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(Accredited by NAAC with Grade A+)

GU/Acad –PG/BoS- CDT /2025-26/653 Date: 18.12.2025

CIRCULAR

The approved syllabus for the Change of Discipline Test (CDT) for **Master of Science in Chemistry** Programme is attached.

The Dean/Vice-Dean (Academic) of the School of Chemical Sciences and the Principals of all the affiliated Colleges are requested to take note of the above and bring the contents of this Circular to the notice of all concerned, including students aspiring to pursue the Master's Programmes.

ASHWIN VYAS LAWANDE
Digitally signed by ASHWIN VYAS LAWANDE
Date: 2025.12.18 15:48:20 +05'30'

(Ashwin V. Lawande)
Deputy Registrar – Academic

To,
1. The Dean, School of Chemical Sciences, Goa University.
2. The Vice-Dean (Academic), School of Chemical Sciences, Goa University.
3. Principals of all the affiliated Colleges.

Copy to:
1. Controller of Examinations, Goa University.
2. Assistant Registrar (Admissions), Goa University.
3. Assistant Registrar Examinations (UG/PG), Goa University.
4. Director, Directorate of Internal Quality Assurance, Goa University for uploading the Syllabus on the University website.

GOA UNIVERSITY

SYLLABUS FOR CHANGE OF DISCIPLINE TEST (CDT)
FOR MASTER OF SCIENCE IN CHEMISTRY PROGRAMME
(ORGANIC/INORGANIC/PHYSICAL/ANALYTICAL/PHARMACEUTICAL)

Effective from AY: 2026-27

Modules	Content
Module 1:	**INORGANIC CHEMISTRY**
	1. Atomic Structure: Review of: Bohr's theory and its limitations, dual behaviour of matter and radiation, de Broglie's relation, Heisenberg Uncertainty principle. Hydrogen atom spectra. Need of a new approach to Atomic structure. What is Quantum mechanics? Time independent Schrodinger equation and meaning of various terms in it. Significance of ψ and ψ2, Schrödinger equation for hydrogen atom. Radial and angular parts of the hydrogenic wave functions (atomic orbitals) and their variations for 1s, 2s, 2p, 3s, 3p and 3d orbitals (Only graphical representation). Radial and angular nodes and their significance. Radial distribution functions and the concept of the most probable distance with special reference to 1s and 2s atomic orbitals. Quantum numbers and their significance, Discovery of spin, spin quantum number (s) and magnetic spin quantum number (ms). Shapes of s, p and d atomic orbitals, nodal planes. Rules for filling electrons in various orbitals, Electronic configurations of the atoms. Stability of half-filled and completely filled orbitals, concept of exchange energy. Relative energies of atomic orbitals, Anomalous electronic configurations. **2. Transition Elements** General characteristic properties of 3d series with special reference to electronic configuration, variable valency, colour, magnetic and catalytic properties. Ability to form complexes and stability of various oxidation states (Latimer diagrams) for Mn, Fe and Cu. Lanthanides: Electronic configurations, oxidation states, colour, magnetic properties, lanthanide contraction, separation of lanthanides (ion exchange method only). Actinides: Electronic configuration and General characteristics.

	3. Chemical Bonding and Molecular Structure Ionic Bonding: General characteristics of ionic bonding. Energy considerations in ionic bonding, lattice energy and solvation energy and their importance in the context of stability and solubility of ionic compounds. Statement of Born-Landé equation for calculation of lattice energy, Born-Haber cycle and its applications, polarizing power and polarizability. Fajan's rules, ionic character in covalent compounds, bond moment, dipole moment and percentage ionic character. **4. Coordination Chemistry** IUPAC system of nomenclature. Bonding in complexes based on Valence Bond Theory (VBT), Inner and outer orbital complexes of Cr, Fe, Co, Ni and Cu (coordination numbers 4 and 6). Different types of structural and stereo-isomerism including optical isomerism in complexes with coordination numbers 4 and 6. Drawbacks of VBT. Werner's theory and its experimental verification Evidences for Covalent bonding in complexes; Stereochemistry of Co-ordination Compounds with different coordination Numbers. Ligand Field Theory: Brief Introduction; Comparison of the CFT and MOT. Molecular Orbital Theory as applied to Octahedral Complexes. Stability of complexes and factors affecting stability. Molecular orbitals diagrams of $[Ti(H_2O)_6]^{+3}$, $[Fe(CN)_6]^{-3}$, $[FeF_6]^{-3}$ and $[Co(NH_3)_6]^{+3}$ Complexes. Effect of π-bonding on splitting parameter. Organometallic chemistry: Definition, nomenclature and classification of organometallic compounds, EAN rule, 18 electron rule. Mononuclear metal carbonyls: Preparation, properties, structure and bonding of $Ni(CO)_4$, $Fe(CO)_5$ and $Cr(CO)_6$. Polynuclear metal carbonyl: Preparation and structures of $Mn_2(CO)_{10}$, $Co_2(CO)_8$, $Fe_2(CO)_9$ and $Fe_3(CO)_{12}$. Sandwich compounds like Ferrocene: preparation, properties, reactions, structure and Bonding (MOT). Preparation and properties of alkyl and aryls of Li, Al, Hg and Ti. Spectra and Magnetic properties: Effect of Crystal Field Splitting on properties of Octahdral Complexes: Magnetic, Spectral. Measurement of 10 Dq for $[Ti(H_2O)_6]^{+3}$ Complex. Determination of ground state term for d1 to d10 metal ions. Electronic Spectra of transition Metal Complexes. Introduction, Types of Electronic transitions. The d-d transitions (d1/d9 and d2/d8), Charge transfer transitions and Ligand-Ligand transitions. Selection Rules (laporte Orbitals and Spin). Applications: Ligand field strength, Colour of complexes, Cis– Trans isomerism and Geometry of complexes. Types of magnetic behaviour, Gouy's method of determining magnetic susceptibility, Spin only formula; application of magnetic moment data for 3d–Metal complexes **5. Crystal Field Theory** Crystal field splitting in octahedral complexes. Crystal field stabilization energy (CFSE), Crystal field effects for weak and strong fields.

	Spectrochemical series. Crystal Field Splitting in Tetrahedral complexes. Calculation of CFSE. Comparison of CFSE for Oh and Td complexes. Factors affecting the magnitude of 10Dq. Merits and Demerits of Crystal Field Theory. **6. Periodicity of Elements:** Properties of the elements with their trends in the periodic table: Atomic radii (van der Waals), Ionic radii and Covalent radii, Effective nuclear charge, shielding or screening effect, Slater rules, Ionization Energy, Successive ionization energies and factors affecting ionization energy., Electron Affinity, Electronegativity, Pauling's/ Mulliken's/ Allred and Rachow's. Calculation of Electronegativity (Paulings Method), Factors affecting Electronegativity. Chemistry of halogens: General methods of preparation, structure, bonding and chemical properties of: i Interhalogens ii) Polyhalide ions iii) Oxyacids of halogens in different oxidation states iv) Pseudohalogens. Noble Gases: Occurrence and uses, inertness of noble gases, Clathrates; preparation properties and structure (VSEPR) of XeF_2, XeF_4 and XeF_6. **7. Solid State Chemistry:** Defects in solids, Point defects; Schottky and Frenkel defects, Colour centre, Extended defects and Non-stoichiometry. Band Theory of solids: Band gaps, Metals, Insulators and Semi-conductors. **8. Oxidation and Reduction:** Oxidation number, single electrode potential, Standard electrode potential and Electrochemical series. Energy cycle for electrode potential. Application of Electrochemical series to check feasibility of reaction. Hydrogen overvoltage and Oxygen overvoltage. The use of reduction potentials, redox cycle, redox stability in water. The diagrammatic presentation of potential data: Frost, Latimer and Poubaix diagrams. Principles involved in the extraction of the elements. **9. Nanochemistry:** Introduction to nano particles, their properties, carbon nanotubes, SWCNT, MWCNT, different types of nanomaterials and their applications. **10. Bio-inorganic Chemistry:** Metalloporphyrins with special reference to haemoglobin and myoglobin. The role of Model systems, The alkali and alkaline earth metals, Metalloenzymes, Nitrogen fixation: Bacterial nitrogenase system (The biological nitrogen cycle). **11. Molecular Symmetry and Atomic Term Symbols:** Symmetry elements like Centre of symmetry, Rotation axis. Mirror Plane, Rotation Reflection Axis, Identity. Determination of point group and its application to H_2O, ethylene, Trans-dichloro ethylene, NH_3, BCl_3, $[PtCl_4]_{-2}$, $SiCl_4$, Benzene, SF_6.

Module 2:	ORGANIC CHEMISTRY
	1. Fundamentals of Organic Chemistry Curved arrow notation, drawing electron movement with arrows, half and double headed arrows, in organic reaction mechanisms. Physical Effects, Electronic Displacements: Inductive Effect, Electromeric Effect, Resonance and Hyperconjugation. Cleavage of Bonds: Homolysis and Heterolysis.Structure, shape and reactivity of organic molecules: Nucleophiles and electrophiles. Reactive Intermediates: Carbocations, Carbanions and free radicals. Strength of organic acids and bases: Comparative study with emphasis on factors affecting pK values. Aromaticity: Benzenoids and Hückel's rule. **2. Aliphatic Hydrocarbons** Functional group approach for the following reactions (preparations & reactions) to be studied in context to their structure. Alkanes: (Upto 5 Carbons). Preparation: Catalytic hydrogenation, Wurtz reaction, Kolbe's synthesis, from Grignard reagent. Reactions: Free radical Substitution: Halogenation. Alkenes: (Upto 5 Carbons) Preparation: Elimination reactions: Dehydration of alkenes and dehydrohalogenation of alkyl halides (Saytzeff's rule); cis alkenes (Partial catalytic hydrogenation) and trans alkenes (Birch reduction). Reactions: cis-addition (alk. $KMnO_4$) and trans-addition (bromine), Addition of HX (Markownikoff's and anti-Markownikoff's addition), Hydration, Ozonolysis, oxymecuration-demercuration, Hydroboration-oxidation. Alkynes: (Upto 5 Carbons) Preparation: Acetylene from CaC_2 and conversion into higher alkynes; by dehalogenation of tetra halides and dehydrohalogenation of vicinaldihalides.Reactions: formation of metal acetylides, addition of bromine and alkaline KMnO4, ozonolysis and oxidation with hot alk. $KMnO_4$. **3. Stereochemistry** Concept of isomerism. Types of isomerism. Stereoisomerism, conformational isomerism. Conformations with respect to ethane, butane and cyclohexane. Interconversion of Wedge Formula, Newmann, Sawhorse and Fischer representations. Concept of chirality (upto two carbon atoms). Configuration: Geometrical and Optical isomerism; Enantiomerism, Diastereomerism and Meso compounds). Threo and erythro; D and L; cis – trans nomenclature; CIP Rules: R/ S (for upto 2 chiral carbon atoms) and E / Z Nomenclature (for upto two C=C systems). **4. Aromatic hydrocarbons** Preparation (Case benzene): from phenol, by decarboxylation, from acetylene, from benzene sulphonic acid. Reactions: (Case benzene): Electrophilic substitution: nitration, halogenation and sulphonation.

	Friedel-Craft's reaction (alkylation and acylation) (upto 4 carbons on benzene). Side chain oxidation of alkyl benzenes (upto 4 carbons on benzene). Huckel's rule of Aromaticity (4n+2) Rule, 4n Rule for antiaromaticity, Electrophilic Aromatic substitution (w.r.t Benzene): Mechanism of Nitration, Sulphonation, Halogenation, Friedel – Crafts alkylation and acylation. Reactivity and orientation of activating, deactivating groups (ortho, para and meta effects). Nucleophilic aromatic substitution of Aryl halides (SNAr mechanism). **5. Alkyl and Aryl Halides** Alkyl Halides (Upto 5 Carbons) Types of Nucleophilic Substitution (SN1, SN2 and SNi) reactions. Preparation: from alkenes and alcohols. Reactions: hydrolysis, nitrite & nitro formation, nitrile & isonitrile formation, elimination vs substitution. Aryl Halides Preparation: (Chloro, bromo and iodo-benzene case): from phenol, Sandmeyer & Gattermann reactions. Reactions (Chlorobenzene): Aromatic nucleophilic substitution (replacement by –OH group) and effect of nitro substituent. Benzyne Mechanism: KNH_2/NH_3 (or $NaNH_2/NH_3$). Reactivity and Relative strength of C-Halogen bond in alkyl, allyl, benzyl, vinyl and aryl halides. **6. Spectroscopic methods in Organic Chemistry:** UV –Visible spectroscopy : Beer-Lambert's law, Types of electronic transitions, λmax, Chromophores and Auxochromes, Bathochromic and Hypsochromic shifts, Intensity of absorption. Visible Spectroscopy: Effect of conjugation on colour. Application of Woodward - Fieser rules for calculation of λmax for the following systems: α, β unsaturated aldehydes, ketones. Conjugated dienes: alicyclic, homoannular and heteroannular, extended conjugated systems (aldehydes, ketones and dienes). Distinction between cis and trans isomers. Infra Red Spectroscopy: Principle of I.R Spectroscopy (Hooke's law), types of molecular vibrations (Stretching and bending). Source, instrumentation and working of I.R spectrophotometer. Functional group region and Fingerprint region. Applications of I. R. Spectroscopy: Functional group analysis, detection of purity of sample, establishing the identity of an unknown molecule, Effect of H-bonding, conjugation, resonance and ring size on IR absorptions. To study the progress of a reaction. Problems based on I.R. spectroscopy (ketone, aldehyde, ester, acid & alcohol). Nuclear Magnetic Resonance Spectroscopy: 1H NMR spectroscopy: Number of signals (Homotopic, Enantiotopic, diastereotopic protons). Position of signals, Chemical shift: Reference standard, Solvent effect, Shielding and deshielding effect, anisotropic effects in alkenes, alkynes, aldehydes, aromatic compounds, factors affecting chemical shift. Intensity of signals: Peak area and proton counting. Spin-Spin coupling: Coupling

constant (J). Interpretation of NMR spectra of simple compounds. (acetone, acetaldehyde, toluene, ethyl bromide, anisole, acetic acid, t-butylbenzene, 2- butanone, propene). Simple problems based on NMR spectral data for identification of molecule.

Carbon-13 Nuclear Magnetic Resonance Spectroscopy and Mass Spectrometry: Principle of 13C spectroscopy. Number of signals: Proton coupled and decoupled spectra (off-resonance). Position of signals. Factors affecting position of signals (hybridisation). Problems based on 13C spectroscopy. Principle, theory, instrumentation of Mass spectrometry. Base Peak, Molecular ion, Metastable ion. Fragmentation pattern for alkanes. Fragmentation pattern of ketones: αcleavage and McLafferty rearrangement. Isotopic effect of alkyl halides.

7. Alcohols, Phenols, Ethers and Carbonyl Compounds

Alcohols: Preparation: Preparation of 1o, 2o and 3o alcohols: using Grignard reagent, Ester hydrolysis, Reduction of aldehydes, ketones, carboxylic acid and esters. Reactions: With sodium, HX (Lucas test), esterification, oxidation (with PCC, alk. $KMnO_4$, acidic dichromate, conc. HNO_3). Oppeneauer oxidation Diols: oxidation of diols using HIO_4. PinacolPinacolone rearrangement with mechanism.

Ethers (aliphatic and aromatic): Williamson's synthesis of ethers. Cleavage of ethers with HI.

Aldehydes and ketones (aliphatic and aromatic): (Formaldehye, acetaldehyde, acetone and benzaldehyde) Preparation: from acid chlorides and from nitriles. Reactions – Reaction with HCN, ROH, $NaHSO_3$, NH_2-G derivatives. Iodoform test. AldolCondensation, Cannizzaro's reaction, Wittig reaction, Benzoin condensation. Clemmensen reduction and Wolff Kishner reduction. Meerwein-Pondorff Verley reduction.

Phenols: (Phenol case) Preparation: Cumene hydroperoxide method, from diazonium salts. Reactions: Electrophilic substitution: Nitration, halogenation and sulphonation. ReimerTiemann Reaction, Gattermann-Koch Reaction, Houben–Hoesch Condensation, Schotten – Baumann Reaction.

8. Carboxylic acids and their derivatives

Carboxylic acids (aliphatic and aromatic),Preparation: Acidic and Alkaline hydrolysis of esters. Reactions: Hell - Volhard - Zelinsky Reaction, Carboxylic acid derivatives (aliphatic): (upto 5 carbons). Preparation: Acid chlorides, Anhydrides, Esters and Amides from acids and their interconversions. Reactions: Comparative study of nucleophilicity of acyl derivatives. Reformatsky reaction, Perkin condensation (mechanism).

9. Amines and Diazonium Salts

Amines (aliphatic and aromatic): (upto 5 carbons), Preparation: from alkyl halides, Gabriel's phthalimide synthesis, Hofmann bromamide reaction (Hofmann rearrangement), Reactions: Hofmann vs. Saytzeff elimination,

	Carbylamine test, Hinsberg test, with HNO_2, Schotten – Baumann reaction. Electrophilic substitution (case aniline): nitration, bromination, sulphonation. Diazonium salts: Preparation from aromatic amines, conversion to benzene, phenol, dyes. **10. Amino Acids and Peptides** Preparation of Amino Acids: Strecker synthesis, Gabriel's phthalimide synthesis. Terms: Zwitterion, Isoelectric point and Electrophoresis. Reactions of Amino acids: Ester of – COOH group, acetylation of –NH2 group, complexation with Cu^{2+} ions, ninhydrin test. Synthesis of simple peptides (upto dipeptides) by N-protection (t-butyloxycarbonyl and phthaloyl) & C-activating groups and Merrifield solid-phase synthesis. **11. Carbohydrates:** Classification and General Properties, Glucose and Fructose (open chain and cyclic structure), Determination of configuration of monosaccharides, absolute configuration of Glucose and Fructose, Mutarotation, Osazone formation, Killiani Fischer synthesis. **12. Alkaloids:** Ziesel's Method, Herzig-Meyer's method, Hoffman's exhaustive methylation method. Structure elucidation of Nicotine, Papaverine and Hygrine. Synthesis of Nicotine from Succinimide. Synthesis of Papaverine using Bischler-Napieralski reaction. Synthesis of Hygrine from Pyrrole. **13. Name Reactions and Rearrangements:** Reaction and mechanism of the following: Benzoin, Aldol, Knoevanagel, Wittig and Darzens Glycidic ester. Rearrangement with mechanism: Beckmann, Wolff Rearrangement and Hofmann. Only Reaction and applications of the following: Baeyer Villiger, Appel, Diekmann and Stobbe. Rearrangements: Schmidt, Claisen, Favorskii ,Curtius. Comparison of Clemmensen reduction and Wolff Kishner reduction. **14. Chemistry of Enolates:** Definition of enolate ion, acidity of carbonyl compounds, pka values, generation of enolate ion, role of bases in enolate ion formation, alkylation of carbonyl compounds with reference to cyclohexanone, acetone, ethylacetoacetate, malonic ester. Claisen condensation for preparation of ethylacetoacetate (reaction and mechanism). Keto-enol tautomerism of ethylacetoacetate. Malonic ester synthesis of carboxylic acids, ethylacetoacetate synthesis of ketones. Alkylation of 1,3-dithianes. Alkylation via enamine synthesis. Michael addition reaction. **15. Photochemistry:** Jablonski diagram, fluorescence, phosphorescence, intersystem crossing and vibrational relaxation. Norrish Type I and Type II cleavage reactions of ketones. Paterno Buchi and Barton reaction. **16. Chemistry of Heterocyclic Compounds:**

	Definition of heterocyclic compounds, Classification with examples for three, four, five and six membered heterocycles. Structure, resonance, stability and industrial source of furan, pyrrole, thiophene and pyridine. Preparation of furan, pyrrole and thiophene using Paal Knorr Synthesis. Reactivity of furan, pyrrole and thiophene: Electrophilic substitution at 2/5 position. Preparation of pyridineusing Hantzsch synthesis. Reactivity of pyridine: Electrophilic substitution at 3 position, Nucleophilic substitution at 2 and 4 position. Definition of bicyclic heterocycles with examples. Structure, resonance, stability and industrial source of indole, quinoline, isoquinoline. Preparation of indole using Fischer indole synthesis. Reactivity of Indole: Electrophilic substitution at 3 position. Skraup synthesis of quinoline and Bischler Napieralski synthesis of isoquinoline. Reactivity of quinoline and isoquinoline: Electrophilic substitution at 5/8 position, Nucleophilic substitution at 2 and 4 position. Oxidation and Reduction of quinoline and Isoquinoline. **17. Vitamins and Hormones:** Structure elucidation of Vitamin A , Vitamin C , Thyroxine and Adrenaline: Synthesis of Vitamin A from β-ionone, Vitamin C from xylose, Adrenaline from Catechol and thyroxine from tyrosine. **18. Terpenes:** Structure elucidation of Citral, α-Terpineol, α-Pinene and Camphor. Synthesis of Methylheptenone, Terebic acid and terpenylic acid. Synthesis of Citral from Methylheptenone. Synthesis of α–Terpineol from p-toluic acid. Synthesis of Norpinic acid, camphoric acid, camphoronic acid. Commercial synthesis of camphor. **19. Carbohydrates:** Open chain reactions of Glucose, Ruff degradation, determination of ring size of Glucose (pyranose and furanose using methylation method). Open chain reactions of sucrose, inversion of canesugar, Evidence of presence of glucose and fructose unit in sucrose. Determination of ring size of Sucrose. (using methylation method). **18. Stereochemistry:** Stereospecific and stereoselective reactions. Addition of bromine to 3-Hexene with mechanism. Addition of hydrogen halides to alkenes: Markownikoff's and antiMarkownikoff's addition rule. Substitution reactions: SN1, SN2, SNi reactions with mechanisms. Elimination reactions: E1, E2, E1cb reactions with mechanism.
Module 3:	**ANALYTICAL CHEMISTRY**
	1. Quantitative analysis: Principles of volumetric analysis: Theories of acid-base, redox, complexometric, iodometric and precipitation titrations: choice of indicators for these titrations. Principles of gravimetric analysis:

precipitation, coagulation, peptization, coprecipitation, post precipitation, digestion, filtration and washing of precipitate, drying and ignition.

2. Sampling Techniques:

Terms encountered in sampling: the population or the universe, Sample, Sampling unit, increment, the gross sample, the sub sample, Analysis sample, Bulk ratio, Size to weight ratio, Random sampling, Systematic sampling, Multistage sampling, Sequential sampling. Sampling of Gases, Liquids and Solids. Preservation, storage and preparation of sample solution.

3. Evaluation of analytical data:

Significant figures and rounding off, accuracy and precision Errors: determinate and indeterminate error, constant and proportionate errors, minimization of errors. Measures of central tendency and dispersion. Standard deviation, Gaussian distribution curve and its characteristics, Histogram and Frequency polygon. Confidence limit. Test of significance: Students t, F test, Rejection of the results: 2.5d & 4d rule and Q test. Linear least squares and Method of averages

4. Solvent Extraction:

Basic Principle, percentage extraction, role of complexing agents in solvent extraction, separation factor, types of extraction (continuous, batch) (Numerical problems are to be solved).

5. Chromatography Techniques:

Column chromatography: Principle, experimental details, theory of development, factors affecting column efficiency and applications. Paper and thin layer chromatography: Principles, techniques and applications of paper and thin layer chromatography. Ion exchange chromatography: Principles, classification of ion exchange materials, Nature of exchanging ions, Ion exchange capacity, applications in analytical chemistry.

Chromatography methods: Gas chromatography: Basic principles of GSC and GLC. Terms involved: Distribution equilibria, rate of travel, retention time, retention volume, relative retention, Height Equivalent to a Theoretical Plate (HETP), Van Deemter equation. Instrumentation: carrier gas, column, injections systems, explanations of factors affecting separation, thermal conductivity and flame ionization detectors. Qualitative and Quantitative analysis: internal standards, determination of peak area. HPLC: Instrumentation, description of pumps, detector choice (UV absorption and refractive index detectors), columns, injection system, packing materials, applications. Introduction to hyphenated techniques: Basic principles of GC-MS and LC-MS. (Numerical problems are to be solved)

6. Electroanalytical methods:

	Electrogravimetric analysis: Introduction, principles, instrumentation, Electrolysis at constant current, apparatus, determination of copper by constant current electrolysis. Coulometry: Introduction, constant Current measuring device, Hydrogen-Oxygen coulometer, Silver coulometer. General characteristics of coulometric method, applications of coulometry in neutralization, complexation, precipitation and redox titrations. Polarography: Introduction, Basic principles of instrumentation, Deposition potential, Dissolution potential, Polarisation of electrode, Polarographic wave, Ilkovic equation, Supporting electrolytes, Interference of oxygen, Applications of polarography – inorganic and organic. **7. Mass spectrometry:** Introduction, theory, making the gaseous molecule into an ion (electron impact, chemical ionization), making liquids and solids into ions (electrospray, electrical discharge), separation of ions on basis of mass to charge ratio. Instrumentation: schematic diagram of single and double focusing. Advantages of Quadrupole Mass Spectrometer, sample introduction, sample purity, spectrum resolution. Applications of mass spectrometry in structure elucidation. Peak matching. **8. X-ray diffraction methods:** Introduction to X-ray absorption and emission methods, Bragg's law, Diffraction of X-rays, production and detection of X-rays, sample preparation, identification of powder diffraction patterns of ZnO, NiO and $MgAl_2O_4$. **9. UV-Visible Spectroscopy:** Interaction of electromagnetic radiation with matter, Quantitative calculations- Beer's and Lambert's law, derivation of Beer-Lambert's law. Principles of instrumentation: Sources, monochromators, cells. Types of instruments: Photoelectric colorimeters and Spectrophotometers: Single & Double beam; comparison between colorimeter and spectrophotometer; applications: qualitative control of purity, quantative analysis; identification of structural groups in a molcule; study of co-ordination compound, cis-trans isomerism; chemical kinetics. Photometric titrations. **10. Atomic spectrometric methods:** Atomic absorption Spectroscopy: Introduction, principle, instrumentation, applications, limitations. Flame photometry and introduction, principle, instrumentation, applications, limitations. Differences between flame photometry and atomic absorption spectroscopy. Fluorimetry: principles of fluorescence, chemical structure and fluorescence. Relationship between concentration & fluorescence intensity, instrumentation & applications. **11. Thermal methods of analysis:**

	Basic principles of differential thermal analysis (DTA) and Differential Scanning Calorimetry (DSC), Differential Thermal Analysis - apparatus and methodology, factors affecting DTA results, quantitative DTA, interpretation of results. Applications to detect polymorphism and pseudopolymorphism in pharmaceuticals by DSC or DTA.
Module 4:	**PHYSICAL CHEMISTRY**
	1. Kinetic Theory of Gases Postulates of Kinetic Theory of Gases, deviation of real gases from ideal behaviour, compressibility factor, causes of deviation. van der Waals equation of state for real gases. Boyle temperature (derivation not required). Critical phenomena, critical constants and their calculation from van der Waals equation. Andrews isotherms for CO_2. Maxwell Boltzmann distribution laws of molecular velocities and molecular energies (graphic representation – derivation not required) and their importance. Temperature dependence of these distributions. Most probable, average and root mean square velocities (no derivation), collision number, collision frequency, collision diameter and mean free path of molecules. **2. Chemical Kinetics** The concept of reaction rates. Effect of temperature, pressure and catalyst on reaction rates. Order and molecularity of a reaction. Derivation of integrated rate equations for zero, first and second order reactions (both for equal and unequal concentrations of reactants). Half–life of a reaction. General methods for determination of order of a reaction. Concept of activation energy and its calculation from Arrhenius equation. Theories of Reaction Rates: Collision theory and Activated Complex theory of bimolecular reactions. **3. Chemical Energetics** Need of thermodynamics and the Laws of Thermodynamics. Important principles and definitions of thermochemistry. Concept of standard state and standard enthalpies of formations, integral and differential enthalpies of solution and dilution. Calculation of bond energy, bond dissociation energy and resonance energy from thermochemical data. Variation of enthalpy of a reaction with temperature – Kirchhoff's equation. Statement of Third Law of thermodynamics and calculation of absolute entropies of substances. **4. Chemical Equilibrium:** Free energy change in a chemical reaction. Thermodynamic derivation of the law of chemical equilibrium. Definition of ΔG and ΔGo, Le Chatelier's principle. Relationships between Kp, Kc and Kx for reactions involving ideal gases. **5. Phase Equilibrium**

	Phases, components and degrees of freedom of a system, criteria of phase equilibrium, Phase diagrams of one-component systems (water, sulphur and CO_2) and two component systems involving eutectics, congruent and incongruent melting points (Zn-Mg, NaCl-H_2O). **6. Solutions** Thermodynamics of ideal solutions: Ideal solutions and Raoult's law, deviations from Raoult's law – non-ideal solutions. Vapour pressure-composition and temperature composition curves of ideal and non-ideal solutions. Azeotropes. Partial miscibility of liquids: Critical solution temperature, distillation and fractional distillation. **7. Liquids** Surface tension and its determination using stalagmometer. Effect of temperature on surface tension. Viscosity of a liquid and determination of coefficient of viscosity using Ostwald viscometer and factors affecting viscosity. **8. Ionic Equilibria:** 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. Salt hydrolysis-calculation of hydrolysis constant, degree of hydrolysis and pH for different salts. Buffer solutions. Solubility and solubility product of sparingly soluble salts. **9. Conductance** Conductivity, equivalent and molar conductivity and their variation with dilution for weak and strong electrolytes. Kohlrausch's law of independent migration of ions. Ionic mobility and factors affecting ionic mobility. Transference number and its experimental determination using moving boundary methods. Applications of conductance measurements: solubility and solubility products of sparingly soluble salts, ionic product of water, conductometric titrations (only acid-base). **10. Electrochemistry** Reversible and irreversible cells. Concept of EMF of a cell. Measurement of EMF of a cell. Nernst equation and its importance. Types of electrodes. Standard electrode potential. Electrochemical series. Thermodynamics of a reversible cell, Concentration cells with transference and without transference. Liquid junction potential and salt bridge. pH determination using hydrogen electrode and quinhydrone electrode. Ion-selective electrodes: Fixed-site membrane, mobile-site membrane, site-free membrane, construction of ion selective electrodes, applications of ion selective electrodes. Decomposition potential, experimental determination of decomposition potential, application of decomposition potential, overvoltage and overpotential, theory of overvoltage, experimental

	determination of overvoltage, factors affecting overvoltage, hydrogen overvoltage, oxygen overvoltage, metal overvoltage. Fuel cells; H_2-O_2, Molten carbonate fuel cell, Proton exchange membrane fuel cell, Solid oxide fuel cell, Electrochemical sensors, principle, advantages and applications. Definition of pH, pOH, pKa, and pKb, Determination of pH using glass electrodes by potentiometric method, Buffer solution, types, buffer action, buffer capacity, mechanics of buffer action, Henderson equation for acidic and basic buffer, amphoteric electrolyte, existence of dipolar ions, isoelectric point, strong electrolytes, Debye Huckel theory of strong electrolytes. Variation of activity coefficient with concentration, ionic strength, Debye Huckel limiting law. Energy sources: Primary and Secondary batteries. Acid and Alkaline battery, Ni-Cd cell, solar cells, Construction, working, advantages and CdS solar cell. **11. Solids** Forms of solids, symmetry elements, unit cells, crystal systems, Bravais lattice. Laws of crystallography - Law of constancy of interfacial angles, Law of rational indices. Miller indices, X–Ray diffraction by crystals, Bragg's law. Particle size determination using powder method. Structures of NaCl, KCl and CsCl. **12. Quantum Chemistry** Postulates of quantum mechanics, quantum mechanical operators and commutation rules, Schrodinger equation and its application to free particle and "particle in a box" (rigorous treatment) quantization of energy levels, zero – point energy and Heisenberg Uncertainity principle, wave functions, probability distribution functions, nodal properties, extension to two and three dimensional boxes, separation of variables, degeneracy. Angular momentum, Rigid rotator model of rotation of diatomic molecule. Schrodinger equation in Catesian and spherical polar coordinates. Separation of variables, Spherical harmonics, Refinement of two approaches (configuration interaction for MO, ionic terms in terms of VB), qualitative description of LCAO-MO treatment of homonuclear and heteronuclear diatomic molecules. (HF, LiF). Qualitative treatment of hydrogen atom and hydrogen–like ions; setting up of Schrodinger equation in spherical polar co-ordinates, radial part, quantization of energy (only final energy expression). Average and most probable distances of electron from nucleus. Setting up of Schrodinger equation for many-electron atoms (He, Li) Need for approximation methods. Statement of variation theorem and application to simple systems (Particle in a box, harmonic oscillator, hydrogen atom) Chemical Bonding: Covalent bonding, valence bond and molecular orbital approaches, LCAO-MO treatment of H2+. Bonding and antibonding orbitals, qualitative

	extension to H_2, comparison of LCAO-MO and VB treatments of H_2 and their limitations. **13. Molecular Spectroscopy** Interaction of electromagnetic radiation with molecules and various types of spectra, Born Oppenheimer approximation. Rotational Spectroscopy: selection rules, intensities of spectral lines, determination of bond lengths of diatomic and linear triatomic molecules, isotopic substitution Vibrational spectroscopy: Classical equation of vibration, computation of force constant, amplitude of diatomic molecular vibrations, anharmonicity, Morse potential, dissociation energies, fundamental frequencies, overtones, hot bands, degree of freedom for polyatomic molecules, modes of vibration, concept of group frequencies. Vibration –rotation spectroscopy: Diatomic vibrating rotator, P, Q, R branches Raman spectroscopy: Qualitative treatment of Rotational Raman effect, Effect of nuclear spin, Vibrational Raman spectra, Raman effect, Stokes and Anti-stokes lines, their intensity difference, Quantum and Classical theories of Raman effect rule of mutual exclusion principle. Electronic Spectroscopy: Franck-Condon principle, electronic transitions, singlet and triplet states, fluorescence and phosphorescence, dissociation and pre dissociation, calculation of electronic transitions of polyenes using free electron model. Nuclear Magnetic Resonance (NMR) spectroscopy: Principles of NMR spectroscopy, Armor precession, Chemical shift and low resolution spectra, different scales, Spin–spin coupling and high resolution spectra, interpretation of PMR spectra of organic molecules. Electron Spin Resonance (ESR) spectroscopy: Principle, hyperfine structure, ESR of simple radicals.
Textbooks:	1. J. D. Lee, Concise Inorganic Chemistry, 5th Ed. Wiley India. 2. Cotton, F.A., Wilkinson, G. & Gaus, P.L. Basic Inorganic Chemistry, 3rd ed., Wiley. 3. Douglas, B.E., McDaniel, D.H. & Alexander, J.J. Concepts and Models in Inorganic Chemistry, John Wiley & Sons. 4. Huheey, J.E., Keiter, E.A., Keiter, R.L. & Medhi, O.K. Inorganic Chemistry: Principles of Structure and Reactivity, Pearson Education India, 2006. 5. Svehla, G. Vogel's Qualitative Inorganic Analysis, Pearson Education, 2012. 6. Mendham, J. Vogel's Quantitative Chemical Analysis, Pearson, 2009. 7. Kotz, J.C., Treichel, P.M. & Townsend, J.R. General Chemistry Cengage Learning India Pvt. Ltd., New Delhi (2009). 8. Mahan, B.H. University Chemistry 3rd Ed. Narosa (1998). 9. Petrucci, R.H. General Chemistry 5th Ed. Macmillan Publishing Co.: New York (1985).

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