Subject: Chemical Science

Existing Syllabus	Proposed Syllabus
Inorganic Chemistry 1. Chemical periodicity 2. Structure and bonding in homo and heteronuclear molecules, including shapes of molocules (VSEPR Theory) 3. Concepts of acids and bases, Hard-Soft acid base concept, Non-aqueous solvents. 4. Main group elements and their compounds: Allotropy, synthesis, structure and bonding, industrial importance of the compounds 5. Transition elements and coordination compounds; structure, bonding theories, spectral and magnetic properties, reaction mechanisms. 6. Inner transition elements: spectral and magnetic properties, redox chemistry, analytical applications. 7. Organometallic compounds: synthesis, bonding and structure, and reactivity, Organometallics in homogeneous catalysis. 8. Cages and metal clusters. 9. Analytical chemistry separation, spectroscopic, electro- and thermoanalytical methods. 10. Bioinorganic chemistry: photosystems, porphyrins, metalloenzymes, oxygen transport, electron transfer reactions; nitrogen fixation, metal complexes in medicine. 11. Characterisation of inorganic compounds by IR, Raman, NMR, EPR, Mössbauer, UV-vis, NQR, MS, electron	CHEMICAL SCIENCES 1. Atomic Structure: Basic principles of quantum chemistry: postulates; operator algebra; exactly solvable systerns: particle-in-a-box, harmonic oscillator, rigid-rotor, and the hydrogen atom. Shapes of atomic orbitals; orbital and spin angular momenta; angular momentum operators, tunneling. Approximate methods of quantum mechanics: Variational principle; first-order perturbation. Many-electron systems and antisymmetry principle. 2. Molecular Structure and Bonding: Chemical bonding; elementary concepts of molecular orbital (MO) and valence bond (VB) theories; Born Oppenheimer (BO) approximation, Hückel theory for conjugated n-electron systems.Valence bond (VB) theory. Molecular orbital (MO) theory: heteronuclear diatomic molecules, polyatomic molecules AH, (n = 2 to 4). Ionic bond, covalent bond, metallic bond, coordinate covalent bond and weak chemical forces. 3. Nomenclature, Structure, and Isomerism of Organic Compounds: Nomenclature, hybridization, resonance, frontier molecular orbitals, aromaticity, acidity and basicity, structure and stability of reactive intermediates (carbocations, carbanions, free

spectroscopy and microscopic techniques.

12. Nuclear chemistry: nuclear reactions, fission and fusion, radio-analytical techniques and activation analysis.

Physical Chemistry:

1. Basic principles of quantum mechanics: Postulates; operator algebra; exactly solvable systems: particle-in-a-box, harmonic oscillator and the hydrogen atom, including shapes of atomic orbitals; orbital and spin angular momenta; tunneling.
2. Approximate methods of quantum mechanics: Variational principle; perturbation theory up to second order in energy, applications.
3. Atomic structure and spectroscopy; term symbols; many-electron systems and antisymmetry principle.
4. Chemical bonding in diatomics; elementary concepts of MO and VB theories; Huckel theory for conjugatedπ -electron systems.
5. Chemical applications of group theory; symmetry elements; point groups; character tables; selection rules.
6. Molecular spectroscopy: Rotational and vibrational spectra of diatomic molecules; electronic spectra; IR and Raman activities selection rules; basic principles of magnetic resonance.
7. Chemical thermodynamics: Laws, state and path functions

radicals, carbenes, benzynes and nitrenes). Isomerism, stereoisomerism (centre, axial, planar and helical chirality), configuration descriptors; topicity and descriptors; conformations of organic molecules.

4. Group Theory and Spectroscopy: Chemical applications of group theory;symmetry elements; point groups; character tables; selection rules. Atomic spectroscopy; term symbols; Molecular spectroscopy; rotational, vibrational and Raman spectra; electronic spectra; basic principles of magnetic resonance.Analytical Techniques for Inorganic Compounds: Ultraviolet-Visible (UV-Vis) spectroscopy, fluorescence spectroscopy, Fourier-transform infrared spectroscopy (FTIR) and Raman spectroscopy, nuclear magnetic resonance (NMR) and electron spin resonance (ESR) spectroscopy, mass spectrometry, cyclic voltammetry.Interpretative Molecular Spectroscopy: Structure elucidation of organiccompounds using Fourier transform infrared spectroscopy (FTIR), ultraviolet-visible (UV-Vis), ^{1}H, ^{13}C nuclear magnetic resonance (NMR) and mass spectra. Determination of configurations and conformations and probing reaction mechanisms.
5. Chemical and Statistical Thermodynamics: Laws of thermodynamics. state and path functions and their applications; thermochemistry, thermodynamic functions and

and their applications; thermodynamic description of various types of processes, Maxwell's relations, spontaneity and equilibria; temperature and pressure dependence of thermodynamic quantities; Le Chatelier principle; elementary description of phase transitions; phase equilibria and phase rule; thermodynamics of ideal and non-ideal gases, and solutions.

8. Statistical thermodynamics: Boltzmann distribution; kinetic theory of gases; partition functions and their relation to thermodynamic quantities calculations for model systems.

9. Electrochemistry: Nernst equation, redox systems, electrochemical cells; Debye-Huckel theory; electrolytic conductance - Kohlrausch's law and its applications; ionic equilibria; conductometric and potentiometric titrations.

10. Chemical kinetics: Empirical rate laws and temperature dependence; complex reactions; steady state approximation; determination of reaction mechanisms; collision and transition state theories of rate constants; unimolecular reactions; enzyme kinetics; salt effects; homogeneous catalysis; photochemical reactions.

11. Colloids and surfaces: Stability and properties of colloids; isotherms and surface area; heterogeneous catalysis.

their relationships; Maxwell's relations; spontaneity and equilibria; temperature and pressure dependence of thermodynamic quantities; Le Chatelier principle; phase transitions, phase equilibria and phase rule; thermodynamics of ideal and non-ideal gases, and solutions. Kinetic theory of gases; Boltzmann distribution; partition functions and their relation to thermodynamic quantities.

6. Electrochemistry: Nernst equation, redox systems, electrochemical cells; Debye-Hückel theory; electrolytic conductance Kohlrausch's law and its applications; ionic equilibria; conductometric and potentiometric titrations.
7. Chemical Kinetics and Surface Chemistry: Empirical rate laws and complex reactions; steady state approximation; mechanism of complex reactions, collision and transition state theories of rate constants; potential energy surfaces, unimolecular reactions, temperature dependence of rate constants; enzyme kinetics; salt effects; homogeneous catalysis; photochemical reactions, fast reactions. Nuclear reaction processes. Kinetics of polymerization and molecular weight determination of polymers. Stability and properties of colloids; isotherms and surface area; principles of heterogeneous catalysis.
8. s and p Block Elements: Periodic trends, hydrides, halides, oxides, oxoacids,

12. Solid state: Crystal structures; Bragg's law and applications; band structure of solids.
13. Polymer chemistry: Molar masses; kinetics of polymerization.
14. Data analysis: Mean and standard deviation; absolute and relative errors; linear regression, covariance and correlation coefficient.

Organic Chemistry

1. IUPAC nomenclature of organic molecules including regio- and stereoisomers.
2. Principles of stereochemistry: Configurational and conformational isomerism in acyclic and cyclic compounds; stereogenicity, stereoselectivity, enantioselectivity, diastereoselectivity and asymmetric induction.
3. Aromaticity: Benzenoid and non-benzenoid compounds - generation and reactions.
4. Organic reactive intermediates: Generation, stability and reactivity of carbocations, carbanions, free radicals, carbenes, benzynes and nitrenes.
5. Organic reaction mechanisms involving addition, elimination and substitution reactions with electrophilic, nucleophilic or radical species. Determination of reaction pathways.
6. Common named reactions and rearrangements applications in organic

nitrides, sulfides. Boranes, carboranes, silicones, silicates, boron nitrides, borazines and phosphazenes. Allotropes of carbon, phosphorous and sulphur. Noble gases. Acids and bases: Lewis, Brønsted, Hard and Soft Acids and Bases (HSAB). Nonaqueous solvent systems, liquid NH3, liquid SOz, superacids.
9. Properties and Reactions of Organic Compounds: Synthesis and reactions of organic compounds alkanes, alkenes, alkynes, arenes, alcohols, phenols, aldehydes, ketones, carboxylic acids, esters, nitriles, halides, nitro compounds, amines, amides, etc. Reactions of aromatic compounds electrophilic and nucleophilic substitutions. Reagents for functional group interconversion, oxidation and reduction. Pericyclic reactions cycloadditions, electrocyclic, sigmatropic, cheletropic andgroup-transfer reactions stereochemical implications, Photochemical reactions.
10. d and f Block Elements:d-block elements and complexes: Structure and isomerism of complexes. Periodic trends. Stability of various oxidation states. Crystal Field Theory (CFT) and Molecular Orbital Theory (MOT) of 4, 5, 6-coordinate complexes. Energy level diagrams, Crystal Field Stabilisation Theory (CFSE), applications of CFT, Jahn-Teller distortion. Metal-metal bonded compounds.Spectroscopy and magnetism: Term symbols, selection rules, Orgel and Tanabe-Sugano diagrams, spectrochemical series,

synthesis.

7. Organic transformations and reagents: Functional group interconversion including oxidations and reductions; common catalysts and reagents (organic, inorganic, organometallic and enzymatic). Chemo, regio and stereoselective transformations.

8.Concepts in organic synthesis: Retrosynthesis, disconnection, synthons, linear and convergent synthesis, umpolung of reactivity and protecting groups.

9. Asymmetric synthesis: Chiral auxiliaries, methods of asymmetric induction substrate, reagent and catalyst controlled reactions; determination of enantiomeric and diastereomeric excess; enantio-discrimination. Resolution -optical and kinetic.

10. Pericyclic reactions-electrocyclisation, cycloaddition, sigmatropic rearrangements and other related concerted reactions. Principles and applications of photochemical reactions in organic chemistry.

11. Synthesis and reactivity of common heterocyclic compounds containing one or two heteroatoms (O, N, S).

12. Chemistry of natural products: Carbohydrates, proteins and peptides, fatty acids, nucleic acids, terpenes, steroids and alkaloids. Biogenesis of terpenoids and alkaloids.

13. Structure determination of organic compounds by IR, UV-Vis, 'H & CNMR and Mass

nephelauxetic effect and Racah parameter, charge-transfer spectra. Magnetic properties.Reaction mechanism: Kinetic and thermodynamic stability, ility, substitution. Electron transfer processes. Photochemistry of $[Ru(bpy)3]^{2+}$ and related complexes.f-block elements: Electronic configuration, oxidation states, spectral and magnetic properties, Lanthanide contraction, separation of lanthanides.

11. Organometallic Compounds: Synthesis, structure and bonding of organometallic compounds: metal-alkyl, carbene, alkylidene and alkylidyne, carbonyl, alkene and arene complexes and metallocenes. Fluxionality in organometallic complexes. Fundamental organometallic reactions. Homogeneous catalysis hydrogenation, hydroformylation, acetic acid synthesis, metathesis, C-X bond forming reactions and olefin oxidation. Heterogeneous catalysis Fischer-Tropsch reaction, Ziegler-Natta polymerization.
12. Bioinorganic Chemistry: O2: Evolution (Photosysterm II), Carriers (Hb, Mb. Hr. Hc), Activation (Cytochrome P450, MMO) and Reduction (Cytc C oxidase); Electron transport (iron sulphur clusters, cytochromes, cofactors); hydrogenase and nitrogenase; Zinc containing enzymes.
13. Solid-state Chemistry and Inorganic Materials: Crystal systems and lattices, X-ray crystallography, Miller planes, crystal packing, crystal defects,

spectroscopic techniques.

Interdisciplinary topics

1. Chemistry in nanoscience and technology.
2. Catalysis and green chemistry.
3. Medicinal chemistry.
4. Supramolecular chemistry.
5. Environmental chemistry.

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Bragg's law, ionic crystals, structures of AX, AX_2, ABX_3 type compounds, spinels, band theory, metals and semiconductors.

14. Reaction Mechanism: Mechanisms of addition, elimination, substitution, condensation, concerted, rearrangement, fragmentation reactions. Generation and reactions of reactive intermediates. Common named reactions and their mechanism. Selectivity (chemo-, regio-, and stereo-selectivity) and stereo-electronic effects. Kinetic and thermodynamic control. Methods for probing reaction mechanisms - Hammond's postulate, reaction kinetics, Hammett equation, kinetic isotope effect, Curtin-Hammett principle.
15. Organic Synthesis: Main group and transition metal-based reagents-formation of carbon-carbon single and multiple bonds. Applications of named reactions. Chemo, regio and stereo-selective transformations. Acid/base catalysis, organocatalysis, transition metal catalysed transformations.Retrosynthesis, disconnection, synthons, linear, convergent, divergent, diverted and iterative synthesis, umpolung, and protecting groups.Asymmetric synthesis: methods of asymmetric induction-substrate, auxiliary, reagent and catalyst controlled reactions; determination of enantiomeric and diastereomeric excess. Resolution, kinetic, parallel and dynamic kinetic resolution, desymmetrisation. Specific

	examples of reactions-epoxidation, dihydroxylation, aldol, carbonyl addition, and hydrogenation. 16. Heterocyclic Chemistry: Synthesis and reactivity of common heterocycliccompounds containing one or more heteroatoms (O, N, S). Chemistry of heterocycles in biological systerns and pharmaceutical molecules. 17. Chemistry of Biological Molecules: Structure, synthesis and reactions ofamino acids, peptides, proteins, carbohydrates, fatty acids, nucleic acids and secondary metabolites (terpenes, alkaloids, polyketides, steroids, etc.)/natural products. 18. Data Analysis and Representation: Precision and accuracy; significantdigits, mean and standard deviation; absolute and relative errors; linear and non-linear regression, covariance and correlation coefficient. Linear, exponential, trigonometric and parabolic functions. Graphs.

NOTE: Part C shall contain 60 questions that shall be of analytical nature where a candidate is expected to apply the scientific knowledge to arrive at the solution to the given scientific problem. The questions in this part shall have multiple correct options. Credit in a question shall be given only on identification of ALL the correct options. No credit shall be allowed in a question if any incorrect option is marked as correct answer. No partial credit is allowed. A candidate shall be required to answer any 25 questions. Each question shall be of 4 marks. The total marks allocated to this section shall be 95 out of 200.