalent nature, oxidation/reduction, hydrolysis, action of heat) of the following:

- **Hydrides:**hydridesofGroup13 (onlydiborane),Group14, Group15, Group16 andGroup 17.
- **Oxides**:oxidesofphosphorus,sulphurandchlorine
- **Oxoacids:**oxoacids ofphosphorusandchlorine;per oxoacids of sulphur
- **Halides:**halidesofsiliconand phosphorus

Unit–IV:Noblegases

Occurrenceanduses,rationalizationof inertnessof noblegases,clathrates;preparationand properties of XeF_2, XeF_4 and XeF_6. Molecular shapes of noble gas compounds (VSEPR theory).

Inorganicpolymer

Preparation,properties,structureandusesofthefollowingcompounds:Borazine,Silicates, silicones, phosphonitrilic halides $\{(PNCl_2)_n$ where n = 3 and 4$\}$, and concept of carbophosphazene.

List ofexperiments

1. Standardizationofsodiumthiosulphatesolutionbystandard$K_2Cr_2O_7$solution.
2. Estimationofcopperusingstandardsodiumthiosulphatesolution(Iodometrically).
3. Estimationofavailablechlorineinbleachingpowderiodometrically.
4. PreparationofCuprouschloride(Cu_2Cl_2)
5. PreparationofManganese(III)phosphate($MnPO_4.H_2O$)
6. PreparationofLeadchromate($PbCrO_4$)

TextBooks:

- ✓ *A.J.Elias,TheChemistryofthep-BlockElements-Syntheses,ReactionsandApplications, University Press (India) Pvt Ltd., 2009.*
- ✓ *J.D.Lee,ConciseInorganicChemistryWileyIndia,5th Edn.,2008.*
- ✓ *J.E.Huheey,E.A.Keiter,R.L.Keiter,InorganicChemistry–Principlesofstructureand reactivity, Pearson Education, 4th Ed. 2002.*

ReferenceBooks:

- ✓ *A.K.Das,Fundamentalsof InorganicChemistry,Vol.I,CBSPublications, 2nd Ed.,2010.*
- ✓ *S.Prakash,G.D.Tuli,S.K.Basu,R.D.Madan,AdvancedInorganicChemistry,Vol.I,7th Ed.,S. Chand & Company Pvt. Ltd., 2021.*
- ✓ *Puri,Sharma,Kalia,PrinciplesofInorganicChemistry,VishalPublicationCo.,33rd Ed.,2017.*
- ✓ *D.E.Shriver,P.W.Atkins,InorganicChemistry,OxfordUniversityPress,5th Ed.,2010.*
- ✓ *G.L.Miessler,P.J.Fischer,D.A.Tarr,InorganicChemistry,5thEd.,Pearson,2014.*
- ✓ *J.Mendham,Vogel'sQuantitativeChemicalAnalysis,6th Ed.,Pearson,2009.*
- ✓ *V.K.Ahluwalia,S.Dhingra,A.Gulati,CollegePracticalChemistry,UniversityPress,2005.*

CoreVI

Chemistryofhalogen,oxygenandsulphurcontainingorganiccompounds

CourseObjectives:

To provide the knowledge on organic compounds containing halogen, alcohol, phenol, thiol, ether, thioether, aldehydes,ketones,carboxylicacidsanditsderivativesasfunctionalgroups.Furthertoknowtheirpreparation, properties and reactivity for developing the skills required for synthesizing a target molecule from a given molecule.

CourseOutcomes:

1. Understandingonpreparation,propertiesandreactionsofhaloalkanes,haloarenes,andorganiccompounds containing C, H, O and S functional groups.
2. Basic knowledge on various name reactions and their mechanisms involving substitution, addition, elimination and condensation.
3. Knowledgeonfunctionalgroupinterconversionandsyntheticapplicationsofdifferentorganiccompounds.
4. Knowledgeon various functional group detection in organic compounds and preparation of derivatives of functional groups.

Unit-I:ChemistryofHalogenatedHydrocarbons

Alkylhalides:Methodsofpreparation,nucleophilicsubstitutionreactions –$SN1$,$SN2$ andSN_imechanisms with stereochemical aspects and effect of solvent and nucleophiles. substitution vs. elimination.
Aryl halides: Preparation, including preparation from diazonium salts, nucleophilic aromatic substitution; SNAr, Benzyne mechanism.
Relativereactivityofalkyl, allyl/benzyl,vinyl andarylhalidestowardsnucleophilicsubstitutionreactions.

Unit-II:Alcohols,Phenols,EthersandEpoxides

Alcohols: preparation, properties and relative reactivity of 1°, 2°, 3° alcohols, Bouvaelt-Blanc Reduction; Preparationandproperties ofglycols: Oxidationbyperiodicacid andleadtetraacetate, Pinacol-Pinacolone rearrangement;
Phenols: Preparation and properties; Acidity and factors effecting it, Ring substitution reactions, Reimer–Tiemann and Kolbe's–Schmidt Reactions, Fries and Claisen rearrangements with mechanism;
EthersandEpoxides:Preparationandreactionswithacids.Reactionsofepoxideswithalcohols,Ammonia derivatives and $LiAlH_4$.
Sulphurcontainingcompounds:Preparation andreactionsofthiolsandthioethers

Unit-III:CarbonylCompounds

Structure, reactivity and preparation. Nucleophilic additions, Nucleophilic addition-elimination reactions with ammonia derivatives with mechanism; Mechanisms of Aldol and Benzoin condensation, Knoevenagel condensation, Perkin, Cannizzaro and Wittigreaction, Beckmann rearrangements, α halo-form reaction and Baeyer-Villigeroxidation,-substitutionreactions,oxidationsandreductions(Clemmensen, Wolff-Kishner, $LiAlH_4$, $NaBH_4$, MPVO.; Addition reactions of unsaturated carbonyl compounds: Michael addition.
Active methylene compounds: Keto-enol tautomerism. Preparation and synthetic applications of diethyl malonate and ethylaceto acetate.

Unit-IV:CarboxylicAcidsandDerivatives

Preparation, physical properties and reactions of monocarboxylic acids: Typical reactions of dicarboxylic acids,hydroxyacidsandunsaturatedacids:succinic,lactic,malic,tartaric,citric,maleicandfumaricacids;
Preparation and reactions of acid chlorides, anhydrides, esters and amides; Comparative study of nucleophilic substitution at acyl group -Mechanism of acidic and alkaline hydrolysis of esters, Claisen condensation, Dieckmann and Reformatsky reactions, Hofmann-bromamide degradation and Curtius rearrangement.

List of Experiments

1. Functionalgrouptestsforamines(*p*-,*sec-tert*-),nitro,amideandimidegroupsinknownorganic compounds.
2. Benzolyation of one of the following amines (aniline, o-, m-, p- toluidines and o-, m-, p- anisidine) and one of the following phenols (β-naphthol, resorcinol, p-cresol) by Schotten-Baumann reaction.
3. Bromination ofanyoneof thefollowing:
   a) Acetanilidebyconventionalmethods
   b) Acetanilideusinggreenapproach(Bromate-bromidemethod)
4. Nitrationofanyoneof thefollowing:
   a) Acetanilide/nitrobenzenebyconventional method
   b) Salicylicacidbygreenapproach(using cericammoniumnitrate).
5. Identification of unknown organic compounds containing one functional group in CHO or CHN systems and their derivative preparation.

Text Books:

- ✓ *R.T.Morrison,R.N.Boyd,S.K.Bhattacharjee,OrganicChemistry,7th Ed.,PearsonEducationIndia, 2010.*
- ✓ *A.Bahl,B.S.Bahl,Advanced OrganicChemistry,5th Ed.,S.Chand,2012.*
- ✓ *N.K.Vishnoi,AdvancedPracticalOrganicChemistry,3rd Ed.,VikasPublishingHouse, 2009.*

o *ReferenceBooks:*

- ✓ *T.W.GrahamSolomons,C.G.Fryhle,S.A.Snyder,Solomons'OrganicChemistry,GlobalEd., Wiley, 2024.*
- ✓ *J.Clayden,N.Greeves, S.Warren, OrganicChemistry,2nd Ed.,OxfordPublisher, 2012.*
- ✓ *R.K.Bansal,OrganicReactionMechanism,3rd Ed.,TataMcGraw-HillPublications,1998.*
- ✓ *P.Sykes,AGuidebooktoMechanisminOrganicChemistry, 6th Ed.,PearsonEducation,2003.*
- ✓ *F.A.Carey,R.J.Sundberg,AdvancedOrganicChemistry,Part-AandPart-B,5th Ed.,Springer2007.*
- ✓ *B.S.Furniss,A.J.Hannaford,P.W.G.Smith,A.R.Tatchell,Vogel'sTextbookofPracticalOrganic Chemistry, 5th Ed., Pearson Education India, 2003.*
- ✓ *O.P.Agarwal,AdvancedPracticalOrganicChemistry,KrishnaPrakashan, 2014.*
- ✓ *V. K. Ahluwalia, R. Aggarwal, Comprehensive Practical Organic Chemistry: Preparation and Quantitative Analysis, Universities Press, 2004.*
- ✓ *H.T.Clarke,AHandbookofOrganicAnalysis:QualitativeandQuantitative,4th Ed.,CBS Publishers, 2021.*

Core VII

Phaseequilibrium,Chemicaldynamics,catalysisandsurfacechemistry

CourseObjectives:

Thiscourseisoffered bySchool of Chemistryasacoresubject fortheB.Sc. programme, withan emphasis on fundamental understandingphaseequilibrium and chemical kinetics. Theobjectiveofthis course is to develop basic and advance concepts regarding of Surface chemistry and catalysis. It aims to study the similarityanddifferencesbetween adsorptionisothermsandreasonsresponsibleforthese.Theobjectiveofthe practical is to develop skills for working in physical chemistry laboratory pertaining to kinetics & adsorption isotherms.Thestudentwillperformexperimentsbasedontheconceptslearntin Physicalchemistry-IIIcourse.

CourseOutcomes:

Bytheend ofthecourse,the students will beableto:

- Establishthephaseruleforone,twocomponentsystems,eutectics;anditsthermodynamicderivation; fundamentals of physical transformation of pure materials.
- Interpretchemical kineticsofchemicalreactions anditsimpactonreactionmechanism.
- Differentiatebetweenhomogenousandheterogenouscatalysis&AcidBaseCatalysis,differentiatebetween Physical adsorption, chemisorption and various adsorption isotherms.
- Determinedistributioncoefficientsofsolutionmixtures,Interpretandusedatageneratedfromkinetic studies by graphical and experimental methods.

Unit-I:PhaseEquilibria-I

Concept of phases, components and degrees of freedom, derivation of Gibbs Phase Rule for nonreactive and reactive systems; Clausius-Clapeyron equation and its applications to solid- liquid, liquid-vapour and solid-vapour equilibria, phase diagram for one component systems, with applications (H_2O and sulphur system). Phasediagramsforsystemsofsolid-liquidequilibriainvolvingeutectic(Pb-Agsystem,desilverisationoflead), congruent (ferric chloride-water) and incongruent (sodium sulphate- water) melting points.

Unit-II:PhaseEquilibria-II

Threecomponentsystems,water-chloroform-aceticacidsystem,triangular plots.
Binary solutions: Gibbs-Duhem-Margules equation, its derivation and applications to fractional distillation of binary miscible liquids (ideal and non-ideal), azeotropes, partial miscibility of liquids, CST, miscible pairs, steam distillation. Nernst distribution law: its derivation and applications.

Unit-III:ChemicalKinetics

Order and molecularityof a reaction, derivation of rate laws (Zero, first, and second order) and its differential andintegratedformofrateexpressionsuptosecondorderreactions,experimentalmethodsofthedetermination of orders. Kinetics of complex reactions (integrated rate expressions up to first order only): (i) Opposing reactions (ii) parallel reactions (iii) consecutive reactions and their differential rate equations (steady-state approximation in reaction mechanisms) (iv) chain reactions (HBr chain reaction).
Temperature dependence of reaction rates; Arrhenius equation; activation energy. Collision theory of reaction rates, qualitative treatment of the theory of absolute reaction rates.

Unit-IV: Catalysis

Types of catalyst, specificity and selectivity, mechanisms of catalyzed reactions at solid surfaces; effect of particle size and efficiency of nanoparticles as catalysts. Enzyme catalysis, Michaelis- Menten mechanism, acid-base catalysis. Surface chemistry: Physical adsorption, chemisorption, adsorption isotherms (Langmuir, Freundlich and Gibb's isotherms), nature of adsorbed state.

List ofexperiments

1. Determinationofdistributioncoefficientsof:
   (a) Iodinebetweenwaterandcarbontetrachloride.
   (b) Acetic/benzoicacidbetweenwaterandcyclohexane.
2. Studytheequilibriumofatleastoneofthefollowingreactionsbythe distribution method:

- $I_2(aq)+I^- \rightarrow I_3^-(aq)$
- $Cu^{2+}(aq)+nNH_3 \rightarrow Cu(NH_3)_n$

3. Studythekineticsofthefollowingreactions.
   (i) Integratedratemethod:
   a) Acidhydrolysis ofmethyl acetatewithhydrochloricacid.
   b) Saponificationofethylacetate.
   (ii) ComparethestrengthsofHCl andH_2SO_4bystudyingkineticsofhydrolysisofmethylacetate.
4. VerifytheFreundlichandLangmuirisothermsforadsorptionofaceticacid onactivatedcharcoal.

TextBooks:

- ✓ *P.W.Atkins,J.dePaula, ElementsofPhysical Chemistry,OxfordUniversityPress,6th Ed., 2006.*
- ✓ *K.J.Laidler,Chemical kinetics,NewYork:Harper&Row1916*
- ✓ *J.Rajaram,J.C.KuriacoseKineticsandMechanismsofChemicalTransformations,PenguinBooksLtd,2000.*

ReferenceBooks:

- ✓ *T.Engel,P.Reid,Physical Chemistry3rd Ed.Pearson2013.*
- ✓ *D.A.McQuarrie,J.D.Simon,MolecularThermodynamics VivaBooksPvt. Ltd.:NewDelhi2004.*
- ✓ *K.L.Kapoor,TextBook ofPhysicalChemistry, MacGrowHill,3rdEdn.2017*

Core VIIISemester IV

Coordination Chemistry, Chemistry of d- and f-block elements,InorganicReactionMechanismandelectron transfer reactions

CourseObjectives:

Toprovidetheknowledgeonthecoordinationcompoundswhichfindmanifoldapplicationsinthediversefields suchasindustrialcatalysis,metallurgy,pharmaceuticalindustry,paintsandpigments.Studentswillachievethe knowledgeaboutthediversekineticaspectsofthecoordinationcompounds.Theywillalsobefamiliarizedwith the chemistry of d- and f-block elements and get an idea about horizontal similarity in a periodin addition to verticalsimilarityinagroup.Besides,theideaofinorganicreactionmechanismandtheimportanceofelectron transferreactionshavebeenreviewed.Synthesisandestimationofinorganiccompoundshave been included to enhance the practical skill of students in this regard.

CourseOutcomes:

1. Understandthechemistryofcoordinationcompounds,andd-andf-Blockelements.
2. Explainmagneticpropertiesand colourofcomplexes onthebasisofCrystalField Theory.
3. Understandingthefundamentalimportanceofinorganicreactionmechanismandelectrontransfer reaction
4. Achieved the knowledge of the preparation of inorganic complex, estimation by EDTA method andgravimetric method.

Unit–I:CoordinationChemistry

Werner's Coordination theory, IUPAC nomenclature of coordination compounds, isomerism in coordination compoundswithcoordinationnumbers4and6.Abriefideaaboutchelateeffect,andlabileandinertcomplexes.

Valencebondtheoryand itsapplicationtocomplexesofcoordinationnumbers4and6.Examplesof innerand outer orbital complexes. Crystal field theory and its application, measurement of Δ_o. Calculation of CFSE in weak and strong fields, concept of pairing energies, factors affecting the magnitude of Δ_o. Octahedral *vs.* tetrahedral coordination, tetragonal distortions from octahedral geometry, Jahn-Teller theorem, square planar geometry. Qualitative aspect of Ligand field theory, and MO Theory (bonding and antibonding interactions, idea about σ, σ^*, π, π^*, n –MO).

Unit– II:Chemistryof d-andf-BlockElements

Chemistryoftransitionmetals:Generalgrouptrendswithspecialreferencetoelectronicconfiguration, colour, variable valency, magnetic properties (no temperature dependence), catalytic properties, and ability to form complexes. Distinction among the first, second and third transition series. Chemistryof Ti, V, Cr, Mn, Fe and Co in various oxidation states (excluding their metallurgy). Some importantcompoundsofCr,Mn,FeandCo andtheirrolesaslaboratoryreagents;Potassiumdichromate,potassiumpermanganate, potassium ferrocyanide, potassium ferricyanide, sodium nitroprusside and sodium cobaltinitrite. Chemistry of Lanthanides and Actinides: electronic configuration, oxidation states, colour, spectral and magnetic properties. Lanthanide contraction (causes and effects), separation of lanthanides by ion exchange method. General features of actinides, separation of Np, Pm, Am from U.

Unit– III:InorganicReactionMechanism

Thermodynamicandkineticstability,Stepwiseandoverallformationconstantsandtheirrelationship,factors affecting stability, Substitution reactions in square planar complexes, trans-effect, theories of trans- effect (electrostatic polarization and π-bonding theory), Substitution reactions in octahedral complexes, acid hydrolysis of octahedral Co(III) complexes with reference to effect of charge, chelation, steric crowding & effects of leaving group, base hydrolysis of octahedral Co(III) complexes: Conjugate base mechanism, test of conjugate base mechanism, anation reaction.

Unit–IV:Electrontransferreaction

Redox reactions: electron tunneling hypothesis, concept of Marcus-Hush theory, atom transfer reactions, one and two electron transfer, complementary and non-complementary reactions, inner sphere and outer sphere reactions, electron transfer through extended bridges, concept of hydrated electron.

Listofexperiments

1. Synthesisofhexaminenickel(II)complex,$[Ni(NH_3)_6]Cl_2$
2. Synthesisoftetraamminecopper(II)sulphate,$[Cu(NH_3)_4]SO_4.H_2O$
3. EstimationofCaandMgfromcementbyEDTAmethod
4. Estimationofnickel(II)usingdimethylglyoxime(DMG)

TextBooks:

- ✓ *J.D.Lee,ConciseInorganicChemistry,WileyIndia,5th Edn.,2008.*
- ✓ *J.E.Huheey,E.A.Keiter,R.L.Keiter, InorganicChemistry–Principlesofstructureandreactivity, PearsonEducation, 4th Ed. 2002.*
- ✓ *F.A.Cotton,G.Wilkinson,AdvancedInorganicChemistryWiley-VCH.,1999.*

Reference books:

- ✓ *A.K.Das, Fundamentals of InorganicChemistry,Vol.II,CBSPublications,2nd Ed.2010.*
- ✓ *G.H.Jeffery,J.Bassett,J.Mendham,R.C.Denney,Vogel'sTextbookofQuantitativeChemical Analysis, John Wiley and Sons, 1989.*
- ✓ *Puri,Sharma,Kalia,PrinciplesofInorganicChemistry,VishalPub.Co.,33rd ed.,2017.*
- ✓ *D.E.Shriver,P.W.Atkins, InorganicChemistry,OxfordUniversityPress,5th Edn.*
- ✓ *V.K.Ahluwalia,S.Dhingra,A.Gulati,CollegePracticalChemistry,UniversityPress(2005).*
- ✓ *S.Gulati,J.L.Sharma,S.Manocha,PracticalInorganicChemistry,1st Edn.,CBSPublishers& Distributors Pvt Ltd., (2017).*

Core-IX

NaturalProducts,HeterocyclicCompounds,NitrogencontainingcompoundsandPolynuclear Hydrocarbons

CourseObjectives:

Imparting information on natural products, nitrogen based organic compounds, heterocyclic compounds and polynuclearhydrocarbonswiththeirchemicalpropertiesandstructuralelucidation.Impartinghandsontraining in estimation and analysis of organic compounds.

CourseOutcomes:

1. Gainingknowledgeonpreparation,propertiesandsyntheticapplicationofnitrogencontainingcompounds including diazonium salts.
2. Understandingonisolation andstructural elucidation ofnatural products andheterocyclic compounds and their chemical reactions.
3. Knowledgeonstructure andpropertiesoffusedaromaticcompounds.
4. Learningonvariousprocedures ofestimationoforganiccompounds.

Unit-I:NitrogenContainingFunctionalGroups

Amines*:* Effect of substituent and solvent on basicity; Preparation from nitro and nitriles and properties: Gabrielphthalimidesynthesis,Carbylaminereaction,Mannichreaction,Hoffmann'sexhaustivemethylation, Hofmann-elimination reaction; Distinction between 1°, 2° and 3° amines with Hinsbergreagent and nitrous acid.

*DiazoniumSalt*s**:**Preparationand theirsynthetic applications.

Unit-II:DyesandPolynuclearhydrocarbonderivatives

Classification, colour and constitution; Mordant and Vat dyes; Chemistry of dyeing. Synthesis and applicationsof:*Azodyes*–MethylorangeandCongored(mechanismofDiazocoupling);*Triphenylmethane dyes*-MalachiteGreen,andcrystalviolet;*Phthaleindyes*–PhenolphthaleinandFluorescein.Edibledyeswith example.

Preparation of Polynuclear Hydrocarbons: Reactions of naphthalene, anthracene, phenanthrene, acenaphthene,pyrene.Preparation andtheirstructureelucidation(naphthalene)andimportantderivativesof naphthalene and anthracene.

Unit-III:HeterocyclicCompounds

Classification and nomenclature, Structure, aromaticityin 5-numbered and 6-membered rings containingone heteroatom, Reaction and mechanism of substitution reactions of: Furan, Pyrrole, Thiophene and Pyridine. Synthesis of Pyrrole (Paal-Knorr synthesis, Knorr pyrrole synthesis), Furan (Paal Knorr synthesis, Fiest-Benary Synthesis), Derivatives of Furan: Furfural and Furoic acid (preparation only) Pyridine (Hantzsch synthesis). Pyrimidine (synthesis from β-keto acid), Bicyclic Heterocyclic compound: Indole (Fischer indole synthesis and Madelung synthesis) Quinoline (Skraup synthesis, Friedlander Synthesis).

Unit-IV:NaturalProducts(11hrs)

Alkaloids

Natural occurrence, General structural features, Isolation and their physiological action. Hoffmann's exhaustive methylation, Emde's modification, Structure elucidation, synthesis and medicinal importance of Hygrine, Nicotine, Quinine and Morphine

Terpenes

Occurrence,classification,isoprenerule;Elucidation ofstructureandsynthesisofCitral,andα-terpineol.

List ofExperiments

1) Qualitativeanalysis ofunknownorganiccompounds containingbifunctional groups
2) EstimationofPhenol/Aniline
3) EstimationofMethylKetone
4) Determinationofpercentagepurityofcarbonylcompound.

TextBooks:

- ✓ *R.T.Morrison,R.N.Boyd,S.K.Bhattacharjee,OrganicChemistry,7th Ed.,PearsonEducationIndia, 2010.*
- ✓ *I.L. Finar,OrganicChemistry,Vol-2,5th Ed.,PearsonPublisher,2002.*
- ✓ *N.K.Vishnoi,AdvancedPracticalOrganicChemistry,3rd Ed.,VikasPublishingHouse, 2009.*

ReferenceBooks:

- ✓ *T.W. GrahamSolomons,C.G. Fryhle,S.A. Snyder,Solomons' OrganicChemistry,GlobalEd., Wiley, 2024.*
- ✓ *J.Clayden,N.Greeves,S.Warren,OrganicChemistry,2nd Ed.,OxfordPublisher, 2012.*
- ✓ *J.A.Joule,K.Mills,HeterocyclicChemistry,5th Ed.,WileyBlackwell,2010.*
- ✓ *R.K.Bansal,HeterocyclicChemistry,5th Ed.,NewAge International, 2017.*
- ✓ *O.P.Agarwal,OrganicChemistry:NaturalProducts,Vol. I,KrishnaPrakashanMedia,2015.*
- ✓ *H.T.Clarke,AHandbookofOrganicAnalysis:QualitativeandQuantitative,4th Ed.,CBS Publishers, 2021.*

Core X

Conductance,electrochemistry,electricalpropertiesofatomsandmolecules

CourseObjectives:

This course offers in introductoryknowledge of electrolytic conductance depth knowledge of electrochemical cells.Studentsareexpectedtohavebackgroundknowledgeinphysicalchemistryandmathematicsuptothe +2 level for this course. The objective of the practical is to develop skills for working in physical chemistry laboratory.Thestudentwillperformexperimentsbasedontheconceptslearntin Physicalchemistry-IVcourse.

CourseOutcomes:

Bytheend ofthecourse,the students will beableto:

1. The text provides an in-depth analysis of the conductance nature of electrolytic solutions, their thermodynamics, Debye-Huckel theory, ionic strength, mean ionic activity coefficient, and the Debye-Huckel limiting law.
2. Explaindynamicelectrochemical processesandskilldevelopmenttoanalyseit.
3. Understandthedynamic electrochemical processesandskilldevelopmenttoanalyseit.
4. Develop skill to solve problems on Electrochemical Cells, electrode potentials, emf & solubility product measurements, potentiometric titrations, pK and pH measurements.

Unit-I:Conductance-I

Arrhenius theory of electrolytic dissociation. Conductivity, equivalent and molar conductivity and their variationwithdilutionforweakandstrongelectrolytes.Molarconductivityatinfinitedilution.Kohlrauschlaw of independent migration of ions. Debye-Hückel-Onsager equation, Wien effect, Debye-Falkenhagen effect, Walden's rules.

Unit-II:Conductance-II

Ionicvelocities,mobilitiesandtheirdeterminations,transferencenumbersandtheirrelationtoionicmobilities, determination of transference numbers using Hittorf and Moving Boundary methods. Applications of conductance measurement: (i) degree of dissociation of weak electrolytes, (ii) ionic product of water (iii) solubility and solubility product of sparingly soluble salts, (iv) conductometric titrations, and (v) hydrolysis constants of salts.

Unit-III:Electrochemistry-I

Quantitativeaspectsof Faraday'slawsofelectrolysis,rulesofoxidation/reductionofionsbasedon half-cell potentials, applications of electrolysis in metallurgy and industry.
Chemical cells, reversible and irreversible cells with examples. Electromotive force of a cell and its measurement,Nernstequation;Standardelectrode(reduction)potentialanditsapplicationtodifferentkindsof half-cells. Application of EMF measurements in determining free energy, enthalpy and entropy of a cell reaction, (ii) equilibrium constants, and (iii) pH values, using hydrogen, quinone-hydroquinone, glass electrodes.

Unit-IV:Electrochemistry-II

Concentration cells with and without transference, liquid junction potential; determination of activity coefficients and transference numbers. Qualitative discussion of potentiometric titrations (acid-base, redox, precipitation). **Electrical properties of atoms and molecules**: Basic ideas of electrostatics, Electrostatics of dielectricmedia.Clausius-MosottiequationandLorenz-Laurentzequation(noderivation),Dipolemomentand molecular polarizabilities and their measurements.

List ofexperiments

I. Determinationofcellconstant.

II. Determinationofequivalentconductance,degreeofdissociationanddissociationconstantofaweak acid.

III. Performthefollowingconductometrictitrations:

i. Strongacidvs. strongbase

ii. Weakacid vs. strongbase

iii. Strongacidvs.weakbase

I Performthefollowingpotentiometrictitrations:

i. Strongacidvs. strongbase

ii. Weakacidvs.strongbase

iii. Dibasicacidvs.strongbase

TextBooks:

- ✓ *P.WAtkins.&J.dePaula,ElementsofPhysicalChemistry,OxfordUniversityPress,6th Ed., 2006.*
- ✓ *J.O.Bockris&A.Reddy.ModernElectrochemistry, KluwerAcademic, 2002.*
- ✓ *S.Glasstone,AnIntroductiontoElectrochemistry:AffiliatedEastWestPressPrivate,Limited.1960*

ReferenceBooks:

- ✓ *T.Engel&P.Reid,PhysicalChemistry3rd Ed.Pearson2013.*
- ✓ *McQuarrie,D.A.&Simon,J. D.MolecularThermodynamicsVivaBooks Pvt. Ltd.:NewDelhi 2004.*
- ✓ *KheterpalS.C.,Pradeep'sPhysicalChemistry,Vol.I&II,PradeepPublications.2002.*

CoreXISemester V

Organic Spectroscopy

CourseObjectives:

To provide knowledge on the principles of different advanced spectroscopic methods such as UV-Visible, FTIR, NMR and Mass-spectrometry and to develop analytical aptitude for interpretation of structure of the organic compounds by applying these spectroscopic methods. Imparting practical knowledge on UV-visible spectroscopy and colour of compounds.

CourseOutcomes:

- GainingknowledgeonprincipleofUV-visibleandInfraredSpectroscopictechniques.
- GainingknowledgeonprincipleofNMRSpectroscopic techniques.
- Gainingknowledgeonprinciple ofMass Spectrometrytechniques.
- Understandingandinterpretationofdifferentspectraoforganic molecules.

Unit-I:UV-VisibleSpectroscopy

Types of electronic transitions, λ_{max}, Lambert-Beer's law and its limitations, Chromophores and Auxochromes, Bathochromic and Hypsochromic shifts, Intensity of absorption; Instrumentation (brief idea only), Application of Woodward rules for calculation of λ_{max} for the following systems: α, β- unsaturated carbonyl compounds, acids and esters; Conjugated dienes, distinction between cis and trans isomers.

Unit-II:FTIRSpectroscopy

Fundamental and non-fundamental molecular vibrations; IR absorption positions of O and N containing functional groups; Effect of H-bonding, conjugation, resonance and ring size on IR absorptions; Fingerprint region and its significance; application in simple functional group analysis

Unit-III:NMRSpectroscopy

NMR Spectroscopy: Basic principles of Proton Magnetic Resonance, chemical shift and factors influencing it; Equivalent and non-equivalent protons, Spin-spin coupling and coupling constant; Anisotropic effects in alkene, alkyne, aldehydes and aromatics; Interpretation of NMR spectra of simple organic compounds. ^{13}C NMR spectroscopy, chemical shift values and interpretation of NMR spectra. preliminary idea on NMR of ^{15}N, ^{19}F, ^{31}P nuclei.

Unit-IV:MassSpectrometry

Introduction,Basicprinciple,Fragmentationpattern,instrumentation,Determinationofmolecularformulae, molecular ions, Parent peak, Base peak, isotopic peak and metastable ion peak. Use of molecular fragmentation, McLafferty rearrangement, Mass spectra of some classes of compounds (hydrocarbons, alcohols, phenols, ketones, aldehydes, acids and esters)

Problemsinvolvingidentificationoforganiccompounds usingUV, IR,NMRandMassspectroscopy.

List ofExperiments

1) Using an UV-visible spectrophotometer, obtain the uv-visible spectrum, determine the λ_{max} value and, after comparing the spectra of the following molecules, predict the effect of auxochrome and conjugation on absorption maxima.

   (a) Takeandanalyzethespectraofbenzene,aniline,and4-methoxyanilineusingasuitablesolvent.Then, compare the results after adding dil hydrochloric acid to it.

   (b) Takeandanalyzethespectraofsalicylicacid,benzoicacidand*p*-aminobenzoicacid,cinnamic acid in neutral and then compare the result after adding dil NaOH to it.

   (c) Takeand analyzethespectraofo-nitrophenol, p-nitrophenolsandnitrobenzeneinneutralandthen compare the result after adding dil NaOH to it.

2) Identificationoflabelled peaksinthe^{1}HNMRspectraoftheknownorganiccompoundsandtoexplain their δ-values and splitting pattern on a supplied NMR spectra.

2)IdentificationoflabelledpeaksintheIRspectrumofacompoundandtoexplaintherelativefrequencies of the absorptions (C-H, O-H, N-H, C-O, C-N, C-X, C=C, C=O, N=O, C≡C, C≡N) of a supplied spectrum.

Text Books:

- ✓ *W.Kemp,OrganicSpectroscopy,2nd Ed.,Macmillan, 2019.*
- ✓ *P.S.Kalsi,SpectroscopyofOrganicCompounds,9th Ed.,NewAge International Publishers,2022.*
- ✓ *D.L.Pavia,G.M.Lampman,G.S.Kriz,J.R.Vyvyan,IntroductiontoSpectroscopy,5thEd.,Cengage India Private Limited, 2015.*

ReferenceBooks:

- ✓ Y.R.Sharma,ElementaryOrganicSpectroscopy,5th Ed.,S.Chand,2013.
- ✓ JagMohan,OrganicSpectroscopy: PrinciplesandApplications,2nd Ed.,NarosaPublishers,2009.
- ✓ J.Singh,JSingh,OrganicSpectroscopy:Principles,ProblemsandtheirSolutions,PragatiPrakashan, 2019.
- ✓ R. M. Silverstein, F. X. Webster, D. J. Kiemle, D. L. Bryce, Spectrometric Identification of Organic Compounds, 8th Ed., Wiley, 2022.

Core XII

Basicquantumchemistry,Molecular&electronicspectroscopy,andphotochemistry

CourseObjectives:

ThiscourseisofferedbySchoolofChemistryasa coresubjectfor the B.Sc.programme,with anemphasison fundamental understanding of Quantum chemistry, molecular spectroscopy, and photochemistry. Students are expectedtohavebackgroundknowledgeinmathematicsuptothe+2levelforthiscourse. Theobjectiveofthe practicalistodevelopskillsforworkinginphysicalchemistrylaboratory.Thestudentwillperformexperiments based on the concepts learnt in Physical chemistry-V course.

Courseoutcomes:

Bytheend ofthecourse,the students will beableto:

- Understandthepostulatesofquantummechanics.ConstructtheSchrödingerwaveequationsfor1-Dbox,3- D box, Rigid rotor, and SHO and able to interpret the solution of Schrödinger equation.
- UnderstandLCAO-MOcomparewithVBTofH2molecule.ApplythefundamentalsofQuantummechanics to interpret molecular spectroscopy.
- Calculatequantumyieldofphotochemicalreactions.
- Interpret the data obtained from graphical methods of Lambert-Beer's law experiments and corelate withUV-Vis spectroscopy.

Unit-I:QuantumChemistry-I

Quantum mechanical operators, Postulates of quantum mechanics, Schrödinger equation and its application to particle in one-dimensional box (complete solution) - quantization of energy levels, zero-point energy, normalization of wave functions, probability distribution functions, nodal properties. Extension to three-dimensional boxes.

Qualitative treatment of simple harmonic oscillator model of vibrational motion: Setting up of Schrödinger equation and discussion of solution and wave functions. Vibrational energy of diatomic molecules and zero-point energy.

Rigid rotator model of rotation of diatomic molecule: Schrödinger equation, transformation to spherical polar coordinates. Derivation of rotational energy expression of diatomic molecule.

UNIT-IIChemicalBonding

Chemical bonding: Covalent bonding, valence bond and molecular orbital approaches, LCAO- MO treatment ofH_2^+.Bondingandantibondingorbitals.QualitativeextensiontoH2.ComparisonofLCAO-MOandVB

treatments ofH_2 (onlywavefunctions, detailedsolution notrequired)and theirlimitations. Localized and non-localized molecular orbitals treatment of triatomic (BeH_2, H_2O) molecules.

Unit-III:MolecularSpectroscopy

Interaction of electromagnetic radiation with molecules and various types of spectra; Born- Oppenheimer approximation.

Rotation spectroscopy: Selection rules, intensities of spectral lines, determination of bond lengths of diatomic molecules, isotopic substitution.

*Vibrationalspectroscopy:*Classicalequationofvibration,computationofforceconstant,amplitudeofdiatomic molecular vibrations, anharmonicity, Morse potential, dissociation energies, fundamental frequencies, overtones, hot bands, degrees of freedom for polyatomic molecules, modes of vibration. Vibration-rotation spectroscopy: diatomic vibrating rotator, P, Q, R branches.

UNIT-IV:MolecularSpectroscopy-II

Raman spectroscopy: Qualitative treatment of Rotational Raman effect; Effect of nuclear spin, Vibrational Raman spectra, Stokes and anti-Stokes lines; their intensity difference, rule of mutual exclusion. ***Electronic spectroscopy:*** Franck-Condon principle, electronic transitions, singlet and triplet states, fluorescence and phosphorescence, dissociation and predissociation.

Photochemistry Lawsofphotochemistry,quantum yield,actinometry,examplesoflowandhighquantum yields, photochemical equilibrium and the differential rate of photochemical reactions, photosensitised reactions, quenching, chemiluminescence.

List ofexperiments

1. Studyofabsorptionspectra(visiblerange)of$KMnO_4$anddeterminetheλ_{max}value.Calculatetheenergies of the transitions in kJ mol^{-1}, cm^{-1}, and eV.
2. VerifyLambert-Beer'slawanddeterminetheconcentrationof$CuSO_4$/$KMnO_4$/$K_2Cr_2O_7$inasolutionof unknown concentration.
3. Determinethedissociationconstantofanindicator(phenolphthalein).
4. Determinethe concentrationofHClagainst 0.1NNaOHspectrophotometrically.
5. Tofindthestrengthofgivenferricammoniumsulfatesolutionof(0.05M)byusingEDTA spectrophotometrically.
6. Tofindout thestrength of$CuSO_4$solution bytitratingwith EDTAspectrophotometrically.
7. Todeterminetheconcentration ofCu (II)andFe (III)solutionphotometricallybytitratingwith EDTA.

TextBooks:

- ✓ *D.A.McQuarrie,QuantumChemistry,Viva Books,IndianStudentEdition,Reprint,2011*
- ✓ *R.K.Prasad,QuantumChemistry,NewAgeInternational,2006*
- ✓ *I. Levine,QuantumChemistry,7th Edition,Pearson,2000*

ReferenceBooks:

- ✓ T.Engel&P.Reid,PhysicalChemistry3rd Ed.Pearson2013.
- ✓ D.A.McQuarrie, &J.D.Simon,MolecularThermodynamicsVivaBooksPvt.Ltd.:NewDelhi2004.
- ✓ S.C.KheterpalPradeep'sPhysicalChemistry,Vol.I&II,PradeepPublications. 2011.

Core XIII

ChemistryofOrganometallicCompounds

CourseObjectives

To provide the basic knowledge and cutting-edge developments in the field of organometallic chemistry. This includes the classification of organometallic compounds, the concept of hapticity and the 18-electron rule governing the stability of a wide variety of organometallic species. Specific organometallic compounds are studied in detail to understand the basic concepts. It familiarizes the versatility of phosphine/NHC ligands as well as metathesis reactions. It provides much fundamentals about the qualitative inorganic analysis having multiple radical mixtures.

CourseOutcomes:

1. Understand the basic concepts of organometallic compounds pertaining to their synthesis, structure and bonding
2. Understandthemechanisticphenomenaoforganometallicbasedcatalyticreactions
3. Get knowledge on the versatility of phosphine/NHC ligands, and industrially important metathesis reactions.
4. Understandandexplainthebasicprinciplesofqualitativeinorganicanalysis

Unit–I:OrganometallicCompounds-I

Definition of organometallic compound, classifications, nature of metal-carbon bond, nomenclature, the 18-electron rule, Concept of hapticity of organic ligands. Metal carbonyls: electron counting of metal carbonyls of 3d series. General methods of preparation (direct combination, reductive carbonylation, thermalandphotochemicaldecomposition)ofmonoandbinuclearmetalcarbonyls of3dseries.Structures ofmononuclearandbinuclearcarbonylsofCr,Mn,Fe,CoandNiusingVBT.π-acceptorbehaviour ofCO (MOdiagramofCOtobediscussed),synergiceffectanduseofIRdatato explainextentofbackbonding. Zeise's salt: preparation and structure, evidence of synergic effect and comparison of synergic effect with that in carbonyls.

Unit– II: OrganometallicCompounds-II

Metal Alkyls: Important structural features of methyl lithium (tetramer) and trialkyl aluminium (dimer), concept of multicentre bonding in these compounds. Role of triethyl aluminium in the polymerisation of ethene and propylene (Ziegler – Natta Catalyst). Ferrocene: preparation and reactions (acetylation, alkylation,metallation,Mannichcondensation,nitration,halogenation,silylation,borylation,sulphonation), structure and aromaticity, comparison of aromaticity and reactivity with that of benzene. Fluxional molecules. Concept of coordinative unsaturation, oxidative addition, reductive elimination, insertion reaction, migratory insertion, intramolecular hydrogen transfer reaction, agostic interaction.

Unit– III: OrganometallicCatalysis

General idea of catalysis, turnover number (TON), turnover frequency (TOF), hydrogenation of alkenes using Wilkinson's catalyst, Tolman catalytic loop, hydroformylation of alkenes (using cobalt catalyst), enantioselective hydrofomylation, wacker process, mosanto acetic acid synthesis, cativa process, hydrosilylationreactions,reductionof carbonmonoxidebyhydrogen(Fischer-Tropschreaction).Concept of Pd-catalyzed cross-coupling reactions.

Unit– IV: NeutralSpectatorLigandsandMetathesisReactions

Steric and electronic structure of phosphine ligands, basicity of phosphine, monodentate and multidentate phosphines, cone angle, bite angle, N-heterocyclic carbenes (NHC), synthesis of NHC, alkene metathesis, mechanismofalkenemetathesis,classificationofmetathesisreactions,significanceofmetathesisreactions.

Lists of Experiment

1. Qualitative analysis of mixtures containing 4 radicals (2 anions and 2 cations). Emphasis should be given to the understanding of the chemistry of different reactions. The following radicals are suggested:

CO_3^{2-},NO_2^-,S^{2-},SO_3^{2-},F^-,Cl^-,Br^-,I^-,NO_3^-,PO_4^{3-},NH_4^+,K^+,Pb^{2+},Cu^{2+},Cd^{2+},Bi^{3+},Sn^{2+},Sb^{3+},Fe^{3+}, Al^{3+}, Cr^{3+}, Zn^{2+}, Mn^{2+}, Co^{2+}, Ni^{2+}, Ba^{2+}, Sr^{2+}, Ca^{2+},Mg^{2+}.

Mixturesmaycontainoneinsolublecomponent($BaSO_4$,$SrSO_4$,$PbSO_4$,CaF_2orAl_2O_3)or combination ofinterfering anions e.g., CO_3^{2-}andSO_3^{2-}; $NO_2^-$and NO_3^-; Cl^-, Br^-, I^-; $Br^-$and I^-; NO_3^-, Br^-, I^-.

TextBooks:

- ✓ *B.D.Gupta,A.J.Elias,BasicOrganometallicChemistry, 2nd Edn.,UniversityPress(2013).*
- ✓ *R.C. Mehrotra,A.Singh, Organometallic Chemistry, New Age InternationalPublishers, 2nd Edn, 2000.*
- ✓ *Vogel'sQualitativeInorganicAnalysis,7th Ed,RevisedbyG.Svehela,4th Ed.,Person,2007.*

ReferenceBooks:

- ✓ *A.K.Das, FundamentalsofInorganicChemistry,Vol.II,CBSPublications,2nd Ed.2010.*
- ✓ *D.E.Shriver,P.W.AtkinsInorganicChemistry, OxfordUniversityPress,5th Edn.*
- ✓ *J.E.Huheey,E.A.Keiter,R.L.Keiter,InorganicChemistry–Principlesofstructureand reactivity,Pearson Education, 4th Ed. 2002.*
- ✓ *B.R.Puri,L.R.Sharma,K.C.Kalia,PrinciplesofInorganicChemistry,VishalPublishingCo., 33rd Ed., 2017.*
- ✓ *J.F.Hartwig,OrganotransitionMetalChemistry:FromBondingtoCatalysis,University ScienceBooks, 2010.*

CoreXIV **Semester VI**

AnalyticalMethodsofChemistry

CourseObjectives:

ThiscourseisofferedbySchoolofChemistryasacoresubjectforboth4-yearB.Sc.withandwithout researchPrograms,withanemphasisonanalyticalmethodsofchemistry.Thiscourseaimstoimpart skills, promotes employability, and entrepreneurships in broad domains such as Thermal industry, pharma, dyes & paints, coating, metal & metallurgical PSUs, research, and academic institutes. Instrumentation proficiency: Students should gain hands-on experience with analytical instrumentationcommonlyusedinchemicalanalysis,suchasspectrophotometers,chromatographs, andmassspectrometers.Theaimsaretoprovideasoundphysicalunderstandingoftheprinciplesof analytical chemistry and to show how these principles are applied in chemistry and related disciplines— especially in life sciences and environmental science.

CourseOutcomes:

1. Performcalibrationandstandardizationproceduresto ensuretheaccuracyandprecisionof analytical measurements, adhering to established protocols and standards.
2. Applyavarietyofanalyticaltechniques, suchas spectroscopy,chromatography, electrochemistry,andtitrimetry,toquantitativelyandqualitativelyanalyzechemical substances.
3. Collect,analyze,andinterpretexperimentaldataaccuratelyusingappropriatestatistical methods and error analysis techniques.
4. Develop critical thinking and problem-solving skills and Implement quality control and assurancepractices,includingtheuseofcontrolchartsandvalidationofanalyticalmethods,to ensure the reliability and reproducibility of analytical results.

UnitI –Tools and DataHandling

Calibration of tools, sampling. Errors and Statistics: significant figures, rounding off, accuracy and precision,determinateandindeterminateerrors,standarddeviation,propagationoferrors,confidence limit, test of data; F, Q and t test, rejection of data, and confidence intervals.

UnitII–Separation Techniques

SolventExtraction:distributionCoefficient,distributionratio,solventextractionofmetals,multiple batch extraction, counter-current distribution. - Chromatographic Techniques: classification, theory ofchromatographicseparation,distributioncoefficient,retention,sorption,efficiencyandresolution. -Column, ion exchange, paper, TLC & amp; HPTLC: techniques and application. - Gas Chromatography:retentiontimeorvolume,capacityratio,partitioncoefficient,theoreticalplateand number, separation efficiency and resolution, instrumentation and application.

UnitIII–Spectroscopic Techniques

Electromagnetic radiation, absorption, and emission of radiation – instrumentation: sources,monochromators, detectors. - Flame spectrometry: flame emission, AAS, ICP, instrumentation and application. - Absorption spectrometry: UV-VIS, IR, instrumentation, techniques and applications.

Unit IV – Thermal and Electroanalytical Techniques

Thermogravimetry:instrumentationandtechniques,TGAcurves,DTAandDSC,applications. Electrogravimetry, coulometry, voltammetry, polarography, conductometry, instrumentation, techniques and application.

Textbooks:

- ✓ *D.C.Harris,QuantitativeChemicalAnalysis,4thEdn.,W.H.Freeman,1995.*
- ✓ *G.D.Christian&J.E.O'Reily,Instrumental Analysis,2ndEdn.,Allyn&Balon, 1986.*
- ✓ *Skoog,HollerandCrouch,PrinciplesofInstrumentalAnalysis,CengageLearning,6th Indian Reprint 2017.*

Referencebooks

- ✓ *W. H. Hobert: Instrumental Methods of Analysis, 7th Ed., Wardsworth Publishing Company,Belmont, California, USA, 1988.*
- ✓ *O.Mikes,&R.A.Chalmes,LaboratoryHandBookofChromatographic&AlliedMethods,Elles Harwood Ltd. London. 2001*
- ✓ *Pavia, Lamman, Kriz and Vyvyan, Introduction to Spectroscopy, Cengage Learning, 3rd Indian Reprint 2017.*

Core XV

Solidandporousmaterials,andmagnetochemistryandpowercells

CourseObjectives:

To provide the basic understanding about the solid and porous materials with their diverse applications. Students will learn fundamentals of magnetochemistry and molecular magnetism which will be helpful for their competitive examinations. Course is designed to develop a comprehensive technological understanding in different power cells.

CourseOutcomes:

- Learnaboutthedifferentmaterials,includingtheoryandmethodsforthedevelopmentofnewmaterials with desired properties.
- Knowhowporescaninfluencethepropertiesofmaterials
- Demonstrateanincreasedknowledgeandunderstandingofmagnetochemistrywithcriticalthoughtand achieve the ability to analyze magnetochemical studies and data
- Explaintheprinciplesthatunderlietheabilityofvariouspowercellsanddevelopnew ideaofconstructing power cell

Unit I

InorganicSolidMaterials

Silicate industry:

Glass: Glassy state and its properties, classification (silicate and nonsilicate glasses), Manufactureandprocessingofglass,compositearmouredpropertiesofthefollowingtypes of glasses: soda lime glass, lead glass, armoured glass, safety glass, borosilicate glass, fluorosilicate, colored glass, photosensitive glass.

Ceramics: Manufacture and types of ceramics, high technology ceramics and their applications,superconductingandsemiconductingoxides,fullerenes,carbonnanotubesand carbon fibers.

Cement:Classificationofcement,ingredientsandtheirrole,manufactureofthecement,and their setting process and quick setting cements.

Unit– II :CrystalEngineeringandPrincipleofDesigningPorousMaterials

Inorganic crystal engineering and design principle of metal-organic frameworks and organic-inorganic hybrids. Principles of ICE in the design of porous materials, their understanding and characterizations using X-ray diffraction and thermal methods. Surface characterizationandsurfacebehaviorofsuchporousmaterialswithspecialreferencetothe gas/solvent vapors sorption. Some special applications of such materials like gas storage, gas/solvent separation, etc. Understanding of the structure-property relationship for the design of functional molecular material or molecular devices- philosophy and the terminologies**.**

Unit– III:Magnetochemistry

Magnetic Substances: Terminology related with magnetic properties, Classification, CooperativeMagnetism,Ferromagneticsubstancesandrelatedaspects,Applicationofhard and soft ferromagnetic substances. Para-, ferro- and antiferro-magnetism: Temperature dependence of magnetic susceptibility, Curie ‘s Law and Curie-Weiss Law, Pathways of ferro- and antiferromagnetism, magnetic properties of an electron, paramagnetism and thermal energy, Spin-orbit Coupling, Magnetic properties of compounds of d- and f-block elements:concentratedanddilutesystems,magneticallyfrustratedsystems,singlemolecule magnet (SMM), single ion magnet (SIM), single chain magnet (SCM).

Unit– IV: Power Cells

Primary and secondary batteries, Battery components and their role, characteristics of battery, working principles of following batteries: Pb-battery, Li-battery, solid state electrolyte battery, fuel cell, solar cell, polymer cell.

TextBooks:

- ✓ *F. Gomez-Granados, J. C. Moreno-Pirajan, L. Giraldo-Gutierrez, Porous Materials: Theory and Its Application for Environmental Remediation (Engineering Materials), Springer Nature Switzerland AG; 1st Ed. 2021.*
- ✓ *R. L. Dutta, A. Syamal, Elements of magnetochemistry, 2nd Ed, Affiliated East-West Press Pvt. Ltd, 2010.*
- ✓ *J. N. Lalena, D. A. Cleary, O. B. M. H. Duparc, Principles of Inorganic Materials Design, 3rd Ed, Wiley, 2020.*

ReferenceBooks:

- ✓ *C.N.R.Rao,K.Biswas,EssentialsofInorganicMaterialsSynthesis,JohnWiley&Sons, Inc.,2015.*
- ✓ *C.Julien,A.Mauger,A.Vijh,K.Zaghib,LithiumBatteries:ScienceandTechnology,Springer, 2015.*
- ✓ *C.S.Solanki,Solar PhotovoltaicTechnologyand Systems: AManual forTechnicians,Trainers and Engineers, Prentice Hall India Learning Pvt. Ltd., 2013.*
- ✓ *D.Pavlov,Lead-AcidBatteries:ScienceandTechnology,ElsevierScience,2015.*
- ✓ *S.P.Jiang,Q.Li,IntroductiontoFuelCells:ElectrochemistryandMaterials,Springer,2022.*
- ✓ *A. Ramanan,G. R. Desiraju,J.J.Vittal, CrystalEngineering: ATextbook,WorldScientific Publishing Co. Pte. Ltd., 2011.*
- ✓ *A.Earnshaw,IntroductiontoMagnetochemistry,AcademicPress,2013.*

Core XVISemester VII

ChemistryofBiomolecules

CourseObjectives:

Theobjectiveofthiscourseistofamiliarizethestudentwithbiomoleculessuchascarbohydrates,amino acids, proteins, peptides, lipids and enzymes. The student will comprehend thestructure, nomenclature, and properties of various biomolecules and their functions in biological systems. It will also help the learnerstobuildtheconceptofmetabolismbystudyingthechemistryand energeticsofbiomoleculesin biochemical reactions.

CourseOutcomes

- Impartingknowledgeonvariousbiomoleculeswiththeirdetailedclassification,structure, nomenclature and functions.
- Understandingthechemistryand energetics offoodto energyconversioninbiologicalsystems.
- Gaining knowledge on typeof enzymes and their roles in metabolism of biomolecules in various biochemical reactions.
- Practically determinesaponificationvalueandiodinenumberof fatandoilanddeterminethe reducing andnon-reducing sugars by Benedict's reagent.

Unit-I:Carbohydrate

Occurrence, classification (mono-, di- and poly- saccharides), chemical structure, constitution and absolute configurationofglucoseandfructose,epimersandanomersrelationships,mutarotation,determinationofring size of glucose and fructose, Haworth projections and Fischer projection conformational structures, interconversions of aldoses and ketoses. Chemical properties of monosaccharides and Killiani-Fischer synthesisandRuffdegradation;SynthesisofDisaccharides–(Sucrose,Lactoseandmaltose)bycondensation reactions.

Unit-II:AminoAcids,Peptides,Proteinsand Nucleicacids

Amino acids: Classification, Synthesis, ionic properties and reactions. Zwitterions, pKa values, isoelectric point and electrophoresis.

Peptides: Classification, Determination of their primary structures-end group analysis, methods of peptide synthesis. Synthesis of peptides using N-protecting, C-protecting and C-activating groups- Solid-phase synthesis.

Proteins:Structureofproteins,proteindenaturationandrenaturation.

NucleicAcids: Componentsofnucleicacids,Nucleosidesandnucleotides;Structure,synthesisandreactions of: Adenine, Guanine, Cytosine, Uracil and Thymine; Structure of polynucleotides.

Unit-III:Lipids

Introduction to oils and fats, common fatty acids present in oils and fats, role of lipids in our body, structure and classification, importance of omega-3 and omega-6 fatty acids and their sources. Physical and chemical properties of oils and fats, acid value, saponification value, iodine value, smoke point, flash point, fire point, and specific gravity. Chemical reactions of oil and fat, rancidity, conversion of oil to fat through hydrogenation, Baudouin test, Halphens test, Hexabromide test.

Unit-IV:Enzymes

Introduction to enzyme nomenclature, classification and characteristics. Salient features of active site of enzymes.Enzyme-substrateformationtheory.Mechanismofenzymeaction,factorsaffectingenzymeaction, coenzymes and cofactors and their role in biological reactions, specificity of enzyme action, enzyme inhibitorsandtheirimportance,phenomenonofinhibition(competitive,uncompetitiveandnon-competitive including allosteric inhibition).

List ofExperiments

(1) DeterminationofSaponification valueofsuppliedoil.
(2) Determinationof Iodinevalueofsupplied oil.
(3) Qualitativeanalysis ofcarbohydrate: aldoses and ketoses,reducingandnon-reducingsugars.
(4) Quantitativeestimationof sugars:
    a) Estimationglucosebytitrationwith Fehling'ssolution.
    b) Estimationglucoseandsucroseina given mixture.
(5) EstimationofglycinebySorenson'sformalin method.
(6) Studyofthetitrationcurveof glycine
(7) Separationand identification ofamino acids bypaper chromatography
(8) Separationofblueandorangedyesfrommethyl orangebypaperchromatography
(9) Separationand identification offooddyes bypaper chromatography
(10) Separationoftwoimmiscibleliquidsbypaper chromatography
(11) Separationofblue andyellowdyes usingisopropanolbypaper chromatography

Textbooks

- ✓ *D. L.Nelson,M.M.Cox,LehningerPrinciplesofBiochemistry,7th Ed.,W.H.FreemanCo.,2017.*
- ✓ *J.L.Jain,S.Jain,N.Jain,FundamentalsofBiochemistry,S. Chand,2016.*
- ✓ *E.J.Wood,WilsonandWalkerPrincipleandTechniquesofPractical Biochemistry, Cambridge University Press, 2009.*

ReferenceBooks:

- ✓ *D.Das,Biochemistry,14thEd.,AcademicPublishers, 2015.*
- ✓ *A.V.S.S.Rao,ATextbookofBiochemistry,9thEd.,UBS,2002.*
- ✓ *R. T. Morrison, R. N. Boyd, S. K. Bhattacharjee, Organic Chemistry, 7th Ed., Pearson Education India,2010.*
- ✓ *G. P. Talwar, L. M. Srivastava, Textbook of Biochemistry and Human Biology,3rd Ed., PrenticeHallIndia, 2002.*
- ✓ *J.M.Berg,J.L.Tymoczko, L. Stryer,Biochemistry, 6th Ed.,W.H.Freeman,2006.*
- ✓ *P.J.Kennelly,K.M.Botham,O.Mcguinness,V.W.Rodwell,P.A.Weil,Harper's IllustratedBiochemistry, 32nd Ed., Lange-McGraw-Hill, 2022.*
- ✓ *T.W.GrahamSolomons,C.G.Fryhle,S.A.Snyder,Solomons'OrganicChemistry,GlobalEd., Wiley,2024.*

Core XVII

PolymerChemistry

CourseObjectives:

ThiscourseisofferedbySchoolofChemistryasacoresubjectforthe4-yearB.Sc.Programme,with an emphasis on fundamental understanding of the type of bond in a polymer and rationally design themonomersforagivenpolymer.Todescribevariousmethodsusedforsynthesizingpolymers.To use analytical methods to characterize a polymer. To study the properties of polymers.

Courseoutcomes:

5. Thelearnerswillbeabletoclassifythepolymersbasedonnature,occurance,modeofsynthesis, thermal properties etc.
6. Todifferentiatebetween methodsandmechanismofpolymerizationprocess.
7. Calculatemolecularweights ofpolymersandstudytheapplications&properties.
8. The learners willbe able todesignthe monomers for thepreparation ofpolymers of interest, characterize and understand the properties polymers.

Unit-I: Introductionandhistoryofpolymeric materials:

Different schemes of classification of polymers, Polymer nomenclature, Molecular forces and chemical bonding in polymers, Texture of Polymers.

Functionality and its importance: Criteria for synthetic polymer formation, classification of polymerization processes, Relationships between functionality, extent of reaction and degree of polymerization. Bi- functional systems, Poly-functional systems.

Unit-II: Mechanism&Kineticsof Polymerization

Polymerizationreactions–additionandcondensation,mechanismandkineticsofstepgrowth,radical chaingrowth,ionicchain (bothcationicandanionic)andcoordinationpolymerizations,Mechanism and kinetics of copolymerization, polymerization techniques. **Crystallization and crystallinity:** Determination of crystalline melting point and degree of crystallinity, Morphology of crystalline polymers, Factors affecting crystalline melting point.

Unit-III: Molecularweightofpolymersandtheirdetermination

(Mn,Mw,Mv,Mz)byend groupanalysis, viscometry and osmotic pressure methods. Molecular weight distribution and itssignificance. Polydispersityindex.Glasstransitiontemperature(Tg)anditsdetermination:WLFequation,outlines of factors affecting glass transition temperature (Tg).

Unit-IV: Propertiesofpolymers

(physical, thermal and mechanical properties). Preparation, structure, properties and applications of the following polymers: polyolefins (polyethylene, polypropylene), polystyrene, polyvinyl chloride, polyvinyl acetate, polyacrylamide, fluoro polymers (Teflon), polyamides (nylon-6 and nylon 6,6). Thermosetting polymers - phenol formaldehyde resins (Bakelite, Novalac), polyurethanes, conducting polymers (polyacetylene, polyaniline). Brief outline of biodegradable polymers.

List ofexperiments

1. Preparationofnylon-6,6/Polyaniline
2. Preparationsofphenol-formaldehyderesin-novalac/phenol-formaldehyderesinresold.
3. Preparationofurea-formaldehyderesin
4. Redoxpolymerizationofacrylamide
5. Precipitationpolymerizationofacrylonitrile
6. Determinationofmolecularweight byviscometry:
   a. Polyacrylamide/Polystyrene
   b. (Polyvinylpyrolidine(PVP)
7. Determinationofacidvalue/saponificationvalueofaresin.
8. Determinationofhydroxylnumberofapolymerusingcolorimetricmethod.
9. EstimationoftheamountofHCHOin thegivensolutionbysodiumsulphitemethod
10. Analysisofsome IRspectraofpolymers–IdentificationoflabelledpeaksinIRspectraof known polymer.

Text Books:

- ✓ *V.R.Gowarikar,JayadevSreedhar,N.V.Viswanathan,PolymerScience1st Edition,NewAge International Publishers, 1986.*
- ✓ *PremamoyGhosh,PolymerScienceandTechnology:Plastics,Rubber,BlendsandComposites, 3rd Edition, McGraw Hill Education, 2010.*
- ✓ *P.Bahadur&N.V.Sastry,Principlesofpolymerscience,NarosaPublishinghouse,New Delhi2002.*

Referencebooks

- ✓ *L.H.Sperling,IntroductiontoPhysicalPolymerScience,4th ed.JohnWiley&Sons (2005)*
- ✓ *MalcolmP.Stevens,PolymerChemistry:AnIntroduction,3rd ed.OxfordUniversityPress (2005)*
- ✓ *Seymour/Carraher'sPolymerChemistry,9th ed.byCharlesE.Carraher,Jr.(2013).*
- ✓ *NayakP.L.,PolymerChemistry,KalyaniPublisher(2017).*
- ✓ *HundiwaleG.D.,AthawaleV.D.,KapadiU.R.andGiteV.V.,ExperimentsinPolymer Science, New Age Publications (2009).*

CoreXVIII

GreenChemistry

CourseObjectives:

BasicintroductionandexplainginggoalsofGreenChemistry.Limitations/Obstaclesinthepursuitofthegoals of Green Chemistry, Principles of Green Chemistry with their explanations and examples and special emphasis on Designing a Green Synthesis using these principles.

Courseoutcomes:

- Discussabouttheroleofprinciplesofgreenchemistry.
- Explaintheimportanceofgreensynthesis.
- Interprettheknowledgeofpreventionofhazardouschemicalsinreactions.
- Evaluatetheefficiencyofgreencatalysts&interprettheuseofbiocatalysts.

Unit-I: IntroductiontoGreen Chemistry

What is Green Chemistry? Need for Green Chemistry. Goals of Green Chemistry. Limitations/ Obstacles in the pursuit of the goals of Green Chemistry.

PrinciplesofGreenChemistryandDesigningaChemicalsynthesis-I

Twelve principles of Green Chemistry. Explanations of principle with special emphasis on - Designinggreensynthesisprocesses:PreventionofWaste/by-products;maximizetheincorporation of the materials used in the process into the final products (Atom Economy) with reference to rearrangement,addition,substitutionandeliminationreactions;Prevention/minimizationof

hazardous/ toxic products; Designing safer chemicals; Use of safer solvents and auxiliaries (e.g. separating agent) - green solvents (supercritical CO_2, water, ionic liquids), solventless processes, immobilized solvents.

Unit-II: PrinciplesofGreenChemistryandDesigningaChemicalsynthesis-II

Explanation of green chemistry principles with special emphasis on: Energy efficient processes for synthesis-useofmicrowavesandultrasonicenergy.Selectionofstartingmaterials(useofrenewable feedstock); avoidance of unnecessary derivatization (e.g. blocking group, protection groups, deprotection);Useofcatalyticreagents(whereverpossible)inpreferencetostoichiometricreagents; designing of biodegradable products use of chemically safer substances for prevention of chemical accidents, inherent safer design greener - alternative to Bhopal Gas Tragedy (safer route to carcarbaryl) and Flixiborough accident (safer route to cyclohexanol); real-time, in-process monitoring and control to prevent the formation of hazardous substances; development of green analytical techniques to prevent and minimize the generation of hazardous substances in chemical processes.

Unit-III: ExamplesofGreenSynthesis/Reactionsandsomereal-worldcases-I

Green Synthesis ofthefollowingcompounds: adipicacid, catechol, methyl methacrylate, urethane, disodium iminodiacetate (alternative to Strecker synthesis), paracetamol, furfural.

Microwave assisted reactions: Applications to reactions (i) in water: Hofmann Elimination, hydrolysis (of benzyl chloride, methyl benzoate to benzoic acid), Oxidation (of toluene, alcohols); (ii)reactionsinorganicsolvents:Diels-AlderreactionandDecarboxylationreaction.

*Ultrasoundassistedreactions:*Applicationstoesterification,saponification,Simmons-Smith Reaction (Ultrasonic alternative to Iodine).

Unit-IV: ExamplesofGreenSynthesis/Reactionsandsomereal-worldcases-II

Surfactants for carbon dioxide – replacing smog producing and ozone depleting solvents with $CO_2$for precision cleaning and dry cleaning of garments; Designing of Environmentally safe marine antifoulant; Rightfit pigment: synthetic azopigments to replace toxic organic and inorganicpigments;Synthesisofacompostableandwidelyapplicableplastic(polylacticacid)from corn; Development of Fully Recyclable Carpet: Cradle to Cradle Carpeting

FutureTrendsinGreenChemistry

Oxidizing and reducing reagents and catalysts; multifunctional reagents; Combinatorial green chemistry;Proliferationofsolventlessreactions; Green chemistryinsustainabledevelopment.(Bio-diesel, bio-ethanol and biogas).

Listofexperiments

1. Acetylationofprimaryamine(AnilinetoN-phenylacetamide)usingZndust.
2. Nitrationofsalicylicacidbygreenmethod(Usingcalciumnitrateandaceticacid).
3. Brominationofacetanilideusingcericammoniumnitrate/KBr.
4. Microwaveassistednitration ofPhenolsusingCu(NO3)2.
5. Detectionofelementsinorganiccompoundsby greenmethod(Sodiumcarbonatefusion)
6. BasecatalyzedAldolcondensation(Synthesisofdibenzalpropanone)
7. VitaminCclockreactionusingvitaminCtablets,tinctureofiodine,hydrogenperoxideand liquid laundry starch. Effect of concentration on clock reaction.
8. Photoreductionofbenzophenonetobenzopinacolinthepresenceofsunlight.
9. DielsAlderreactioninwater:Reactionbetweenfuranandmaleicacidinwaterandatroom temperature rather than in benzene and reflux.
10. Preparationandcharacterizationofnanoparticles(Cu,Ag)usingplantextract.

Text Books:

- ✓ *P.T.Anastas&J.K.Warner,GreenChemistry-TheoryandPractical,OxfordUniversityPress 2000.*
- ✓ *V.K.Ahluwalia&M.Kidwai.:NewTrendsinGreenChemistry,AnamalayaPublishers,New Delhi 2004.*
- ✓ *V.KumarAnIntroductiontoGreenChemistry,VishalPublishingCo.,2015.*

ReferenceBooks:

- ✓ *A.S.Matlack. IntroductiontoGreenChemistry,Marcel Dekker2001.*
- ✓ *AK.DasandM.Das,EnvironmentChemistrywithGreenChemistry,BooksandAllied(P) Ltd. 2010.*
- ✓ *R.K. Sharma, I.T. Sidhwani &, M.K Chaudhari. I.K. Green Chemistry Experiment:A monographInternationalPublishingHousePvtLtd.NewDelhi.BangaloreCISBN978-93- 81141-55-7, 2013.*
    - ✓ ***E-Contents:****Thesupportingmaterialscanbefoundonthe****websiteoftheBerkeleyCenterfor Green Chemistry (http://bcgc.berkeley.edu/)****.*
    - ✓ ***CaseStudy:****https://shorturl.at/cjuHI*

CoreXIX

Oxidation,Reduction,Reagents,RearrangementsandName Reactions

Unit-I:OxidationReactions

Oxidation of (a) alcohols to carbonyls by chromium, manganese, aluminium, silver, ruthenium, DMSO, hypervalent iodine and TEMPO based reagents, (b) alkenes to epoxides by peroxides/per acids, Sharpless asymmetric epoxidation, Jacobsen epoxidation, Shi epoxidation (c) alkenes to carbonyls with bond cleavage by Manganese, Osmium, Ruthenium and lead based oxidants and ozonolysis (d) alkenes to alcohols/carbonyls without bond cleavage, Wacker oxidation, selenium, chromium based allylic oxidation process.

Unit-II:ReductionReactions

Reduction reactions (a) in heterogeneous medium by Palladium/Platinum/Rhodium/Nickel (Resenmund reduction) and in homogeneous medium (Wilkinson reaction). Noyori asymmetric hydrogenation. (b) Metal based reductions using Li/Na in liquid ammonia (Birch reduction), Sodium, Magnesium, Zinc, Titanium and Samarium. (c) Reduction by hydride transfer reagents: Aluminium alkoxide, Sodium borohydride (NaBH4), di-isobutylaluminium hydride (DIBAL-H), Sodiumcyanoborodydride,Lithiumtrialkylborohydride,reductionwithhydrazine(Wolff-Kischner reduction), reduction with trialkyltinhydride.

Unit-III:ReagentsinOrganicSynthesis

Functionalized Grignard reagents, organozinc, organo-lithium, organocopper, organopalladium, lithiumdiisopropylamide(LDA),Dicyclohexylcarbodiimide(DCC),organosilicon,organoborane, organotin, crown ethers, Dichlorodicyano benzoquinone (DDQ), Osmium tetroxide, 1,3-Dithiane, Trimethyl silyl iodide, Tri-n-butyl tin hydride.

Unit-IV:RearrangementandNameReactions

Nature of migration and migratory aptitude of groups in rearrangements reaction, Wagner-Meerwein, Favorskii, Fries, Benzil-Benzilic acid, Arndt-Eistert synthesis, Neber, Beckmann, Hofmann, Schmidt, Lossen, Shapiro reaction, Von-Richter, Sommelet-Hauser rearrangement, Wolff, Stevens reaction.

RecommendedTextbooks:

- ✓ S.N.Sanyal,Reactions,RearrangementsandReagents,4th Ed.,BharatiBhawanPublishers& Distributors, 2019.
- ✓ R.K.Bansal,OrganicReactionMechanism,3rd Ed.,TataMcGraw-HillPublications,1998.
- ✓ R. K. Bansal, Synthetic Approaches in Organic Chemistry, Narosa Publishing House, India, 1996.

ReferenceBooks:

- ✓ W.Carruthares,I.Coldham,ModernMethodsofOrganicSynthesis,4th Ed.,Cambridge University Press, 2015.
- ✓ F.A.Carey,R.J.Sundberg,AdvancedOrganicChemistry,Part-AandPart-B,5th Ed.,Springer 2007.
- ✓ J. March, M. B. Smith, March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure, 6th Ed., Wiley, 2013.
- ✓ I.L. Finar,OrganicChemistry,Vol-2,5th Ed.,PearsonPublisher,2002.
- ✓ R.O.C. Norman,J. M.Coxon,PrincipleofOrganicSynthesis, 3rd Ed.,CRCPress,2017.

CoreXX Semester VIII

Quantumchemistry&StatisticalThermodynamics

CourseObjectives:

This course is offered by School of Chemistry as a core subject for the B.Sc. programme, with an emphasis on fundamental understanding of Quantum chemistry, molecular spectroscopy, and photochemistry. Students are expected to have background knowledge in mathematics up to the +2 level for this course. The objective of the practical is to develop skills for working in physical chemistrylaboratory.Thestudentwillperformexperimentsbasedontheconceptslearntin Physical chemistry-V course.

CourseOutcomes:

Bytheend ofthecourse,the students willbeableto:

- Understandtheapproximationmethodencompassing Linearvariationprinciple,perturbation theory.
- ApplyHMOto differentconjugated systems.
- Acquire a firm knowledge of statistical methods, Ensambles, and apply the concept of molecular partition functions to macroscopic systems.
- Comparethethermodynamicpropertiesofdifferent statistics.

Unit-I:

ApproximationMethods:Thevariationtheorem,linearvariationprinciple,Perturbationtheory(firstorder and non-degenerate). Applications of variation method and perturbation theory to the Helium atom.

Unit-II:

Huckell theory of conjugated systems, Calculation of π-bond energy, delocalization energy, electronic & charge density calculation, and bond order. Applications to ethylene, butadiene, cyclopropanol radical, and cyclobutadiene.

Unit-III:

FundamentalsofStatisticalmethods,Starling'sapproximation,StatisticalThermodynamics:mathematical
&thermodynamicprobability.MaxwellBoltzmandistributionbetweenpartitionfunction.TypesofPartition functions: translational, rotational, vibrational and electronic partition functions.

Unit-IV:

TypesofStatistics-Bose-Einsteinstatistics,Maxwell-Boltzman,Fermi-Diracstatistics.Calculationofresults of three types of statistics.

Text Books:

- ✓ *D.A.McQuarrie,QuantumChemistry,VivaBooks,Reprint,2011,IndianStudentEdition*
- ✓ *StatisticalThermodynamics:M.C.Gupta,NewAgePvtPublication*
- ✓ *StatisticalMechanicsandThermodynamics,C.Garrod,OxfordUniv.Press,NewYork.*

ReferenceBook:

- ✓ *Atkin'sPhysicalChemistry:P.W.Atkins,J.D.Paula,OxfordUniversityPress*
- ✓ *StatisticalMechanics,D.A.McQuarrie,UniversityScienceBooks,California.*
- ✓ *StatisticalMechanics-AConciseIntroductionforChemistsB.Widom,CambridgeUniversityPress*

Core XXI

Chemicalgrouptheory,electronicspectraofmetal complexes, and nuclear chemistry

CourseObjectives:

Toprovidebasicknowledgeonsymmetryofmoleculesappliedthroughmathematicalgrouptheory.

Gives idea about the electronic transitions between d-orbitals, L-S coupling, qualitative Orgel diagrams for different d^n systems, selection rules for electronic spectral transitions, charge transfer phenomena,

Nuclearchemistryhasbeenintroducedtoinculcatestudentsaboutthechemistryofinnercoreofatoms.Lab work has been designed for preparing key inorganic compounds and estimating important ingredients of day-to-day use in a product in order to make students competent in this regard.

CourseOutcomes:

- Learn a significant knowledge on formal group theory for understanding molecular spectroscopy.
- Explorethefundamentals ofelectronicspectraof coordinationcomplexes.
- Understandthestabilityofnucleusanditsreactions,andtheapplicationsofradioisotopesin different fields.
- Achieve the knowledge on quantitative estimation of important ingredients in various commonly used products, and also get the synthetic skills of preparing key inorganic compounds

Unit–I: Fundamentalsofgrouptheory

Symmetry operation, symmetry element, classification of symmetry elements, definition of group, subgroup, cyclic groups, molecular point groups, group multiplication table, group generators,symmetryofplatonicsolids,conjugacyrelationandclasses,matrixrepresentationof symmetry elements.

Unit– II: Charactertableand normal modes

Character of a representation, reducible and irreducible representation, Great orthogonality theorem (qualitative description only), properties of irreducible representation. Character table (explanation and significance), construction of character tables for C_{2v} and C_{3v} point groups, direct product, standard reduction formula, Normal modes for $C_{2v}$and C_{3v}molecules.

Unit– III: Electronicspectraofmetalcomplexes

Electronic transitions between d-orbitals, L-S coupling, Orgel diagrams for $3d^1$ to $3d^9$ ions. Selection rules for electronic spectral transitions, relaxation in selection rules. spectrochemical series of ligands, nephelauxetic series, Evaluation of Dq, B and beta (β) parameters for the complex, charge transfer spectra (elementary idea). Significance of Tanabe-Sugano diagram.

Unit– IV: NuclearChemistry

Nuclear stability, magic numbers, radioactivity, general characteristics of radioactive decay particles, decay kinetics, nuclear reaction, Bethe's notation, types of nuclear reaction, nuclear crosssection,compoundnuclear theory,nuclearfission,liquiddropmodel,shellmodel,hardcore preformation theory, fission fragments and their mass distribution, charge distribution, ionic charge of fission fragments, working principle of nuclear reactor, concept of boron-neutron capture therapy, concept of nuclear fusion.

List ofexperiments:

1. Estimationofiodineiniodizedcommonsalt iodometrically
2. Estimationofphosphoricacidincoladrinksbymolybdenumbluemethod
3. Preparationofpotashalumfromscrapaluminum
4. Preparationofpotassiumoftrioxalatoferrate(III)trihydrate,$K_3[Fe(C_2O_4)_3].3H_2O$
5. DeterminationofalkalicontentinantacidtabletusingHCl
6. Determinationofaceticacidincommercialvinegar

TextBooks:

- ✓ *K.V.Ready,SymmetryandSpectroscopyofMolecules,NewAge Int.Publishers,2nd Ed, 2009.*
- ✓ *H.J.Arnikar,EssentialsofNuclearChemistry,NewAgeInternationalPvt.Ltd.,4thEd. 2011.*
- ✓ *A. Sakthivel , D. T. Masram, M. Sathiyendiran,S. Kaur-Ghumaan, Electronic and MagneticPropertiesofTransitionandInnerTransitionElementsandTheirComplexes, Publish with Nova Science Publishers, 2017.*

ReferenceBooks:

- ✓ *F.A.Cotton,ChemicalApplicationsofGroupTheory,Wiley India(P) Ltd.,3rd Ed, 2009.*
- ✓ *G.L.Miessler,P.J.Fischer, D.A.Tarr,Inorganicchemistry,5thEd., 2014.*
- ✓ *D.E.Shriver,P.W.Atkins, InorganicChemistry,OxfordUniversityPress,5thEdn.*
- ✓ *D.Gabel,R.Moss,BoronNeutronCaptureTherapy:TowardClinicalTrialsofGlioma Treatment, Springer-Verlag New York Inc., 1st Ed, 2012.*
- ✓ *A.J.Elias,GeneralChemistryExperiments,UniversityPress, 2007.*
- ✓ *Y.R.Sharma,ModernApproachtoPracticalChemistry,KalyaniPublishers,2008.*
- ✓ *Vogel'sQualitativeInorganicAnalysis,7thEd,RevisedbyG.Svehela,4thEd.,Person, 2007.*

CoreXXII

Pericyclicreactions,Photochemistryand Retrosynthesis

CourseObjective

Impartingknowledgeinthetheoryandapplicationsofvariousaspectsofpericyclicreactions and photochemistry and synthetic aptitutde of organic molecules. It will also help to understand the synthesis and mechanisms of various reactions.

CourseOutcome

- Understandthe conceptsrelated toorganicsynthesis, mechanisms.
- Applytheirunderstandingaboutthephotochemicalreactionsofindustrial significance.
- Evaluatethephotochemicalreactionsbased ontheinfluenceofthesubstituents on substrate
- molecules.
- Designnewphotochemicalreactionsinordertoachievetherequiredproduct(s).

nit-I:PericyclicReaction-I:

Molecular orbital symmetry, Frontier orbitals of ethylene, 1,3-butadiene, 1,3,5-hexatriene and allyl system. Classification of pericyclic reactions. Woodward-Hoffmann rules, Correlation diagrams, FMOandPMOapproaches.Electrocyclicreactions-Conrotatoryanddisrotatorymotions,4n,4n+2 and allyl systems.

Unit-II:PericyclicReaction-II:

Cycloaddition reactions - suprafacial and antarafacial additions, 4n and 4n+2 systems, Correlation diagrams and FMO method, Allowed and forbidden reactions. Diels-Alder reactions: retro Diels-Alder reaction- FMO mechanism for endo- and exo-selectivity, stereochemistry, inter- and intramolecular reactions.

Sigmatropic rearrangements: [i,j] H-shifts and C-shifts, supraand antarafacial migrations, retention and inversion of configurations, Sommelet-Hauser, Claisen, thio-Claisen, Cope, Oxa and aza-Cope rearrangements, Ene reaction.

Unit-III:Photochemistry:

First order Photochemical processes Light absorption, Fluorescence and Phosphorescence. Photochemistry of Alkene: Isomerization, Intramolecular reactions of the olefinic bond,di-π-methane,oxadi-π-andazadi-π-methanerearrangements,Photochemistryofvision.Photochemistry of Carbonyl compounds: Norrish type I and II reaction, Paterno-Buchi reaction, Photoreduction. PhotochemistryofArenes:Photochemicalaromaticsubstitution,additionandisomerisationreaction.

Photo-Fries reactions of anilides, Barton reaction, the mechanisms of reactions involving free radicals- Sandmayer, Gomberg- Bachmann, Pschorr, Ulmann and Hunsdiecker reactions. Singlet molecular oxygen reactions.

Unit-IV:Retro synthesis:

An introduction to synthons and synthetic equivalents, disconnection approach, functional group interconversions,theimportanceoftheorderofeventsinorganicsynthesis.onegroupC-Xandtwo group C-Xdisconnections,chemoselectivity, reversalofpolarity, cyclisationreactions.One Group C-C disconnection: Alcohols and carbonyl compounds, regioselectivity, Alkene synthesis, use of acetylenesandaliphaticnitrocompoundsinorganicsynthesis.TwogroupC-CDisconnections:

Diels-Alder reaction, 1,3-difunctionalised compounds, α, β- unsaturated carbonyl compounds, controlincarbonylcondensations,1,5-difunctionalisedcompounds.MichaeladditionandRobinson annulation.Protecting Groups, Principle of protection of alcohol, amine, carbonyl and carboxyl groups.

List ofExperiments

(1) Photoreductionofbenzophenonetobenzopinacolinthepresenceof sunlight.
(2) DielsAlderreactioninwater:Reactionbetweenfuranandmaleicacidinwateratroom temperature rather than in benzene under reflux condition.
(3) Preparationsofthefollowingcompounds:Aspirin/Paracetamol/Barbituricacid/
(4) Synthesisofmethyl orange.
(5) Synthesisofamidederivativefromcarboxylicacidandamineorfrom esters
(6) Synthesisofestersbyrefluxingglacialaceticacidandethanolin presenceofsulphuric acid.
(7) Retrosyntheticanalysisofbiomolecules.

Textbooks

- ✓ *S.Warren,P.Wyatt,Organicsynthesis,thedisconnectionapproach,2nd Ed.,Wiley, 2012.*
- ✓ *J.Singh,JSingh,PhotochemistryandPericyclic Reactions,NewAgeScience,2009.*
- ✓ *B.S.Furniss,A.J.Hannaford,P.W.G.Smith,A.R.Tatchell,Vogel'sTextbookofPractical Organic Chemistry, 5th Ed., Pearson Education India, 2003.*

ReferenceBooks:

- ✓ *S. Kumar, V. Kumar, S. P. Singh, Pericyclic Reactions: A Mechanistic and Problem-SolvingApproach, Academic Press, 2015.*
- ✓ *W.Carruthares,I.Coldham,ModernMethodsofOrganicSynthesis,4thEd.,Cambridge University Press, 2015.*
- ✓ *J. March, M. B. Smith, March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure, 6th Ed., Wiley, 2013.*
- ✓ *R.K.Bansal,OrganicReactionMechanism,3rdEd.,TataMcGraw-HillPublications,1998.*
- ✓ *R. K. Bansal, Synthetic Approaches in Organic Chemistry, Narosa Publishing House, India, 1996.*
- ✓ *J.Clayden,N.Greeves,S.Warren,OrganicChemistry,2nd Ed.,OxfordPublisher, 2012.*
- ✓ *T.L.Gilchrist,R.C.Storr,OrganicReactionsandOrbitalSymmetry,2ndEd., Cambridge University Press, 1979.*

- ✓ *F.A.Carey,R.J.Sundberg,AdvancedOrganicChemistry,Part-AandPart-B,5th Ed.,Springer 2007.*
- ✓ *I.L.Finar,OrganicChemistryVol.I&Vol.II, Longman,Cambridge,2011.*

CoreXXIII

ResearchMethodologyforChemistry

CourseObjectives:

- Tomakethestudentsawareoffundamentalbutmandatoryethicalpracticesinchemistry.chemistry.
- To introduce the concept of data analysis.
- To learn to perform literature survey in different modes.
- To make the students aware of safety handling and safe storage of chemicals.
- To make students aware about plagiarism and how to avoid it. To teach the use of different e-resources.

CourseOutcomes:

Bytheend ofthecourse,the students will beableto:

- Followethicalpracticesinchemistry
- DoData analysis
- Literaturesurveyindifferentmodes
- Usee-resources.
- Avoidplagiarism,understandtheconsequencesandhowtoavoid

Unit-I:ScopeofResearch,ResearchDatabasesandMetrics

Define research problem, review literature, formulate hypothesis, design research/experiment, collect and analyse data, interpret and report, importance and future scope. **Print Database (traditional)**: Sources of information: Primary, secondary, tertiary sources; **Digital: Databases (modern source):** Google Scholar, Web of science, Scopus, UGC INFONET, SciFinder, PubMed, ResearchGate, E-consortium, e-books; **EBSCO:** e-Resources Gateway for Universities of Odisha (odisha university | OSHEC | e-Resources for Universities and Colleges of Odisha); **Research metrics**:ImpactfactorofJournal,h-index,i10index,Altmetrics,Citationindex;**Authoridentifiers/ profiles:** ORCID, Publons, Google Scholar, ResearchGate, VIDWAN.

Unit-II:Statisticaltoolsandvalidationforchemists

Types of data, data collection-Methods and tools, data processing, hypothesis testing, Normal and Binomial distribution, tests of significance: t-test, F-test, chi- square test, ANOVA, multiple range test, regression and correlation. Features of data analysis with computers and softwares -Microsoft Excel, Origin, SPSS.

Unit-III:ResearchandPublicationethics:

Ethics with respect to science and research, Scientific Misconducts: falsification, fabrication and plagiarism, similarity index, software tools for finding plagiarism (Turnitin, Drillbit/Urkund etc), redundantpublications;**PublicationEthics:**Introduction,COPE(CommitteeonPublicationEthics) guidelines;conflictsofinterest,**publicationmisconduct:**problemsthatleadtounethicalbehaviour and vice versa, types, violation of publication ethics, authorship and contributorship, predatory publishers and journals; **IPR** - Intellectual property rights and patent law, commercialization, copy right, royalty, trade related aspects of intellectual property rights (TRIPS)

Unit-IV:ScienceCommunications:

Types of scientific documents: Full length research paper, book chapters, reviews, short communication, project proposal, Letters to editor, and thesis; Thesis writing – Windows and/or linux operatingsystem, programmingfundamentals, basics ofhigh level programminglanguage-C: editing, compilation and running a programme, storing data, elementary numerical methods, different steps and software tools (Word processing, LaTeX, Chemdraw, Chemsketch etc) in the design and preparation of thesis, layout, structure (chapter plan) and language of typical reports, Illustrationsandtables,bibliography,referencing:Styles(APA,Oxfordetc),annotatedbibliography, Citation management tools: Mendeley, Zotero and Endnote; footnotes; Oral presentation/posters – planning, software tools, creating and making effective presentation, use of visual aids, importance of effective communication, electronic manuscript submission, effective oral scientific communication and presentation skills.

Text Books:

- ✓ *Dean,J.R.,Jones,A.M.,Holmes,D.,Reed,R.,Weyers,J.&Jones,A.(2011)Practicalskillsin chemistry. 2nd Ed. Prentice-Hall, Harlow.*
- ✓ *Hibbert,D.B.&Gooding,J.J.(2006)Dataanalysisforchemistry.OxfordUniversityPress.*
- ✓ *Topping,J.(1984)Errorsofobservationandtheirtreatment. FourthEd.,ChapmanHall,London.*

ReferenceBook:

- ✓ *Harris,D.C.Quantitativechemicalanalysis.6thEd.,Freeman(2007)Chapters3-5.*
- ✓ *Levie,R.de,howtouseExcelinanalyticalchemistryandingeneralscientificdataanalysis. Cambridge Univ. Press (2001) 487 pages.*
- ✓ *Chemicalsafetymatters –IUPAC–IPCS,CambridgeUniversityPress, 1992. OSUsafetymanual 1.01*

E-Contents:

1. GoogleScholar
2. Scopuspreview-Scopus-Welcometo Scopus
3. WebofScience
4. CASInsights|CAS
5. Revealonlineattentiontoresearch- Altmetric
6. odishauniversity|OSHEC|e-ResourcesforUniversitiesandCollegesofOdisha