Assistant Professor in Chemistry- Collegiate Education Syllabus

Module 1
Inorganic Chemistry-1

Structure and bonding in molecules- Chemical periodicity- Chemistry of Hydrogen and s block elements- Chemistry of p block elements and d block elements- Extractive chemistry of various metals of commercial importance- Chemistry of Nontransition elements like Glass

Theories of acids and bases- HSAB concept- solvent effects, linear free energy relationship – mechanism and methods of determination, super acids - Reactions in Non-aqueous solvents- Protic and Aprotic solvents- Chemistry of Isopoly and Heteropoly acids ; Silicon-Oxygen compounds; Zeolites ; Xenon and Krypton compounds including their organic and coordination compounds

Synthesis, reactions, structure and bonding in Sulphur-Nitrogen compounds ; Sulphur-Phosphorus compounds ; Phosphorous-Nitrogen compounds ; Boron - Nitrogen compounds ; Boron hydrides; Organoboranes; Carboranes and metallocarboranes- STYX and WADE rules

Chemistry of Lanthanides and Actinides including their extraction and applications as well as their coordination complexes and spectral behaviour

Theories of Coordination Chemistry in detail: Werner's theory - Crystal field theory – Ligand field theory – Molecular orbital theory- Stereochemistry of coordination compounds- Jahn Teller distortion- Detailed study of Stability and reactions of metal complexes- Electron transfer, Substitution and Photochemical reactions and their kinetics

Module 2
Inorganic Chemistry-2

Construction of energy level diagrams. Correlation diagram. Method of descending symmetry. Term symbols; Correlation diagrams for d^n and d^{10} ions in octahedral and tetrahedral fields ; Orgel and Tanabe-Sugano diagrams. Symmetry and Selection rules for electronic spectra , IR and Raman Theory of Electronic, IR, NMR, ESR and Mossbaur spectra of complexes. Different aspects of magnetic properties of complexes and their determination.

Spectroscopic Methods in Inorganic Chemistry- Structural elucidation of coordination compounds containing the following molecules/ ions as ligands- NH_3, H_2O, CO, NO, OH^-, SO_2^- , CN^- , SCN^- , NO^-, NO^-, CH_3COO^- and X^- (X=halogen). changes in ligand vibration on coordination with metal ions.- CD and ORD spectra of metal complexes- NMR of metal nuclides with emphasis on ^{11}B, ^{31}P and ^{19}F NMR.- ESR spectra: Application to Cu(II) complexes and inorganic free radicals such as PH_4, F^- and $[BH]^-$. Mossbauer Spectroscopy: Application of the technique to the studies of iron and tin complexes

Nomenclature, synthesis, structure, properties and bonding of organo-metallic compounds - metal carbonyls and cyanides – Complexes with linear π donor ligands: Olefins, acetylenes, dienes and allyl complexes. Complexes with cyclic π donors: Cyclopentadiene, benzene complexes. Structure and bonding of ferrocene and dibenzenechromium complexes - Metal –Metal bonds and metal atom clusters. Tri , Tetra and hexa nuclear clusters, Isoelectronic and isolobal relationships, Low nuclearity and High nuclearity carbonyl clusters (LNCCs and HNCCs). Cubane Clusters, Chalcogenide Clusters, Chevrel Phases. Zintl Anions and Cations – Capping Rule Catalysis by organo metallic compounds and metal clusters- hydrogenation, hydroformylation and polymerization.

Essential and trace metal elements in biological systems, . Role of Iron,Calcium, Copper, Lithium, Aluminium, Magnesium and other metals in biological systems structure and functions of biological membranes, mechanism of ion transport across membranes, sodium- potassium pump. - Role and effects : Coenzymes, Cytochromes, chlorophylls and hormones. Photosynthesis, porphyrin ring system, chlorophyll, PS I and PS II. Synthetic model for photosynthesis. Inorganic medicinal chemistry. Metals in medicine.

Module 3
Inorganic Chemistry-3

Nuclear reactions - structure and stability- Magic numbers – Detailed study of different nuclear models- radio active equilibria and equations of radioactive decay and growth - Nuclear reactions: Direct nuclear reactions, heavy ion induced nuclear reactions, photonuclear reactions. Neutron captures cross section and critical size -Applications of nuclear reactions- fission and fusion; neutron activation analysis – counting techniques.

Solid State Chemistry: Crystal symmetry- Point groups and space groups. Miller indices and Bravais Lattices- Close packed structures: BCC, FCC and HCP. Voids. Coordination number.

X-ray diffraction by crystals: Applications and calculations using Bragg's equation and indexing methods. Different types of Crystal defects and consequences

Electronic structure of solids. Different theories about conductors, insulators and semiconductors and their applications. Doping and band gap adjustments. AX, AX_2, A_mX_2, ABX_3, Spinels and Inverse spinel structures. Structure and theories of Liquids- Liquid crystals and their applications.

Temperature dependence of conductivity, carrier density and carrier mobility in semiconductors - Superconductivity, Photoconductivity Photovoltaic effect.

Colour in inorganic solids. - Dielectric properties. Dielectric materials. Ferroelectricity, pyroelectricity, piezoelectricity and ionic conductivity. Applications of ferro, piezo and pyroelectrics.

Inorganic Advanced materials : Solid Electrolytes: Mixed oxides, cationic, anionic solid electrolytes, mixed ionic-electronic conductors- Solid Oxide Fuel Cells (SOFC), Rechargeable battery materials- Solid state chemistry of metal nitrides and fluorides, chalcogenides, intercalation chemistry and metal-rich phases.- Inorganic pigments, Inorganic

phosphors- Molecular materials and fullerides, basic idea of molecular materials chemistry like One dimensional metals, Molecular magnets and Inorganic liquid crystals.

Module 4
Organic Chemistry-1

Nomenclature of organic compounds - Cyclic, fused polycyclic and bridged polycyclic hydrocarbons, bridged and fused hydrocarbon systems, Spirocyclic hydrocarbon systems, Heterocyclic systems containing Nitrogen and Oxygen.

Molecular symmetry and chirality, axial chirality, planar chirality and helicity, relative configuration, stereochemical nomenclature, R and S, E and Z. Stereo chemistry of biphenyl and allenes - Topicity and prostereo isomerism -asymmetric synthesis. Axial stereochemistry: atropisomerism and its designation - biphenyls, allenes, spiranes- M and P configurations. Stereoselectivity: enantioselectivity, diastereoselectivity & stereoconvergence. Stereospecific and stereoselective synthesis. stereotopicity & stereoprojections. Prochiral centre and prochiral faces - Pro R and Pro S, Re face and Si face, Importance of prochirality in biological systems. Geometrical isomerism . , Conformational analysis in acyclic and cyclic systems , Application of Cram's rule, Felkin–Ahn model

Basic concepts of Organic reactions - Electron displacement effects –Aromaticity and antiaromaticity. Non aromatic, homoaromatic, hetero and non–benzenoid aromatic systems. Aromaticity of annulenes, mesoionic compounds, metallocenes, cyclic carbocations and carbanions.

Mechanism and applications of common substitution, addition, elimination and rearrangement reactions. Stereochemistry and factors affecting Aliphatic and Aromatic SN1 and SN2 reactions. S_N1', S_N2', S_Ni S_NAr and benzyne mechanisms – NGP and Nonclassical carbocations- Generation and reactions of Nitrenes, Carbenes and free radicals like Triphenyl methyl, TEMPO, Dibenzoyl peroxide, NBS , Tributyl Tinhydride and AIBN. - Chlorination of alkane, addition of HX, S_RN1 mechanism- Acyloin condensation, Alkyne coupling reactions- Reimer-Tiemann, Vilsmeier-Haack reactions. Mitsunobu reaction and Chichibabin reactions.

Mechanism of Addition of H_2O, X_2, HX, and boranes to C=C systems- Cis and trans hydroxylation of cycloalkenes- Mechanism and applications of Michael addition and Robinson Annulation- Aldol condensation- Stork enamine, Cannizzaro, Perkin, Ritter, Stobbe, Knoevenagel, Darzen, Reformatsky and benzoin condensations- Grignard, Mannich, Thorpe reactions and Dieckmann condensation

Mechanism and regio and stereo aspects of E1, E2 and E1cb reactions in cyclic and acyclic systems. Hoffmann and Saytzeff elimination- Elimination Vs substitution- Mechanism and applications of Shapiro reaction, Peterson and Julia olefination, Wittig and Wittig - Horner reactions; Chugaev reaction and Cope eliminations- Sodium in liquid ammonia and Lindlars catalyst in conversion of alkynes to alkenes

Module 5
Organic Chemistry-2

Mechanism with evidence of Wagner – Meerwein, Pinacol, Demjanov, Hofmann, Curtius, Schmidt, Lossen, Beckmann, Fries, Hofmann–Martius, Dienone–phenol, Benzilic acid, Benzidine, Favorskii, Stevens and Wolf rearrangement.

Oxidation and Reduction reactions in organic synthesis- Reduction using boranes, hindered boranes and derivatives- $NaBH_4$, and $LiAlH_4$, DIBAL-H, tri-n-butyltin hydride, diimide, and aluminium alkoxide. Birch reduction, Clemmensen reduction and Wolff - Kishner reduction, Huang - Minlon modification, Rosenmund reduction - allylic and benzylic oxidation, Sharpless epoxidation, oxidation using SeO_2, manganese (IV) oxide, lead tetraacetate, ozone, peracids, DDQ, silver carbonate and Cr(VI) reagents. Jones oxidation, Swern oxidation, Moffatt oxidation, Sommelet reaction. Applications of HIO_4, OsO_4 and mCPBA

Linear Free Energy Relations, The Hammett equation and its applications. Significance of sigma (σ) and rho (ρ) reactions with negative and positive ρ, low and high ρ, abnormal Hammet plot, Taft equation. Hammet plot and applications- Primary, secondary, inverse kinetic isotope effects. Salt effects and special salt effects in SN reactions

Retrosynthetic analysis and disconnection approach in organic synthesis- Olefin metathesis- Grubbs' catalysts. Umpolung concept-1,3-Dithiane, benzoin condensation. Heck, Negishi, Sonagashira, Kumada, Stille coupling and Suzuki coupling

Use of various organic, inorganic and organometallic reagents in organic synthesis- Grignard reagents, Alkyl lithiums, Lithium Dialkylcuprates, Alkynyl copper reagents, Tebbe reagent etc. Use of various protecting groups in peptide synthesis. Phase transfer catalysis and its applications.

Module 6
Organic Chemistry-3

Photochemical processes. Singlet and triplet states and their reactivity, Jablonski diagram, Energy transfer, sensitization and quenching. Photoreactions of carbonyl compounds, enes, dienes and arenes. Patterno-Buchi and Barton reactions, Hofmann-Löffler- Freytag reaction, photo-Fries and Di-π methane, di- π methane rearrangements. Applications of photochemistry.

Classification of pericyclic reactions, FMO, Correlation diagram, Mobius and Huckel theory of electrocyclic and cyclo addition reactions- Stereo and region selectivity and industrial applications of Diels Alder reaction, 1,3–Dipolar cycloaddition and Sigmatropic rearrangements

Chemistry of Natural Products : Terpenes, steroids, alakaloids, carbohydrates, proteins, nucleic acids, vitamins, prostoglandins, hormones and enzymes.

Combinatorial organic synthesis, introduction, methodology, automation, solid supported and solution phase synthesis, study of targeted or focused libraries and small molecule libraries. Application of Drug design and development- various steps

Fundamentals of polymerization - structure - property relationship of polymers and polynucleotides- Protein sequencing by Edmans method.

Protein denaturation - Synthesis of stereo regular polymers. Ziegler-Natta catalyst. Polymers in organic synthesis - supports, reagents and catalysts. Biodegradable polymers biopolymers

Spectrocopic methods in Organic chemistry- Applications of UV, IR, H^1NMR, C^{13}NMR and Mass Spectroscopy - 2D NMR techniques - NOE, DEPT, and 2D techniques such as COSY-HSQC, HMQC and HMBC. Spectral interpretation and structural elucidation. Solving of structural problems on the basis of numerical and spectrum based data. ORD and CD - theory and applications

Module 7
Physical Chemistry-1

Gaseous State- Maxwell's distribution and equation- Transport phenomena- Chapman equation- Equations of state of real gases- vander Waals, Virial and other equations- Inter molecular forces and consequences.

Electronic Structure of Solids - Crystal Symmetry - Theories of Solids - Properties of Solids : Electrical, Magnetical and Optical - Crystal defects. Structure and Theories of Liquids- XRD of liquids- Theories and calculation of Surface tension and Viscosity - Liquid Crystals and their applications

Laws of Thermodynamics - Entropy and its dependence on variables of a system- Equations of state- Euler's relation, Gibbs and Helmholtz equations and energies. Maxwells relations- Gibbs Duhem equation- Partial Molar Quantities- Chemical potential- Fugacity- Activity coefficients. Thermodynamics of Solutions – Duhem Marghules equation- vant Hoff's equations, isochore and isotherm. Thermodynamics of irreversible process – Fundamentals and advances in the study of Phase Equilibria - Two and Three Component Systems

Statistical thermodynamics - Molecular Partition Function - Quantum Statistics - Heat capacities of Solids and Gases- Relationship between partition functions and thermodynamic properties, Sackur-Tetrode equation. The principle of equi-partition of energy

Chemical equilibrium, Law of mass action, Transformation of the equilibrium expressions. Statistical derivation.

Module 8
Physical Chemistry-2

The gas-solid interphase, types of adsorption. Monolayer and multilayer adsorption - Adsorption Isotherms Heat of adsorption and its determination .-Adsorption from solutions -Determination of surface area of solids-Harkins–Jura absolute method, point B method, Langmuir method and BET method- - Principles of LEED, SEM, TEM, ECSA, Photoelectron spectroscopy, scanning probe microscopy, Auger electron spectroscopy

Electrochemistry and Ionics: Activity and activity coefficient of electrolytes, determination of activity coefficient.- Electrodes and Electrochemical Cells - Nernst, Debye-Huckel, Omsager Equations - Over potentials: Butler-Volmer equation. Tafel and Nernst equation, Tafel plot and its significance - Electrolytic Polarization- Fuel cells: H2-O2, zinc-air and solid oxide fuel cells- Theory and applications of electro Analytical Methods : Potentiometry, Polarography , Coulometry, Conductometry, Cyclic Voltametry, Stripping Voltametry and Amperometry- Colloids - Zeta Potential - Electrokinetic Phenomena

Basic principles of Kinetics - Kinetics of Complex reactions - steady state approximation -Theories of Reaction Rates - Arrhenius equation - fast reactions and methods of study. Reactions in solution: Factors affecting reaction rates in solutions, effect of dielectric constant and ionic strength, cage effect, Bronsted-Bjerrum equation - Kinetic effects: Primary and secondary kinetic salt effect, influence of solvent on reaction rates, significance of volume of activation, linear free energy relationship. Hammet equation and Taft equation.

Catalysis: Mechanism and theories of homogeneous and heterogeneous catalysis. Bimolecular surface reactions. Langmuir–Hinshelwood mechanism. Enzyme catalysis.

Module 9
Physical Chemistry-3

Classical mechanics and its limitations –need of quantum mechanics, de Broglie relation and its experimental proof, uncertainty principle and its consequences- Formulation of Quantum Mechanics - Postulates of quantum mechanics- Application of Quantum mechanics to Exactly Solvable Model Problems- Translational motion- Quantum mechanical tunnelling- Vibrational motion- and Rotational motion –SHO, Rigid Rotor- Legendre polynomials and associated Legendre functions Approximation Methods and Chemical Bonding - Hydrogen like Atoms -Multi Electron Systems - Angular Momentum – SCF and variation method - MO diagram of homo nuclear diatomic molecules Li_2, Be_2, B_2, C_2, O_2 and F_2 and hetero nuclear diatomic molecules LiH CO, NO and HF-

Wave functions for multi electron systems, wave equation for multi electron systems, symmetric and anti- symmetric wave functions, Pauli’s anti-symmetry principle, and the postulate of spin- Spin orbitals. Spin- orbit coupling. Vector atom model-Term symbols, selection rules and exp anation of spectral lines of hydrogen atom- Applications- Chemical Bonding in Diatomic and Polyatomic Molecules

Computational Chemistry - Computational methods : ab initio, Semi Empirical methods - Molecular Mechanics

Quantum statistics- Bose-Einstein statistics, Thermodynamic probability- Maxwell Boltzmann, Bose Einstein and Fermi-Dirac statistics- Quantum theory of heat capacity - calculation of heatcapacity of gases- Dulong and Petit’s law, Kopp’s law; limitations.- Einstein theory and Debye theory of heat capacity

Symmetry elements and symmetry operation. Basic principles of Group Theory - Character Tables - . Point groups and their systematic identification.- Multiplication of

operations - Setting up of character table of C_{2v}, C_{3v} and C_{2h} groups –Applications to MO Theory, Chemical Bonding and Spectroscopy

Electronic Spectroscopy of Atoms – Basic principles of Molecular spectroscopy: Microwave, Infrared, Raman, Electronic, NMR, ESR, Raman and Mossbaur

Module 10
Analytical, Environmental, Material and Supramolecular chemistry

Evaluation of analytical data: Accuracy and precision. Standard deviation, variance and coefficient of variation. Student ‘t’ test, ‘Q’ test, and ‘F’ test. Confidence limits- Errors and their minimisation- Significant figures- Correlation analysis- Calculation of R by method of least squares

Theory and practice of : Quantitative and Qualitative analysis- Inorganic analysis- Organic analysis and preparations - physical chemistry experiments (Post graduate level)

Applications of TG, DTA and DSC in the study of metal complexes, ceramics and polymers.

Theory of chromatographic techniques -Column, TLC, Paper, GC, HPLC and ion exchange chromatographic techniques. Solvent extraction. Extraction using supercritical liquid CO_2, Craig’s technique of liquid-liquid extraction

Twelve principles of green chemistry and issues in sustainable chemistry - Green synthesis - Application of Phase Transfer Catalysts -Green Reactions- Applications of Microwave and sonication in the synthesis of organic compounds.

Chemistry of Atmosphere, Hydrosphere and Lithosphere.

Nanostructures - ID, 2D and 3D structures - Synthesis and applications of nanomaterials..

Chemistry behind Piezoelectric, magnetostrictive, halochromic, chromogenic, electrochromic, thermochromic, magnetocaloric and thermoelectric materials

Supramolecular chemistry - Molecular recognition : Synthetic Receptors, Cyclodextrin, Calixiranes, Cyclophanes, Crown Ethers- Drug design and Drug action.