DEPARTMENT OF CHEMISTRY
RESTRUCTURED SYLLABUS
effective from Session 2013–14

Semester I

Physical Chemistry

ThermodynamicsI **12**

Lectures

a. Basicconceptsanddefinitions – Applicabilityofthermodynamics, thermodynamicsystemsandtheirclassification, Universe, system, surroundings and differenttypesofboundaries
b. Zerothlawandtemperature
c. Thermometry
d. Processes,reversibleandirreversibleprocess,thermodynamicequilibriumandsteadystate.
e. Workandheatinvolvedinathermodynamicprocess.
f. FirstlawandConceptofinternalenergy
g. Applicationtovariouskindsofprocesses
h. Stateandpathfunctions,exactandinexactdifferentials
i. ChangeinInternalenergy
j. Joule'sexperimentandconsequences
k. Enthalpy
l. Specificheatatconstantvolumeandpressure,relationshipbetweenthemandtheir differences
m. Standardstates
n. Kirchoff'sequations
o. Thermo-chemistry

ChemicalKinetics and Catalysis **12**

Lectures

a. Rateofareaction
b. Ratelawsandrateconstants
c. Orderandmolecularity
d. Integratedratelaws
e. Halflifeanditssignificance
f. Determinationoforderofareaction
g. Unimolecularreactionandreactionmechanism
h. Multistepreactions
i. Ratedeterminingstep
j. Zeroandfractionalorderreactions
k. SteadystateapproximationandEquilibriumapproximation
l. Rateexpressionforcomplexreactions
m. Molecularreactiondynamicsandconceptofreactiveencounters
n. Collisiontheory
o. Energyandstericrequirements(Basicqualitativeoverview)
p. Catalystsandinhibitors
q. Homogeneouscatalysis
r. Arrheniusandvan'tHoffcomplexes
s. Generalizedacid-basecatalysis
t. Identificationofhomogeneousandheterogeneouscatalysis
u. Activationenergydiagrams

KineticMolecularTheoryofgases **12**

Lectures

a. Assumptions
b. Expressionforaveragepressure
c. Arrivaltoothergaslaws
d. Conceptoftemperature
e. Maxwelldistributionofmolecularvelocityandspeed(in1,2,and3dimensions), their derivation,natureandcharacteristics
f. Wallcollisionfrequency
g. Calculationofaveragequantities
h. Mostprobablespeed
i. Energydistributionfunction,averageenergyandmostprobableenergy
j. Principleofequipartitionofenergy
k. Maxwell-BoltzmannDistribution
l. Specificheatofgases
m. Gaseouscollisions
n. Meanfreepath
o. Viscosity of gases
p. Effect of temperature and pressure on viscosity of ideal gases

Inorganic Chemistry

(A) Atomic Structure

H-Spectra; Wave mechanical model; de Broglie relation; Heisenberg Uncertainty Principle & its significance; Schrödinger Wave Equation (qualitative approach); Radial and Radial Probability Fuctions; Angular and angular probability functions (qualitative idea only); s, p and d – type atomic orbital envelope diagrams; nomenclature of atomic orbitals. Exchange energy, Hund'srule , limitations of Auf Bau Principle.

(B)PeriodicTable

Modern form of Periodic Table (IUPAC version), Nomenclature of Super-heavy elements (Z >100), screening effect and Slater's rules.

Inert Pair Effect, trends in atomic/ionic size, ionization energy, electronegativity and electron affinity of the s-, p-, d- and f- block elements, ionic potential and diagonal relationship in the Periodic Table. Scales of Electronegativity :Mulliken Scale, Pauling Scale and Alred–Rochow Scale. Variation of electronegativity with bond order and oxidation states.

(C) Radioactivity

Atomic nucleus – nuclear stability, n/p ratio and different modes of decay, nuclear binding energy, nuclear forces, Meson field theory, Nuclear Shell Model (elementary idea) and magic numbers.

Nuclear reactions – nuclear fission, nuclear fusion, spallation and transmutation of elements.Uses of isotopes in Chemistry.

Organic Chemistry

(A) General Introduction and Bonding Features in Organic Molecules (12 lectures)

DBE, steric effects, inductive effects, bond energy, bond polarity & bond polarizability, bond distance, Resonance, Steric inhibition of resonance, hyperconjugation, bond moment, dipole moment, orbital pictures of ethylene, acetylene, allene, formaldehyde and carbene. Orbital pictures of dienes, enynes, enones, vinylcyanide; π- MO diagrams of butadiene,1,3,5-hexatriene, allyl systems, benzene:concepts of HOMO & LUMO ; Aromaticity, Huckel's (4n+2) rule,Frost diagram, anti-aromaticity, Homoaromaticity,application of Huckel's rule to benzenoid and nonbenzenoid compounds. Relative strength of organic Acids-Bases.

(B)Stereochemistry of Acyclic Compounds (12 lectures)

Representation of molecules in Fischer, flying wedge, Saw-horse and Newman projection formulae and their inter-translations. Chirality, elements of Symmetry, simple axis of symmetry, plane of symmetry, centre of symmetry, alternating axis of symmetry.Asymmetry &disymmetry, optical activity, meso/dl, specific rotation, molar rotation.Enantiomerism&Diastereoisomerism, Stereogenic centres involving C=C, C=N, Absolute configuration: D/L, R/S,Relative configuration: E/Z, syn/ anti, cis/trans,erythro/threo, like/unlike nomenclature.

Isomerism involving two like/unlike stereogenic centres (AA and ABA types), pseudoasymmetric centres, stereogenicity, chirotopicity, achirotopicity**.**

C) Reaction Mechanism (6 lectures)

Bond Cleavage & Bond Formation- heterolytic&homolytic bond cleavage at stereogenic (single) and non-stereogenic centres, racemization, formation of racemic products. Reactive intermediates: Electrophiles, nucleophiles, radicals. Carbocations (onium and enium ions), carbanions, carbenes; Structure and stability.

Semester II

Physical Chemistry

ThermodynamicsII **12**

Lectures

a. NeedfortheSecondLaw
b. Carnot'sheatengineandrefrigerator
c. Statementsofthesecondlawandtheirequivalence
d. Thermodynamictemperaturescale
e. Carnot'stheorem
f. Entropyasastatefunction
g. Entropychangeofvariousprocesses(reversibleandirreversible)
h. Clausiusinequality
i. Combinedfirstandsecondlaw
j. Thermodynamicequationofstate
k. Auxiliarystatefunctions – GibbsandHelmholtzenergies
l. Maxwellrelations
m. Joule-Thomsonexperiment
n. TemperaturedependenceofGibbsfreeenergy(Gibbs-Helmholtz equations)
o. Gibbsfreeenergyofrealgasesandfugacity
p. Spontaneityandequilibrium
q. Gibbs-Helmholtzequation
r. Conceptofchemicalpotentialofpuresubstances
s. Partialmolarquantities
t. Gibbs-Duhemequation

Realgases **12**

Lectures

a. DeviationfromidealbehaviourwithreferencetoAndrew'sandAmagat'sexperiment,Joule (qualitative idea) andJoule-Thompsonexperiment(qualitativeidea).
b. Compressibilityfactor
c. Conceptofattractiveandrepulsiveforcesamongrealgasmolecules.Temperature dependence
d. vanderWaal'sequationofstate
e. Criticalstate,criticalpressure,volumeandtemperature,andtheirformforavanderWaal's gas.
f. BoyletemperatureandtheirformforavanderWaal'sgas.
g. Briefreviewofotherequationofstates(Dieterici).
h. Virialequationofstate, first and secondvirialcoefficient,theirrelationtootherconstants and their significance.
i. ReducedequationofstateandtheLawofcorrespondingstates
j. Continuityofstates
k. NatureofIntermolecularforces

QuantumMechanicsI

a. Blackbodyradiation,ClassicalTheoryofRayleigh-Jean,Ultravioletcatastropheand Planck'stheory,Thermodynamicviewpoint
b. Photoelectriceffect,Einstein'sQuanta,
c. Comptoneffect,
d. Dualnatureofelectromagneticradiation
e. deBroglie'shypothesis
f. Waveparticleduality
g. Matterwave
h. Conceptofwavepackets
i. Uncertaintyprinciple,itsvariousmathematicalformsanditsjustifications

Inorganic Chemistry

(A) Ionic Bonding

Packing of ions in crystals, radius ratio rules – applications & limitations; lattice energy – Born- Lande' equation and its applications

Born-Haber Cycle and its applications; solvation energy, dissolution of ionic solutes in polar solvents; Polarizability&Fajan's Rules; Stoichiometric and non–stoichiometric defects in crystals (non – mathematical approach), Van der Waal's forces, Hydrogen bonding and its applications.

(B) Coordination Chemistry – I

Double salts , Complex salts, Werner's Coordination Theory, mono- poly- and ambidentate ligands, Chelate complexes, Inner metallic complexes, IUPAC nomenclature of complexes, application of chelates in qualitative and quantitative chemical analysis.

(C) Covalent Bonding – I

Formal Charge, VSEPR theory and structure of inorganic molecules, Berry pseudorotation, hybridization, Bent's rule, dipole moment, resonance.

Organic Chemistry

(A) Energetics of reaction (10L)

Free energy profile for one-step & two-step reaction. Hammond postulate, Kinetically Controlled Vs Thermodynamically Controlled reactions, Investigation of reaction mechanism: Kinetic studies, study of intermediates, cross over experiments, stereochemical proof, isotope labelling- kinetic & non-kinetic, primary kinetic isotopic effect (kH/kD) only.

(B)Tautomerism (3L)

Application of thermodynamic principles in tautomericequilibria [keto-enoltautomerism, composition of theequilibrium in different systems (simple carbonyl, 1,3 and 1,2- dicarbonyl systems, phenols and related system), substituent and solvent effect].

(c)Nucleophilic substitution and elimination reactions (8L)

Nucleophilic substitution and elimination reactionsof alkyl halides; S_N1, S_N2, S_Ni, NGP, E1, E2, E1cB mechanisms; Elimination vs Substitution; Saytzeff and Hoffmann rules; reactivity of aryl, vinyl, allyl and benzyl halides.

(D) Stereochemistry of acyclic compounds (14L)

Axial chirality, systems with odd and even number of cumulated double bonds, atropisomerism in biphenyl systems, R/S nomenclature of axially chiral systems.Resolution of recemic acids, bases and alcohols; Optical purity/enantiometricexcess.Topicity of ligands and faces (elementary idea).Homotopic, Enantiotopic&Diastereotopic ligands and faces; pro-chirality, pro-R,Pro-S, and re/si descriptors.

Conformational Nomenclature- eclipsed, staggered, gauche, anti; dihedral angle, energy barrier of rotation, relative stability of conformers on the basis of steric effects; dipole-dipole interaction, H-bonding; conformational analysis of ethane, propane, n-butane, 1,2-dchloroethane, 2-methylbutane, 1,2-glycols, invertomerism of trialkylamines.

Semester III

Physical Chemistry

ChemicalEquilibrium **12 Lectures**

a. Thermodynamicsofmixingofidealgases
b. Conditionsofspontaneityandequilibriumintermsofinternalenergy,Enthalpy,Gibbsand Helmholtzfreeenergy
c. Gibbsfreeenergychangeofamixtureofgases
d. Gibbsfreeenergychangeofareaction
e. Definitionofmolar Gibbsfreeenergychangeofareaction
f. Equilibriuminidealgasmixtureandheterogeneousreaction
g. ConceptofEquilibriumconstant, concept of activity and concentration
h. Effectoftemperatureandpressureonequilibrium
i. ThermodynamicderivationofvantHoffequation
j. Temperaturedependenceofequilibriumconstantandvant Hoffisotherm
k. Variousequilibriumconstantsandtheirinterrelation
l. Temperaturedependence of K_c
m. Conceptofstandardstatefreeenergychangeofareactioninpressureandconcentration scale
n. LeChatelierprinciple
o. Solubilityequilibria
p. Salteffect
q. Nernstdistributionlaw and generalised Distributionequilibrium

Electrochemistry I **12 Lectures**

a. Activity,ionicactivities,meanionicactivities
b. Activitycoefficientandmeanionicactivitycoefficient
c. Debye-HuckelLimitinglaw(withoutderivation)
d. Flowofelectricalcharge through a solution and its consequences
e. Specificandequivalentconductance
f. Effectofdilution,dielectricconstantofsolvent,viscosityofsolventandtemperatureon conductanceofstrongandweakelectrolytes
g. ElectrophoreticandAssymetriceffect
h. Determinationofacidityconstantofaweakacid:Ostwalddilutionlaw,ionicproductof water,determinationofionicradii
i. Kohlrausch'slaw
j. Ionicmobilities
k. Transportnumberanditsdetermination(Hittorf'sandmovingboundarymethod)
l. Effectofconcentrationandtemperatureontransportnumber
m. Abnormaltransportnumber
n. Transport number in a mixture of two nonreactive electrolytes

QuantumMechanicsII **12 Lectures**

a. Operators,Linearoperators
b. Hermitianoperators
c. PostulatesofQuantumMechanics
d. Schrödingerequation
e. SolutionofSchrödingerequationaswavefunctionandenergy(eigenvaluesand eigenfunctions)
f. Commutatorsandtheirimplicationwithrespecttox, p_x.
g. Expectationvalues
h. Propertiesofeigenfunctions
i. Energyquantization

j. Simplesystems:1-D,2-D,3-Dbox(eigenvalues,eigenfunctions,expectationvalues, quantumnumbers,degeneracy,probabilitydensity)

k. SimpleHarmonicOscillator:SettingtheSchrödingerequation,derivation,eigenvalues andeigenfunctions,zeropointenergy

l. Tunneling-Basicconcepts

Inorganic Chemistry

(A) Redox Equilibrium

Balancing redox reactions by the ion–electron method; Standard redox potential, Nernst equation, influence of pH, precipitation and complexation on redox potential, formal potentials, feasibility of redox titrations, redox potential at equivalent point, redox indicators; redox diagrams – Latimer and Frost diagrams of concerned elements and their applications (typical examples).

(B) Group Chemistry – I : Group 1 and 2

Solutions of alkali metals in liquid ammonia; complexation with crown–ethers, cryptands and related ligands; basic beryllium acetate; detection of metal ions – Na^+, K^+, Mg^{2+}, Ca^{2+}, Sr^{2+}, Ba^{2+} in qualitative analysis.

(C)Group Chemistry – II : Groups 13 & 14

General trends in the oxidation states, hydrides, oxides, halides of B, Al, Ga, In, Tl; special features in the chemistry of boron trihalides, diborane, boron nitride and borazine; General trends in the oxidation states, catenation property, hydrides, halides and oxides of C, Si, Ge, Sn, Pb; special features in the chemistry of graphite, fullerenes, silicates, silicones and chloroflurocarbons; ultra–pure silicon.

(D) Covalent Bonding – I

Molecular orbital theory : Qualitative approach to molecular orbital theory; MO energy level diagrams of H_2, Li_2 to N_2, O_2, F_2, CO,NO,CN^-, HF, HF_2^-, BeH_2, CO_2.

Metallic bonding :qualititative treatment of Band Theory; conductors, semiconductors and insulators.

Organic Chemistry

(A) **Aromatic substitution reactions (6L)**

Aromatic electrophilic substitution reactions:π-complex, σ-complex, activating and deactivating groups, orienting influence of groups. Aryl halides: activated aromatic nucleophilic substitution, cine substitution. Ipso substitution.

(B) **Mechanism of free-radical substitution (2L)**

Alkane H, allyl/benzyl H; reactivity and selectivity of substitution by chlorine and bromine;

(C) Addition to carbon-carbon multiple bonds (12L)

Reactivity, regioselectivity (Markownikoff's rule), stereoselectivity, chemoselectivity; halogenation, hydrogenation,hydration,oxymercuration-demercuration,hydroboration-oxidation, epoxidation,hydroxylation, ozonolysis, carbene addition to alkynes, allenes,; free radical addition to C=C bond, peroxide effect; electrophilic and free radical addition to conjugated dienes;1,2- vs 1,4-addition; Michael addition; Birch reduction of alkadienes and alkynes; reactions involving alkynic C-H cleavage; Diels-Alder reaction (simple treatment).Interconversion of constitutional isomers of alkene and alkynes, Interconversion of E and Z isomers of alkenes.

D) Spectral Methods in Organic Chemistry- UV & IR and NMR Spectra (15L)

UV-Spectra: Electronic Transitions ($\sigma \rightarrow \sigma^*, n \rightarrow \sigma^*, \pi \rightarrow \pi^*, n \rightarrow \pi^*$), Relative position of λ_{max} considering conjugative effect, steric effect, solvent effect, effect of pH, relative intensity of absorption of allowed transitions, bathochromic shift, hypochromic shift, hyperchromic shift, hypsochromic shift with typical examples.

IR-Spectra: Modes of molecular vibrations, application of Hooke's law, Characteristic stretching freqeuncies of O-H, N-H, C-H, C-D, C=C, C=N, C=O; factors affecting stretching frequencies.

NMR Spectra

Nuclear spin, NMR-active nuclei, principle of PMR, equivalent & non-equivalent protons, anisotropy, chemical shifts, shielding/deshielding protons, upfield& downfield shifts.NMR peak area, relative peak positions of Toluene, nitro-benzene, o, m, p- dichloro- and dinitro-benzenes &chloronitobenzenes; spin-spin coupling in ethanol (ordinary grade),ethyl bromide; 1,1-dibromoethane; 1,2-dibromoethane; 1,1,2-tribromoethane.

Semester IV

Physical Chemistry

Electrochemistry II **12**

Lectures

a. Electrochemicalcells
b. Electrode,electrolyte
c. Electrodereactionandcellreaction
d. Nernstequation
e. Standardelectrodepotentialandapplication
f. Formalpotentialanditsapplication
g. Thermodynamicfunctionsfromcellpotentialmeasurement
h. Concentrationcells(withandwithouttransference)
i. Liquidjunctionpotential,it'sdeterminationandelimination
j. Applicationofe.m.f.measurement(relatedtopracticalexperiments)

StatisticalMechanics and Reaction Rate Theories **12**

Lectures

a. Energystatesandlevels
b. Microandmacrostates
c. Thermodynamicprobability
d. Entropyandprobability
e. Maxwell-Boltzmannstatistics
f. Distributionofmolecularstates:Boltzmanndistribution
g. ApplicationtoMaxwell'svelocitydistributionandbarometricdistribution
h. Partitionfunctionandit'ssignificance
i. Translational, rotational and vibrationalpartitionfunctionand their significance
j. Thermodynamicproperties(internalenergy,enthalpy,Helmholtzfreeenergy,Gibb's freeenergy,chemicalpotential,entropyandvalueofbeta)
k. ReactioncoordinateandPES
l. Transitionstatetheoryandactivatedcomplex
m. Expressionofrateconstantintermsofpartitionfunction,theEyringequation

Liquid and Solid state **12**

Lectures

a. General features of liquid state (short and long range order/disorder, hole theory)
b. Vapourpressure
c. YoungandLaplaceequation
d. Surfacetension
e. Surfaceenergy
f. Excesspressure
g. Capillarity phenomenon
h. Workofadhesionandcohesion
i. Contactangle
j. Spreadingofliquids
k. Dupreequation
l. Temperaturedependenceofsurfacetension
m. measurement of surface tension
n. Viscosityofliquids
o. Temperaturedependenceofviscosityofliquids
p. Poiseuille'sequation and Measurementofsurfaceviscosity

Solid state **12**

Lectures

a. Typesofsolids:crystallinestateandit'sproperties
b. Typesofcrystals
c. Latticepoints
d. Latticeplanes
e. Unitlattice
f. Basis
g. Bravaislatticeandit's14latticetypes
h. Millerindices
i. X-raydiffraction
j. Bragg'slaw
k. Calculationofbasisperunitcrystal,volume,densityperunitcell
l. Diffractiontechniques(Qualitativetreatmentonly):singlecrystalandpowder
m. StructureelucidationofNaCl,Kcl, CsCl, diamond, graphite and hcp
q. Specificheatofsolids(DulongPetitlaw,Einsteinstheory,Debyecorrection qualitatively)

QuantumMechanicsIII **12**

Lectures

a. ParticleonaRing
b. Conceptoftheeffectivepotential
c. Particle on a sphere: coordinate system
d. FormofSchrodingerequationinpolarcoordinates
e. FormofSchrodingerequationforatwoparticlesysteminCartesianco-ordinatesand reductiontooneparticlesystem
f. Thediatomicrigidrotor:solutionof thetaandphipart(basicexpressionsonly)
g. Expression of L^2, L_z inpolarcoordinate,physicalsignificance
h. Concept of effective potential
i. CentralforceproblemandformulationoftheSchrodingerequation for hydrogen atom

Colloids, Polymers andSurfaceProcesses **12**

Lectures

a. Colloids:Definition,generalproperties
b. Opticalpropertiesofcolloids
c. Rayleighequationandit'soutcomes
d. Qualitativeunderstandingofelectrokineticphenomenon:electrophoresis, electroosmosis,streamingpotentialandsedimentationpotential
e. Electricaldoublelayer,Zetapotential
f. Mechanismofcoagulation
g. Schulze-Hardyrule
h. Goldnumber
i. SurfaceexcessandGibbsadsorptionisotherm
j. Surfactant
k. Criticalmicellarconcentration,it'stensiometricandconductometricdetermination
l. Micelles
m. Thermodynamicsofmicellization
n. Liquid crystals
o. Polymeranddegreeofpolymerization
p. Molecularweightofpolymer(numberandweightaveragemolecularweight)
q. Numberdistributionandweightdistributionfunction
r. Expressionofnumberaverageandweightaveragemolecularweightand their interrelation

s. Reactiononsurfaces-Physisorptionandchemisorption
t. Adsorptionisotherms, derivation of Langmuir adsorption isotherma
u. Mechanismofsurfacereactions
v. DerivationofLangmuiradsorptionisotherm

Inorganic Chemistry

(A) Definition of acids and bases; solvents

Recapitulation of Arrhenius concept, Bronsted–Lowry definition, solvent system definition, Lux–Flood definition; Relative strength of hydracids, strength of oxoacids, Pauling's rules; HSAB principle, superacids; Solvent properties of water and liquid ammonia; reactions in liquid ammonia.

(B) Acid – Base equilibria

pH (of strong acid/base solution and weak acid/base solution), buffer solution, pH of a buffer solution, Hendersen's equation, buffer capacity; salt hydrolysis, pH of salt solutions (salt of strong acid/weak base; strong base/weak acid and weak acid / weak base); indicators, indicator constant, choice of indicators in acid – base titrations.

(C) Solubility equilibria

Solubility product & common ion effect; applications in group analysis – precipitation of sulphides and hydroxides.

(D) Group Chemistry – III : Group 15, 16, 17 and 18

Group 15 : Catenation, oxidation states, trends in the hydrides, halides, and oxides ; special features in the chemistry of hydrazine, hydroxylamine, hydrazoic acid/azides and phosphonitrilic compounds.

Group 16 : Catenation, atomicity, trends in the halides and hydrides; oxides and fluorides of S and Te; special features in the chemistry of the oxoacids of sulphur; Structure and bonding in O_2F_2, polythiazyl, tetrasulphurtetranitride.

Group 17 : Trends in the Chemistry of oxides, oxoacids and hydracids; special features in the chemistry of interhalogens, polyhalides, pseudohalogens, uses of potassium bromate and potassium hydrogen iodate in quantitative analysis.

Group 18 : Trends in the ionization energy and reactivities of He, Ne, Ar, Kr, Xe; reactivity, structure and bonding in fluorides and oxofluorides of Xe.

Organic Chemistry

A) Alcohols & Ethers (4 lectures)

Relative reactivity of 1°, 2°, and 3° alcohols in reactions via H-O and C-O cleavages; reactions of alcohols as nucleophiles, nucleophilic substitution reactions at carbinol C, S_Ni, dehydration, dehydrogenation, oxidation of alcohols. Reactions of epoxides and ethers via C-O cleavage, reactions of α-glycols: cyclic ketal/acetal formation, complex formation with H_3BO_3, oxidative cleavage of glycolic bond.

B) Aldehydes & Ketones (12 Lectures)

Nucleophilic addition to C=O bond: reactivity of carbonyl compounds, relative stability of adducts, formation of acetal, ketal, thioacetal, thioketal, and cyanohydrin, Grignard reaction, $LiAlH_4$ and $NaBH_4$ reductions, electrolytic reductions, reductive coupling, M.P.V reduction, Cannizzaro reaction, Internal Cannizzaro reaction, benzil-benzilic acid rearrangement; nucleophilic addition to α, β- unsaturated carbonyl compounds, reactions of benzoquinones, reactions with derivatives of NH_3, Wolff-Kishner reduction, Aldol condensation, Claisen

condensation, Directed Aldol condensation, Wittig reaction,Acyloin condensation(use of Me_3SiCl)

Mannich reaction, Enamine reaction, Reformatsky reaction, Darzen's reaction, Perkin reaction, Benzoin condensation, Tischenko reaction. Electrophilic substitution at α–position of carbonyl compounds, D-exchange, Nitrosation, halogenation.,Haloform reaction, SeO_2 oxidation.

C) Carboxylic Acids &Derivatives(6 lectures)

Nucleophilic substitution reaction at the acyl carbon of acyl halide, anhydride, ester, amide; tetrahedral mechanism, esterification of carboxylic acid and hydrolysis of esters:$A_{Ac}2$, $A_{Ac}1$, $A_{Al}1$, $B_{Ac}2$, $B_{Al}1$, $B_{Al}2$ mechanisms. Reactions via cleavage of α-C-H (use of trimethylsilyl chloride): HVZ reaction, Claisen ester condensation, Bouveault Blanc reduction, decarboxylation, Hunsdiecker reaction, action of heat on hydroxy acids.

Group-II

D) Organometallic compounds and Organonitogen Compounds (10 lectures)

i) Grignard reagents: Preparation and synthetic applications of Grignard reagents and organolithiumcompounds.Organocoppercompounds:Corey-House,Organocuprates.

ii) Organonitogen Compounds: Acidity of α-H of nitroalkanes, reduction of aromatic nitro compounds, alkyl cyanides and isocyanides and their hydrolysis, Von Richter reaction. Distinction among 1°, 2°, and 3° amines and their separation, Hofmann's exhaustive methylation, carbylamine reaction, partial reduction of aromatic nitro compounds.

Amines: Ring substitution vs N-substitution in aromatic amines, diazotisation and coupling reactions, synthetic applications of aromatic diazonium compounds. Preparation and synthetic uses of diazomethane and diazoacetic ester.

E) Rearrangement Reactions (8 lectures)

Rearrangements involving electron deficient C, N and O: Allylic rearrangement, Wagner rearrangement, Wolff rearrangement, Arndt-Eistert synthesis, Baeyer-Villigeroxidation,Cumene peroxide-phenol rearrangement, Dakin reaction, Beckmann rearrangement,Schmidt rearrangement, Hofmann rearrangement, Lossen rearrangement, Curtius rearrangement, rearrangements of N-azo to C-azo compounds, Orton rearrangement,Hofmann-Martius rearrangement, benzidine rearrangement.

F) Phenols (4 lectures)

Ambident nucleophile, ring substitution Vs O-Substitution. Reactions of phenols:Reimer-Tiemann reaction,Kolbe reaction,Houben-Hoesch reaction alkylation, acylation, Fries rearrangement, Claisen rearrangement, nitration, sulphonation, halogenation,

Semester V

Physical Chemistry

Phaseequilibria **12**

Lectures

a. Definitionofphase
b. Phaseboundaries
c. Components
d. Thermodynamicconditionforphaseequilibrium
e. Phaseruleanditsderivation
f. Phaseequilibriumforonecomponentsystem (for example H2O, S, CO2)
g. Firstandsecondorderphasetransition
h. Clapeyronequation
i. Clausius-Clapeyronequation
j. Trouton'srule
k. Liquidvaporequilibriumfortwocomponentsystem
l. ReviewoftheGibbs-DuhemandtheDuhem-Margulesequation
m. Constantboilingmixture
n. Criticalsolutiontemperature
o. Completelyimmisciblesystems
p. Thermodynamicsofmixingofbinarysolutions
q. Simpleeutecticsystems

SpectroscopyI **12**

Lectures

a. Spectroscopy-Natureofelectromagneticradiation,rangeofwavelength
b. Transitionmomentintegral(qualitativeidea)andallowedtransitions
c. Separationofelectronicandnuclearmotion – Born-Oppenheimerapproximation
d. Signaltonoiseratio
e. Widthandintensityoftransition,linebroadening

<u>Rotationalspectroscopy</u>

f. Rigidrotor(diatomiconly)
g. Selectionrule
h. Spectrum: position and intensity of spectral lines.
i. Non-rigidrotorandit'seffectonenergylevels
j. Selectionruleandspectrum
k. Application
l. Isotopeeffect

AtomicStructureandAtomicSpectra **12**

Lectures

a. AppripriatetreatmentofScrodingerequationforHydrogenicsystem
b. Solutionofradial,thetaandphipart(Generalexpression)
c. Shapesofs,p,dorbitals
d. Hydrogenicwavefunctionsupton=3
e. Atomicorbitalsandtheirenergies
f. Spectroscopictranstionsandselectionrules.
g. Conceptofelectronicspin
h. Spectraofcomplexatoms-singletandtripletstates
i. Spin-orbitcouplingandfinestructure
j. Term-Symbol and LS coupling

Inorganic Chemistry

(A) Isomerism, Reactivity and Stability of coordination complexes

Constitutional, Geometrical and optical isomerism with respect to C.N. = 4 and 6; Mills and Quibell complex, examples of purely inorganic optically active complexes; labile and inert complexes; substitution in square planar complexes and trans – effect (examples and applications); choice of ligands and stability of various oxidation states of the 3d metal ions; stability constant of complexes.

(B) Structure and Bonding in coordination complexes

VBT, CFT, splitting of d^n configurations in octahedral and tetrahedral fields, crystal field stabilization energy in weak and strong fields, pairing energy, Jahn – Teller distortion and its application; MOT (elementary idea), sigma and pi – bonding in octahedral complexes (a pictorial approach)

(C) Organometallic Chemistry

18 electron rule and its application to carbonyls (including carbonyl hydrides and carbonylates), nitrosyls, cyanides, metal–carbon sigma and pi – bonded organometallic complexes of transition metals; bonding and IR spectra of carbonyls and nitrosyls; Zeise's salt – its preparation properties and structure; ferrocene – its preparation, properties and sturture; elementary idea of fluxional molecules; oxidative addition, reductive elimination and insertion reactions; homogenous catalysis of organometallic compounds – hydrogenation, hydroformylation, and polymerization of alkenes (Ziegler – Natta catalyst)

Organic Chemistry

A) Synthetic strategies and asymmetric synthesis (14 lectures)

Disconnection approach towards synthesis of bifunctional molecules (both cyclic and acyclic): concepts of synthons, synthetic equivalents (ethyl acetoacetate, ethyl cyano acetate and diethyl malonate as examples). Functional group interconversion (FGI).Protection and deprotection of common functional groups (-OH, carbonyl, $-NH_2$, $-CO_2H$) in synthetic route, activation of synthetic equivalents.Umpolung: Illogical electrophiles and nucleophiles. Disconnection and synthesis of 1,3; 1,4 and 1,5-dioxygenated compounds. Robinson ring annulation, applications of Claisen rearrangement, Favorskii rearrangement and Demjanov rearrangements involving electron deficient C, O, N. Large ring synthesis: High dilution techniques. Asymmetric synthesis:

B)Pericyclic reactions (8 lectures)

Definition and classification.Electrocyclic reactions: FMO approach, examples of electrocyclic reactions (thermal and photochemical) involving 4 and 6 π-electrons and corresponding cycloreversion reactions. Cycloaddition reactions: FMO approach, Diels-Alder reaction, photochemical [2 + 2] reactions. Sigmatropic shifts and their order. [1,3]and [1,5] H-shifts. [3,3]-shifts with reference to Claisen and Cope rearrangements.

C) Stereochemistry of alicyclic compounds and Dynamic stereochemistry (12 lectures)

Stereoisomerism of di-substituted ring compounds, ring size strain and Baeyer strain theory, concept of I-strain. Conformational analysis of cyclohexanes: energy profile of ring inversion of cyclohexane, symmetry properties of chair,boat and skew-boat conformations, conformational analysis of mono- and di-substituted cyclohexanes.E2, S_N2 and NGP, lactonisation reactions of cyclohexane systems, oxidation of cyclohexanols with chromic acid, pinacol-pinacolonerearrangements,esterification,saponification of esters, steric assistance and steric hindrance.

Analytical Chemistry

[33L] UNIT 1:

CONVENTIONAL METHODS OF ANALYSIS 15L

(a) Redox Titrimetric analysis of Fe, Cu, Zn, Cr, Mn. Formol titration, estmation of sugars and vitamin C (principles only).

(b) Complexometric Titrations – Metal ion indicators, masking, demask agents (examples). Principles for the estimation of (Ca + Mg), (Fe + Al), and (Cu + Zn) in a mixture of complexometry.

(c) Basic concepts and simple application of chromatography – Thin layer, paper and column chromatography, R_f-values. Ion exchange chromatography (IEC): Ion exchange resins and their ion exchange capacities, deionization of water. Solvent extraction: Definition, types, principle and efficiency; factors affecting extraction, extraction with a metal chelator, gass chromatography, HPLC, extraction with dithiozone.

UNIT 2: INSTRUMENTAL METHODS OF ANALYSIS 10L

(a) Flame Spectrometry – Introduction, Principles, Elementary Theory and Instrumentation of atomic absorption and atomic emission spectrometry; Determination of Ca and Mg in tap water (application).

(b) Radiochemical methods and Environmental analysis. Basic instrumentation, Measurement of radioactivity, Neutron activation analysis, Isotope dilution analysis, radiometric titrations, hazards of radiation and safety measures.

UNIT 3: ERROR ANALYSIS AND ANALYSIS OF SAMPLES 8L

(a) Error Analysis – Errors and their classifications, determinate and indeterminate errors, systematic and random errors, accuracy and precession, distribution of random errors; statistical analysis of data; methods of least squares and standard deviation, confidence interval, significance testing

Semester VI

Physical Chemistry

Thermodynamics III 12

Lectures

a. TheNernstheattheorem
b. Thirdlawofthermodynamics
c. Residualentropy
d. Raoult's law
e. Henry'sLaw
f. Positiveandnegativedeviationfromidealbehaviour
g. Idealsolution and ideallydilutesolution
h. Definitionandthermodynamicoriginofcolligativeproperties

i. Thermodynamicderivationofcolligativepropertiesofsolutionusingchemicalpote
ntial andtheirinterrelationships(loweringofvapour pressure,depressionoffreezing point,elevationofboilingpointandosmoticpressure)
j. Abnormalcolligativeproperties

SpectroscopyII **12**
Lectures
a. Vibrationofadiatomicmoleculeandsimpleharmonicoscillator
b. ReviewofSolutionofquantumharmonicoscillator(generalexpression)
c. Selectionruleforharmonicoscillator
d. Spectrum
e. Anharmonicityanditseffectonenergylevels
f. Selectionruleforanharmonicoscillator
g. Vibrationalspectrum
h. Rotational – vibrationalcoupling in the limit of Born-Oppenheimer approximation
Ramanspectroscopy(Qualitative)
i. RayleighandRamanscattering
j. Polarizabilityellipsoids
k. FeaturesandconditionforRamanactivity(forlinearandnon-linearAB_2molecule)
l. RotationalandvibrationalRamanspectraanditscharacteristics

Photochemistry **12**
Lectures
a. Potentialenergycurvesforelectronicstates,Frank-Condonprinciple
b. Decayofexcitedstatesbyradiativeandnon-radiativepaths
c. Timescales
d. Fluorescenceandphosphorescence
e. Jablonskidiagram
Mechanismofrelaxationthroughnon-radiativepaths(Unimolecularandbimolecular mechanism(colision,energytransfer))
f. Photophysicsoftheexcitedstate
g. Lawsofphotochemistry
h. Quantumyieldandit'smeasurementforphotochemicalprocesses
i. Photostationarystate
j. Photosensitizedreactions
k. Photochemistry of Photosynthesis

Inorganic Chemistry

(A) Magnetism and Spectra of Coordination Complexes
Orbital and spin magnetic moments, spin only magnetic moments of $3d^n$ ions and their correlation with effective magnetic moments, quenching of magnetic moments in presence of crystal field; ferromagnetic and anti– ferromagnetic coupling (elementary idea with examples only); d –d spectra, weak–field splitting schemes, qualitative Orgel diagrams for d^n systems and their spectroscopic ground states, selection rules for spectral transitions, charge transfer spectra (elementary idea with examples only).
(B) Bioinorganic Chemistry
Essential and trace elements of life; role of metal ions in biology – Na^+, K^+, Ca^{2+}, Mg^{2+}, $Fe^{2+/3+}$, $Cu^{+/2+}$,Zn^{2+}; active site structures and bio-functions of myoglobin, haemoglobin, cytochromes, ferredoxins, carbonic anhydrase; photosynthesis – PS–I and PS–II, sodium ion pump and ionophores, metal ion induced toxicity and chelation therapy, metal ion as drugs (cisplatin and a few gold drugs)
(C) Chemistry of the Lanthanides

General characteristic with respect to electronic configuration, oxidation states and ionization enthalpies, lanthanide contraction, separation of lanthanides by ion – exchange method.

Organic Chemistry

A) Heterocyclic compounds (12 lectures)

Synthesis (including retrosynthetic approach),Knorrpyrole synthesis, Hantz pyridine synthesis, Fischer indole synthesis, Skraup'squinoline synthesis, Bischler-Napieralski synthesis, reactivity, orientation and important reactions of furan, pyrrole, thiophene, pyridine, indole, quinoline, and isoquinoline.

B) Carbohydrates (10 lectures)

Monosaccharides- classification, osazone formation, stepping up and stepping down of aldoses, interconversion of aldoses to ketoses and vice versa, epimerisation. Constitution and configuration of D-glucose and D-fructose, ring structure and conformational aspects of D-glucose and its derivatives, anomeric effect, mutarotation of D-glucose.Disaccharides: structure of sucrose.

C) Amino acids (10 lectures)

Synthesis of α-amino acids (Gabriel, Strecker, azlactone, acetamido, malonic ester methodologies). Isoelectric popint, ninhydrin reaction, resolution of amino acids.Peptides: geometry of peptide linkage, peptide synthesis including Merrifield synthesis,structure determination of peptides, C-terminal and N-terminal unit determination,determination of amino acid sequence.

Biochemistry

A) Structural aspects of Biomolecules 9 lectures

Proteins- Introduction and classification. Protein structure- primary, secondary, tertiary
and quaternary structure(Forces that stabilizes structure of proteins: H-bonds, hydrophobic bond, electrostatic attraction, Vanderwaals interaction, dipole-dipole interaction.) Denaturation and renaturation of proteins.Behavior of proteins in solutions, salting- in and salting -out of proteins. Structure and biological function of fibrous proteins (keratins, collagen and elastin)
*(Globular proteins and structural aspects of carbohydrates are excluded as Chem (H) students study these in details in Bioinorganic Chemistry).

Nucleic acids- Nucleosides and nucleotides.Nature of genetic material. Composition ofRNA and DNA, generalized structural plan of nucleic acids, nomenclature used in writing structure of nucleic acids, complementary base- pairings, features of DNA doublehelix (Watson-Crick model). Denaturation and annealing of DNA, structure and role ofdifferent types of RNA.Size of DNA of prokaryotic and eukaryotic cells.

Lipids- Definition and classification.Fatty acids- properties of saturated and unsaturatedfatty acids.Esters of fatty acids-formation and hydrolysis; Essential fatty acids.Triacylglycerols. Reactions and characterization of fats – hydrolysis, saponification value, iodine number, rancidity of fats, Reichert- Meissel number. Biological significance of fats.Characterization of fats, Phospholipids, Micelle bilayer, liposomes, Glycolipids, steroids and sterols.

B) **Bioenergetics and Metabolism**: (2.**5 marks)** **2 lectures**
Principles of Bioenergetics: Bioenergetics and Thermodynamics, Phosphoryl group transfers and ATP generation, Biological Oxidation and Reduction reaction.

C) **Carbohydrate metabolism: (5 marks)** **5 lectures**
Intracellular metabolism of glucose - glycolysis, reaction and energetic of TCA cycle, (gluconeogenesis, glycogenesis, glycogenolysis, reactions and physiological significance of pentose phosphate pathway, regulation of glycolysis, TCA cycle, and glycogen metabolism).

D) **Oxidative phosphorylation and electron transport chain: (2.5 marks) 2 lectures**
Structure of mitochondria, sequence of electron carriers, ATP synthesis, inhibitors of ETC, basic concept of oxidative phosphorylation, inhibitors and uncouplers of oxidative phosphorylation, photophosphorylation.

E) **Lipid metabolism: (2.5 marks)**
Metabolism (anabolism and catabolism) of triglyceride, Transport of fatty acid into mitochondria, Beta-oxidation of fatty acids, reactions and energetic of beta oxidation, biosynthesis of saturated and unsaturated fatty acids, metabolism of ketone bodies, biosynthesis of phospholipids and cholesterol.

F) **Amino acid metabolism: (5 marks)**
General reactions of amino acid metabolism (oxidative
deamination, transamination, decarboxylation etc), glucogenic and ketogenic amino acids, urea cycle, biosynthesis and catabolism of amino acids (glycine, phenylalanine, glutamic acid), inborn errors of amino acid metabolism.

G) **Nucleotide metabolism: (2.5 marks)**
Biosynthesis and catabolism of purines and pyrimidines
(Adenine and cytosine)

H) **Enzymes: (20 marks)**
Cofactors – Definition, examples of a) metal ions b) coenzymes c) prosthetic group Definition, examples of holoenzymes, Apoenzyme.
Classification of enzymes, IUPAC system, Name & examples of each class
Mechanism of enzyme activity—standard free energy change in a reaction-transition state, activation energy both in non-enzymatic and enzymatic reaction, reaction rate, rate
constant, rate limiting step, rate equation, binding energy, specificity of enzymes geometric and stereo specificity with example, lock & key hypothesis, induced fit hypothesis, proximity and orientation effect, strain and distortion theory, enzyme catalysis-i) acid- base catalysis, ii)metal ion catalysis iii) covalent catalysis – Examples .

Regulatory enzyme- allosteric enzyme, definition & example, allosteric modulators, feedback inhibition, kinetic properties of allosteric enzyme, K enzymes, M enzymes, sequential model & symmetry model, examples, regulation by covalent modification (likephosphorylation), example, regulation by proteolytic cleavage of protein, zymogens,example

Isozymes-Definition and basis of difference, example-lactate dehydrogenase.