HSNC University, Mumbai

The Faculty of Science and Technology

For the Course

Chemistry

Curriculum – First Year Postgraduate Program

Semester-I and Semester –II

First Year Semester I – Units – Topics- Teaching Hours

Semester I			
Units	**Papers**	**Lectures**	**Credits**
Paper- I Physical Chemistry(MS-FCH-101**)**			**3**
1	Thermodynamics-I	**12**	
II	Quantum Chemistry-I	**11**	
III	Chemical Dynamics-I and Nuclear Chemistry	**11**	
IV	Electrochemistry	**11**	
Paper- II Inorganic Chemistry(MS-FCH-102**)**			**3**
I	Chemical Bonding	**12**	
II	Molecular Symmetry and Group Theory	**11**	
III	Materials Chemistry and Nanomaterial	**11**	
IV	Characterisation of Coordination compounds	**11**	
Paper -III Organic Chemistry(MS-FCH-103**)**			**3**
I	Physical Organic Chemistry	**12**	
II	Nucleophilic substitution reactions and Aromaticity	**11**	
III	Stereochemistry	**11**	
IV	Oxidation and Reduction	**11**	
Paper -IV Analytical Chemistry MS-FCH-104**)**			**3**
I	Language of Analytical Chemistry and Quality in Analytical Chemistry	**12**	
II	Calculations based on Chemical Principles	**11**	
III	Optical Methods	**11**	
IV	Thermal Methods and Automation in chemical analysis	**11**	

	Practicals		
I	MS-FCH-1P1 Physical Chemistry	**30**	**1**
II	MS-FCH-1P2 Inorganic Chemistry	**30**	**1**
III	MS-FCH-1P3 Organic Chemistry	**30**	**1**
IV	MS-FCH-1P4 Analytical Chemistry	**30**	**1**

SEMESTER- I

Paper –I PHYSICAL CHEMISTRY (MS-FCH-101**)**

Sr No	Topics	No. of Lectures
UNIT-I	**Thermodynamics-I**	**12**
1	• State function and exact differentials. • Maxwell equations, Maxwell thermodynamic Relations; it's significance and applications to ideal gases, • Joule Thomson experiment, Joule Thomson coefficient, inversion temperature, Joule Thomson coefficient in terms of van der Waals constants. **[6L]**	
2	• Third law of Thermodynamics, • Entropy change for a phase transition, absolute entropies, determination of absolute entropies in terms of heat capacity, standard molar entropies and their dependence on molecular mass and molecular structure, residual entropy. **[6L]**	
UNIT- II	**Quantum Chemistry**	**11**
	• Classical Mechanics, failure of classical mechanics: Need for Quantum Mechanics. Particle waves and Schrödinger wave equation, wave functions, properties of wave functions. • Normalization of wave functions, orthogonality of wave functions. • Operators and their algebra, linear and Hermitian operators, operators for the dynamic variables of a system such as, position, linear momentum, angular momentum, total energy, eigen functions, eigen values and eigen value equation, • Schrödinger wave equation as the eigen value equation of the Hamiltonian operator, average value and the expectation value of a dynamic variable of the system, • Postulates of Quantum Mechanics, Schrodinger's Time independent wave equation from Schrodinger's time dependent wave equation. • Application of quantum mechanics to the following systems: a) Free particle, wave function and energy of a free particle. b) Particle in a one, two and three dimensional box, separation of variables, Expression for the wave function of the system, expression for the energy of the system, concept of quantization introduction of quantum number, degeneracy of the energy levels. c) Harmonic oscillator, approximate solution of the equation, Hermite polynomials, expression for wave function, expression for energy, use of the recursion formula.	

UNIT- III	**Chemical Dynamics-I and Nuclear Chemistry**	**11**
1	**Composite Reactions: [6L]** • Recapitulation: Rate laws, Differential rate equations Consecutive reactions, • Steady state Approximation, rate determining steps, Microscopic Reversibility and Detailed Balanced Chain reactions-chain initiation processes. • Some inorganic mechanisms: formation and decomposition of phosgene, decomposition of ozone, Reaction between Hydrogen and Bromine and some general examples • Organic Decompositions: Decomposition of ethane, decomposition of acetaldehyde Gas phase combustion: Reaction between hydrogen and oxygen, Semenov – Hinshelwood and Thompson mechanism, Explosion limits and factors affecting explosion limits.	
2	**Nuclear Chemistry: [5L]** • Types of Radioactive decay: α decay, β decay,γ decay and Spontaneous fission. • Kinetics of Radioactive decay • Half life : Statistical aspects of radioactive decay, Mean life and branching decay • Mixture of Radioactive Nuclides: Parent Daughter Equilibria, Growth of Daughter Product, Growth of Radioactive Product, radioactive Equilibrium, Types of Equilibria	
UNIT- IV	**Electrochemistry**	**11**
	• Recapitulation – basics of electrochemistry. • Debye-Hückel theory of activity coefficient, Debye-Hückel limiting law and it's extension to higher concentration (derivations are expected). • Electrolytic conductance and ionic interaction, relaxation effect,. • Debye-Hückel- Onsager equation (derivation expected). • Validity of this equation for aqueous and non- aqueous solution, deviations from Onsager equation, • Debye -Falkenhagen effect (dispersion of conductance at high frequencies), Wien effect. Batteries: Alkaline fuel cells, Phosphoric acid fuel cells, High temperature fuel cells [Solid –Oxide Fuel Cells (SOFC) and Molten Carbonate Fuel Cells]Bio-electrochemistry: Introduction, cells and membranes, membrane potentials, theory of membrane potentials, interfacial electron transfer in biological systems, adsorption of proteins onto metals from solution, electron transfer from modified metals to dissolved protein in solution, enzymes as electrodes, electrochemical enzyme-catalysed oxidation of styrene. Goldmann equation. (derivations are expected)	

SEMESTER-I Paper I (PRACTICALS)

Paper-I (MS-FCH-1P1**)**
Non – Instrumental
1) To determine the heat of solution (ΔH) of a sparingly soluble acid (benzoic /salicylic acid) from solubility measurement at three different temperature
2) To study the variation of calcium sulphate with ionic strength and hence determine the thermodynamic solubility product of $CaSO_4$ at room temperature
3) To investigate the reaction between acetone and iodine.
4) To study the variation in the solubility of $Ca(OH)_2$ in presence of NaOH and hence to determine the solubility product of $Ca(OH)_2$ at room temperature
5) Plotting of mathematical functions –linear, exponential and trigonometry and identify whether functions are acceptable or non-acceptable?
Instrumental
1) To determine the mean ionic activity coefficient of an electrolyte by e.m.f. measurement.
2) To study the effect of substituent on the dissociation constant of acetic acid conductometrically.
3) To determine pKa values of phosphoric acid by potentiometric titration with sodium hydroxide using glass electrode.
4) To verify Ostwald's dilution law and to determine the dissociation constant of a weak mono-basic acid conductometrically.
5) To determine the mean ionic activity coefficient of an electrolyte by e.m.f. measurement.

Paper- II- INORGANIC CHEMISTRY (MS-FCH-102**)**

Sr No	Topics	No. of Lectures
UNIT- I	**Chemical Bonding**	**12**
	• **Recapitulation of hybridization** Derivation of wave functions for *sp*, sp^2, *sp3* orbital hybridization types considering only sigma bonding. • Discussion of involvement of *d* orbitals in various types of hybridizations. Concept of resonance, resonance energy derivation expected. Formal charge with examples. • Critical analysis of VBT. • Molecular Orbital Theory for diatomic species of First transition Series. • Molecular Orbital Theory for Polyatomic species considering σ bonding for SF_6, CO_2, B_2H_6, I_3^-molecularspecies. • Weak forces of attraction: Hydrogen bonding – concept, types, properties, methods of detection and importance. Van der Waal's forces, ion-dipole, dipole-dipole, London forces.	
UNIT- II	**Molecular Symmetry and Group Theory**	**11**
	• Symmetry criterion of optical activity, symmetry restrictions on dipole moment. A systematic procedure for symmetry classification of molecules. • Concepts of Groups, Sub-groups, Classes of Symmetry operations, Group Multiplication Tables. Abelian and non-Abelian point groups. • Representation of Groups: Matrix representation of symmetry operations, reducible and irreducible representations. The Great Orthogonality Theorem and its application in construction of character tables for point groups C_2v, C_3v and D_{2h}, structure of character tables. • Applications of Group Theory a) Symmetry adapted linear combinations (SALC), symmetry aspects of MO theory, sigma bonding in AB_n (Ammonia, CH_4) molecule. b) Determination of symmetry species for translations and rotations. c) Mulliken's notations for irreducible representations. d) Reduction of reducible representations using reduction formula. e) Group-subgroup relationships. f) Descent and ascent in symmetry correlation diagrams showing relationship between different groups.	
UNIT- III	**Materials Chemistry and Nano material**	**11**
1	**Solid State Chemistry: [8L]** • Electronic structure of solids and band theory, Fermi level, K Space and Brillouin Zones. • Structures of Compounds of the type: AB [nickel arsenide (NiAs)], AB_2 [fluorite (CaF_2) and anti-fluorite structures, rutile (TiO_2) structure and layer structure [cadmium chloride and iodide ($CdCl_2$,CdI_2)]. • Methods of preparation for inorganic solids: Ceramic method, precursor method, sol-gel method (applications in Biosensors), microwave synthesis (discussion on principles, examples, merits and demerits are expected)	

2	**Nanomaterials: [3L]** • Preparative methods: Chemical methods, Solvothermal, Combustion synthesis, Microwave, Co-precipitation, • Characterisation of nanomaterials • Langmuir Blodgett(L-B) method, • Biological methods: Synthesis using microorganisms. • Applications of nanomaterials	
UNIT- IV	**Characterisation of Coordination compounds**	**11**
	• Formation, thermal studies, Conductivity measurements, electronic spectral and magnetic measurements, IR, NMR and ESR spectroscopic methods. • Spectral calculations using Orgel and Tanabe-Sugano diagram, calculation of electronic parameters such as Δ, B, C, Nephelauxeticratio. • Determination of formation constants of metal complexes (Overall and Stepwise): Comparative studies of Potentiometric and spectralmethods.	

Semester- I Paper II- Practicals

Paper- II (MS-FCH-1P2**)**
Inorganic Preparations (Synthesis and Characterization)
1) Bis- (tetraethylammonium) tetrachloroCuprate(II)
2) Bis- (tetraethylammonium) tetrachloroNickelate (II) $(Et_4N)_2[NiCl_4]$
3) Bis- (tetraethylammonium) tetrachloroCobaltate (II) $(Et_4N)_2[CoCl_4]$ (Any two from above preparations)
4) Tetramminemonocarbanato Cobalt(III)Nitrate
5) Bis (ethylenediammine) Copper(II)Sulphate
Instrumentation
1) Determination of equilibrium constant by Slope intercept method for Fe^{+3}/ SCN^- system
2) Determination of Electrolytic nature of inorganic compounds by Conductance measurement.

Paper- III ORGANIC CHEMISTRY (MS-FCH-103)

Sr No	Topics	No. of Lectures
UNIT- I	**Physical Organic Chemistry**	**12**
	• **Thermodynamic and kinetic requirements of a reaction:** rate and equilibrium constants, reaction coordinate diagram, transition state (activated complex), nature of activated complex, Hammond postulate, Reactivity *vs* selectivity, Curtin-Hammett Principle, Microscopic reversibility, Kinetic *vs* thermodynamic control of organic reactions. • **Determining mechanism of a reaction:** Product analysis, kinetic studies, use of isotopes (Kinetic isotope effect – primary and secondary kinetic isotope effect). Detection and trapping of intermediates, crossover experiments and stereo chemical evidence. • **Acids and Bases:** Factors affecting acidity and basicity: Electronegativity and inductive effect, resonance, bond strength, electrostatic effects, hybridization, aromaticity and solvation. Comparative study of acidity and basicity of organic compounds on the basis of pKa values, Leveling effect and non-aqueous solvents. Acid and base catalysis – general and specific catalysis withexamples.	
UNIT- II Nucleophilic substitution reactions and Aromaticity		**11**
	• **Nucleophilic substitution reactions: [7 L]** Aliphatic nucleophilic substitution: SN1, SN2, SNi reactions, mixed SN1 and SN2 and SET mechanisms. SN reactions involving NGP - participation by aryl rings, α- and pi-bonds. Factors affecting these reactions: substrate, nucleophilicity, solvent, steric effect, hard-soft interaction, leaving group. Ambident nucleophiles. SNcA, SN1' and SN2' reactions. SN at sp2 (vinylic) carb Aromatic nucleophilic substitution: SNAr, SN1, benzyne mechanisms. Ipso, cine, tele and vicarious substitution. Ester hydrolysis: Classification, nomenclature and study of all eight mechanisms of acid and base catalyzed hydrolysis with suitable examples. • **Aromaticity: [4 L]** Structural, thermochemical, and magnetic criteria for aromaticity, including NMR characteristics of aromatic systems. Delocalization and aromaticity. Application of HMO theory to monocyclic conjugated systems. Frost-Musulin diagrams. Huckel's (4n+2) and 4n rules. Aromatic and antiaromatic compounds up-to 18 carbon atoms. Homoaromatic compounds. Aromaticity of all benzenoid systems, heterocycles, metallocenes, azulenes, annulenes, aromatic ions and Fullerene (C60).	

UNIT- III	Stereochemistry	11
	• Concept of Chirality: Recognition of symmetry elements. • Molecules with tri- and tetra-coordinate centres: Compounds with carbon, silicon, nitrogen, phosphorous and sulphur chiral centres, relative configurational stabilities. • Molecules with two or more chiral centers: Constitutionally unsymmetrical molecules: erythro-threo and syn-anti systems of nomenclature. Inter conversion of Fischer, Sawhorse, Newman and Flying wedge projections. Constitutionally symmetrical molecules with odd and even number of chiral centres: enantiomeric and meso forms, concept of stereogenic, chirotopic, and pseudo asymmetric centres. R-S nomenclature for chiral centres in acyclic and cyclic compounds. • Axial and planar chirality: Principles of axial and planar chirality. Stereochemical features and configurational descriptors (R,S) for the following classes of compounds: alkenes, alkylidene cycloalkanes, spirans, biaryls (buttressing effect) (including BINOLs and BINAPs), ansa compounds, cyclophanes, trans-cyclooctenes. • Prochirality: Chiral and prochiral centres; prochiral axis and prochiral plane. Homotopic, heterotopic (enantiotopic and diastereotopic) ligands and faces. Identification using substitution and symmetry criteria. Nomenclature of stereoheterotopic ligands and faces. Symbols for stereoheterotopic ligands in molecules with i) one or more prochiral centres ii) a chiral as well as a prochiralcentre,iii) a prochiral axis iv) a prochiral plane v) pro-pseudo asymmetric centre. Symbols for enantiotopic and diastereotopic faces.	
UNIT- IV	**Oxidation and Reduction**	**11**
	• Oxidation: General mechanism, selectivity, and important applications of the following: • Dehydrogenation: Dehydrogenation of C-C bonds including aromatization of six member rings using metal (Pt, Pd, Ni) and organic reagents (chloranil, DDQ). • Oxidation of alcohols to aldehydes and ketones: Chromium reagents such as KCr2O7HSO4 (Jones reagent), CrO3-pyridine (Collin's reagent), PCC (Corey's reagent) and PDC (Cornforth reagent), hypervalent iodine reagents (IBX, Dess-Martin periodinane). DMSO based reagents (Swern oxidation), Corey-Kim oxidation - advantages over Swern and limitations; and Pfitzner-Moffatt oxidation-DCC and DMSO and Oppenauer oxidation. • Oxidation involving C-C bonds cleavage: Glycols using HIO4; cycloalkanones using CrO3; carbon-carbon double bond using ozone, KMnO4, CrO3, NaIO4 and OsO4; aromatic rings using RuO4 and NaIO4. • Oxidation involving replacement of hydrogen by oxygen: oxidation	

	of CH2 to CO by SeO2, oxidation of arylmethanes by CrO2Cl2 (Etard oxidation). • Oxidation of aldehydes and ketones: with H2O2 (Dakin reaction), with peroxy acid (Baeyer-Villiger oxidation) • Reduction: General mechanism, selectivity, and important applications of the following reducing reagents: • Reduction of CO to CH2 in aldehydes and ketones- Clemmensen reduction, Wolff- Kishner reduction and Huang-Minlon modification. • Metal hydride reduction: Boron reagents ($NaBH_4$, $NaCNBH_3$, diborane, 9-BBN, $Na(OAc)_3BH$, aluminium reagents ($LiAlH_4$, DIBAL-H, Red Al, L and K- selectrides). • NH_2NH_2 (diimide reduction) and other non-metal based agents including organic reducing agents (Hantzschdihydropyridine). • Dissolving metal reductions: using Zn, Li, Na, and Mg under neutral and acidic conditions, Li/Na-liquid NH_3 mediated reduction (Birch reduction) of aromatic compounds and acetylenes.	

Semester I Paper III -Practicals

Paper- III (MS-FCH-1P3**)**
One step preparations (1.0 g scale)
1. Bromobenzene top-nitrobromobenzene
2. Anthracene to anthraquinone
3. Benzoin tobenzil
4. Anthracene to Anthracene maleic anhydride adduct
5. 2-Naphthol to BINOL
6. p-Benzoquinone to1,2,4-triacetoxybenzene
7. Ethyl acetoacetate to3-methyl-1-phenylpyrazol-5-one
8. *o*-Phenylenediamine to2-methylbenzimidazole
9. *o*-Phenylenediamine to2,3-diphenylqunooxaline
10. Urea and benzil to 5,5-diphenylhydantoin

Paper- IV ANALYTICAL CHEMISTRY (MS-FCH-104)

Sr No	Topics	No. of Lectures
UNIT- I	**Language of Analytical Chemistry and Quality in Analytical Chemistry**	**12**
1	**Language of Analytical Chemistry: [7 L]** • Analytical perspective, Common analytical problems, terms involved in analytical chemistry (analysis, determination, measurement, techniques, methods, procedures and protocol) • An overview of analytical methods, types of instrumental methods, instruments for analysis, data domains (only introduction), detectors, selection of an analytical method, accuracy, precision, selectivity, sensitivity, detection limit and dynamic range. • Errors, determinate and indeterminate errors. Types of determinate errors, tackling of errors. • Quantitative methods of analysis: calibration curve, standard addition and internal standard method. (numerical problems expected)	
2	**Quality in Analytical Chemistry: [5 L]** • **Quality Management System (QMS):** Evolution and significance of Quality Management, types of quality standards for laboratories, total quality management (TQM), philosophy implementation of TQM (reference of Kaizen, Six Sigma approach & 5S), quality audits and quality reviews, responsibility of laboratory staff for quality and problems. ISO certification procedure for analytical laboratory. • **Safety in Laboratories**: Basic concepts of Safety in Laboratories, Personal Protection Equipment (PPE), OSHA, Toxic Hazard (TH) classifications, Hazardous Chemical Processes (including process calorimetry / thermal build up concepts). Transportation and Storage of hazardous and reactive material • **Good Laboratory Practices (GLP)** Principle, Objective, OECD guidelines, The US FDA 21CFR58, Klimisch score	
UNIT- II	**Calculations based on Chemical Principles**	**11**
	• **The following topics are to be covered in the form of numerical problems only.** a) Concentration of a solution based on volume and mass units: N, m, M, F and their inter conversion. b) Calculations of ppm, ppb and dilution of the solutions, concept of m mol. c) Stoichiometry of chemical reactions, concept of kg mol, limiting reactant, theoretical and practical yield. d) Buffer solution – definition and Preparation of buffer pH 4, 10 and 7 etc. e) Calculations of pH of buffers. f) Concept of formation constants, stability and instability constants, stepwise formation constants. g) Oxidation number and balancing of redox reaction (various conditions)	

UNIT- III	Optical Methods	11
1	• **Molecular Ultraviolet and Visible Spectroscopy: [4 L]** Derivation of Beer- Lambert's Law and its limitations, factors affecting molecular absorption, types of transitions [Emphasis on charge transfer absorption], pH, temperature, solvent and effect of substituents, deviations from Beer- Lambert's Law. Applications of Ultraviolet and Visible spectroscopy: 1) On charge transfer absorption 2) Simultaneous spectroscopy 3)Derivative Spectroscopy Dual spectrometry – Introduction, Principle, Instrumentation and Applications (numerical expected on Beers Law)	
2	• **Infrared Absorption Spectroscopy: [4 L]** Instrumentation: Sources, Sample handling, Transducers, Dispersive, non-dispersive instrument FTIR and its advantages Applications of IR [Mid IR, Near IR, Far IR]: Qualitative with emphasis on "Finger print" region, Quantitative analysis, Advantages and Limitations of IR Introduction and basic principles of diffuse reflectance spectroscopy.	
3	• **FT Technique: [3 L]** Introduction to F T techniques, instrumentation (source, sample containers, detectors) , Advantages and applications.	
UNIT- IV Thermal Methods and Automation in chemical analysis		**11**
1	• **Thermal Methods: [7 L]** **Introduction,** Recapitulation of types of thermal methods, comparison between TGA and DTA **Differential Scanning Calorimetry-** Principle, comparison of DTA and DSC, Instrumentation, Block diagram, Nature of DSC Curve, Factors affecting curves (sample size, sample shape, pressure). Heat of reaction, Specific heat, Safety screening, Polymers, liquid crystals, Percentage cystallinity, oxidative stability, Drug analysis, Magnetic transition. e.g. Analysis of Polyethylene for its crystallinity. • **Automation in chemical analysis: [4 L]** Need for automation, Objectives of automation, An overview of automated instruments and instrumentation, process control analysis, flow injection analysis, discrete automated systems, automatic analysis based on multilayered films, gas monitoring equipments, Automatic titrators.	

Semester – I –Paper IV - Practicals

Paper- IV (MS-FCH-1P4)	
1)	To carry out assay of the sodium chloride injection by Volhard's method Statistical method.
2)	To determine (a) the ion exchange capacity (b) exchange efficiency of the given cation exchange resin.
3)	To determine amount of Cr(III) and Fe(II) individually in a mixture of the two by titration with EDTA.
4)	Separation of Iron and Magnesium from the given solution by solvent extraction and To determine amount of total iron present.
5)	To determine the lead and tin content of a solder alloy by titration with EDTA.
6)	To determine amount of Cu(II) present in the given solution containing a mixture of Cu(II) and Fe(II).
7)	To determine number of nitro groups in the given compound using $TiCl_3$.

SEMESTER II

First Year Semester II – Units – Topics- Teaching Hours

Semester II			
Units	**Papers**	**Lectures**	**Credits**
Paper -I Physical Chemistry(MS-FCH-201**)**			**3**
I	Chemical Thermodynamics II	**12**	
II	Quantum Chemistry II	**11**	
III	Chemical Kinetics and Molecular Reaction Dynamics	**11**	
IV	Solid State Chemistry and Phase Equilibria	**11**	
Paper- II Inorganic Chemistry(MS-FCH-202**)**			**3**
I	Inorganic Reaction Mechanism	**12**	
II	Organometallic Chemistry of Transition metals	**11**	
III	Environmental Chemistry	**11**	
IV	Bioinorganic Chemistry	**11**	
Paper- III Organic Chemistry MS-FCH-203**)**			**3**
I	Alkylation of nucleophilic carbon intermediates and reactions of carbon nucleophiles with carbonyl groups	**12**	
II	Reactions and rearrangements	**11**	
III	Introduction of MOT for organic chemistry and applications of UV and IR spectroscopy	**11**	
IV	NMR Spectroscopy and Mass Spectrometry	**11**	
Paper -IV Analytical Chemistry(MS-FCH-204**)**			**3**
I	Chromatography	**12**	
II	Spectroscopy	**11**	
III	Surface Analytical Techniques, NMR and ESR	**11**	
IV	Electroanalytical Methods	**11**	

	Practicals		
I	MS-FCH-2P1 Physical Chemistry	**30**	**1**
II	MS-FCH-2P2 Inorganic Chemistry	**30**	**1**
III	MS-FCH-2P3 Organic Chemistry	**30**	**1**
IV	MS-FCH-2P4 Analytical Chemistry	**30**	**1**
	Total	**480**	**24**

SEMESTER II

Paper- I PHYSICAL CHEMISTRY (MS-FCH-201)

Sr No	Topics	No. of Lectures
UNIT- I	**Chemical Thermodynamics II**	**15**
	• Fugacity of real gases, Determination of fugacity of real gases using graphical method and from equation of state. Equilibrium constant for real gases in terms of fugacity. Gibbs energy of mixing, entropy and enthalpy of mixing. • **Real solutions:** Chemical potential in non ideal solutions excess functions of non ideal solutions calculation of partial molar volume and partial molar enthalpy, Gibbs Duhem Margules equation. • **Thermodynamics of surfaces**, Pressure difference across curved surface (Laplace equation), vapour pressure of droplets (Kelvin equation), Gibbs adsorption isotherm, BET isotherm (derivations expected). • Bioenergetics: standard free energy change in biochemical reactions, exergonic, endergonic. Hydrolysis of ATP, synthesis of ATP from ADP. •	
UNIT- II	**Quantum Chemistry - II**	**15**
	• Rigid rotor, spherical coordinates Schrödinger wave equation in spherical coordinates, separation of the variables, the phi equation, wave function, quantum number, the theta equation, wave function, quantization of rotational energy, spherical harmonics. • Hydrogen atom, the two particle problem, separation of the energy as translational and potential, separation of variables, the R the □ * and the □ equations, solution of the equation, introduction of the four quantum numbers and their interdependence on the basis of the solutions of the three equations, total wave function, expression for the energy, probability density function, distances and energies in atomic units, radial and angular plots., points of maximum probability, expressions for the total wave function for 1s,2s, 2p and 3d orbitals of hydrogen. • Application of the Schrödinger equation to two electron system, limitations of the equation, need for the approximate solutions, methods of obtaining the approximate solution of the Schrödinger wave equation. • Hückel Molecular Orbitals theory for ethylene , 1,3-butadiene and benzene.(Derivation expected)	

UNIT- III Chemical Kinetics and Molecular Reaction Dynamics		11
	• **Elementary Reactions in Solution:-** Solvent Effects on reaction rates, Reactions between ions- influence of solvent Dielectric constant, influence of ionic strength, Linear free energy relationships Enzyme action • **Kinetics of reactions catalyzed by enzymes** -Michaelis-Menten analysis, Lineweaver-Burk and Eadie Analyses**.** • **Inhibition of Enzyme action**: Competitive, Non-competitive and Uncompetitive Inhibition. Effect of pH, Enzyme activation by metal ions, Regulatory enzymes. • **Kinetics of reactions in the Solid State:-** Factors affecting reactions in solids • **Rate laws for reactions in solid**: The parabolic rate law, The first order rate Law, the contracting sphere rate law, Contracting area rate law, some examples of kinetic studies.	
UNIT- IV Solid State Chemistry and Phase Equilibria		**11**
	• **Solid State Chemistry [5L]** **Recapitulation:** Structures and Defects in solids. **Types of Defects and Stoichiometry** a) Zero dimensional (point)Defects b) One dimensional (line)Defects c) Two dimensional (Planar)Defects d) Thermodynamics of formation of defects (Mathematical derivation to find concentration of defects and numerical problems based on it) • **Phaseequilibria [6L]** **Recapitulation:** Introduction and definition of terms involved in phase rule. Thermodynamic derivation of Gibbs Phase rule. **Two component system:** Solid –Gas System : Hydrate formation, Amino compound formation Solid – Liquid System: Formation of a compound with congruent melting point, Formation of a compound with incongruent melting point. (with suitable examples) **Three component system** Type-I : Formation of one pair of partially miscible liquids Type-II: Formation of two pairs of partially miscible liquids Type-III: Formation of three pairs of partially miscible liquids	

Paper I (MS-FCH-2P1**)Practicals**
Non – Instrumental
1) Polar plots of atomic orbitals such as 1*s*, $2P_z$,$3d_z$ orbitals by using angular part of hydrogen atom wave functions.
2) To study the influence of ionic strength on the base catalysed hydrolysis of ethyl acetate.
3) To study phase diagram of three component system water – chloroform /toluene – acetic acid.
4) To determine the rate constant of decomposition reaction of diacetone alcohol by dilatometric method.
Instrumental
1) To determine the formula of silver ammonia complex by potentiometric method.
2) To determine CMC of sodium Lauryl Sulphate from measurement of conductivities at different concentrations.
3) To determine Hammette constant of *m*- and *p*- amino benzoic acid/nitro benzoic acid by pH measurement.
4) To determine the Michaelis – Menten's constant value (Km) of the enzyme Beta Amylase spectrophotometrically.

Paper- II INORGANIC CHEMISTRY (MS-FCH-202**)**

Sr No	Topics	No. of Lectures
UNIT- I	**Inorganic Reaction Mechanism**	**12**
	• Rate of reactions, factors affecting the rate of reactions, techniques for determination of rate of reaction (Direct chemical analysis, spectrophotometric method, electrochemical and flow methods). • Ligand substitution reactions of: a) Octahedral complexes without breaking of metal-ligand bond (Use of isotopic labelling method) b) Square planar complexes, trans-effect, its theories and applications. Mechanism and factors affecting these substitution reactions. • Redox reactions: inner and outer sphere mechanisms, complimentary and non- complimentary reactions. Stereochemistry of substitution reactions of octahedral complexes. (Isomerization and racemization reactions and applications.)	
UNIT- II	**Organometallic Chemistry of Transition metals**	**11**
	• Eighteen and sixteen electron rule and electron counting with examples. Preparation and properties of the following compounds (a) Alkyl and aryl derivatives of Pd and Pt complexes (b) Carbenes and carbynes of Cr, Mo and W (c) Alkene derivatives of Pd and Pt (d) Alkyne derivatives of Pd and Pt (e) Allyl derivatives of nickel (f) Sandwich compounds of Fe, Cr and Half Sandwich compounds of Cr, Mo. • Structure and bonding on the basis of VBT and MOT in the following organometallic compounds: Zeise's salt, bis(triphenylphosphine) diphenylacetylene platinum(0) [Pt(PPh3)2(HC≡CPh)2], diallyl nickel(II), ferrocene and bis (arene) chromium(0), tricarbonyl (η2-butadiene) iron(0). • Applications of Organometallic compounds	
UNIT- III	**Environmental Chemistry**	**11**
	• Conception of Heavy Metals: Critical discussion on heavy metals • Toxicity of metallic species: Mercury, lead, cadmium, arsenic, copper and chromium, with respect to their sources, distribution, speciation, biochemical effects and toxicology, control and treatment. • Estimation of Arsenic in contaminated water • Case Studies: (a) Itai-itai disease for Cadmium toxicity, (b) Arsenic Poisoning in the Indo-Bangladesh region. (c) Minamata Disease for mercury poisoning • Interaction of radiation in context with the environment: Sources and	

	biological implication of radioactive materials. Effect of low level radiation on cells- Its applications in diagnosis and treatment, Effect of radiation on cell proliferation and cancer. • Air Pollution	
UNIT- IV	**Bioinorganic Chemistry**	**11**
	• Biological oxygen carriers; hemoglobin, hemerythrene and hemocyanine-structure of metal active center and differences in mechanism of oxygen binding, Differences between hemoglobin and myoglobin: Cooperativity of oxygen binding in hemoglobin and Hill equation, pH dependence of oxygen affinity in hemoglobin and myoglobin and it's implications. • Activation of oxygen in biological system with examples of mono-oxygenases, and oxidases- structure of the metal center and mechanism of oxygen activation by these enzymes. • Copper containing enzymes- superoxide dismutase, tyrosinase and laccase: catalytic reactions and the structures of the metal binding site Nitrogen fixation-nitrogenase, hydrogenases Metal ion transport and storage:Ionophores, transferrin, ferritin and metallothionins Medicinal applications of cis-platin and related compounds	

Paper II (MS-FCH-2P2) Practicals
Ores and Alloys
1) Analysis of Devarda's alloy
2) Analysis of Cu – Ni alloy
3) Analysis of Tin Solder alloy
4) Analysis of Limestone.
Instrumentation
1) Estimation of Copper using Iodometric method Potentiometrically.
2) Estimation of Fe+3 solution using Ce(IV) ions Potentiometrically

Paper- III ORGANIC CHEMISTRY (MS-FCH-203)

Sr No	Topics	No. of Lectures
UNIT- I Alkylation of Nucleophilic Carbon Intermediates and reaction of Carbon Nucleophiles with Carbonyl groups		**12**
1	**Alkylation of Nucleophilic Carbon Intermediates: [6L]** Generation of carbanion, kinetic and thermodynamic enolate formation, Regioselectivity in enolate formation, alkylation of enolates. Generation and alkylation of dianion, medium effects in the alkylation of enolates, oxygen versus carbon as the site ofalkylation. Alkylation of aldehydes, ketones, esters, amides andnitriles. Nitrogen analogs of enols and enolates- Enamines and Imines anions, alkylation of enamines andimines. Alkylation of carbon nucleophiles by conjugate addition (Michaelreaction). **Reaction of carbon nucleophiles with carbonyl groups: [6L]** Mechanism of Acid and base catalyzed Aldol condensation, Mixed Aldol condensation with aromatic aldehydes, regiochemistry in mixed reactions of aliphatic aldehydes and ketones, intramolecularAldol reaction and Robinson annulation. Addition reactions with amines and iminium ions; Mannichreaction. Amine catalyzed condensation reaction: Knoevenagelreaction. Acylation of carbanions.	
UNIT- II Reactions and Rearrangements		**11**
	Reactions and Rearrangements: Mechanisms, stereochemistry (if applicable) and applications of the following: Reactions:Baylis-Hilman reaction, McMurry Coupling, Corey-Fuchs reaction, Nef reaction, Passerinireaction. **Concerted rearrangements:** Hofmann, Curtius, Lossen, Schmidt, Wolff, Boulton- Katritzky. **Cationic rearrangements:** Tiffeneau-Demjanov, Pummerer, Dienone-phenol, Rupe, Wagner-Meerwein. **Anionic rearrangements:** Brook, Neber, Von Richter, Wittig, Gabriel–Colman, Payne.	
UNIT- III Introduction to Molecular Orbital Theory for Organic Chemistry and Applications of UV and IR Spectroscopy		**11**
1	**Introduction to Molecular Orbital Theory for Organic Chemistry: [5L]** **Molecular orbitals:** Formation of σ- and π-MOs by using LCAO method. Formation of π MOs of ethylene, butadiene, 1, 3, 5-hexatriene, allylcation, anion and radical. Concept of nodal planes and energies of π-MOs **Introduction to FMOs:** HOMO and LUMO and significance of HOMO-LUMO gap in absorption spectra as well as chemical reactions. MOs of formaldehyde: The effect of electro negativity perturbation and orbital polarization in formaldehyde. HOMO and LUMO (π and π* orbitals) of formaldehyde. A brief description of MOs of nucleophiles and electrophiles.	

	Concept of 'donor-acceptor' interactions in nucleophilic addition reactions on formaldehyde. Connection of this HOMO-LUMO interaction with 'curved arrows' used in reaction mechanisms. The concept of hardness and softness and its application to electrophiles and nucleophiles. Examples of hard and soft nucleophiles/ electrophiles. Identification of hard and soft reactive sites on the basis ofMOs. Application of FMO concepts in (a) $S_N2$reaction, (b) Lewis acid base adducts (BF_3- NH_3complex), (c) ethylene dimerization to butadiene, (d) Diels-Aldercycloaddition, (e) regioselective reaction of allylcation with allyl anion (f) addition of hydride to formaldehyde. • **Applications of UV and IR spectroscopy: [6L]** **Ultraviolet spectroscopy:** Recapitulation, UV spectra of dienes, conjugated polyenes (cyclic and acyclic), carbonyl and unsaturated carbonyl compounds, substituted aromatic compounds. Factors affecting the position and intensity of UV bands – effect of conjugation, steric factor, pH, and solvent polarity. Calculation of absorption maxima for above classes of compounds by Woodward-Fieser rules (using Woodward-Fieser tables for values for substituents). **Infrared spectroscopy:** Fundamental, overtone and combination bands, vibrational coupling, factors affecting vibrational frequency (atomic weight, conjugation, ring size, solvent and hydrogen bonding). Characteristic vibrational frequencies for alkanes, alkenes, alkynes, aromatics, alcohols, ethers, phenols, amines, nitriles and nitro compounds. Detailed study of vibrational frequencies of carbonyl compounds, aldehydes, ketones, esters, amides, acids, acid halides, anhydrides, lactones, lactams and conjugated carbonyl compounds.	
UNIT- IV	**NMR Spectroscopy and Mass Spectrometry**	**11**
1	**NMR spectroscopy and Mass spectrometry (11 L)** **Proton magnetic resonance spectroscopy:** Principle, Chemical shift, Factors affecting chemical shift (Electronegativity, H-bonding, Anisotropy effects). Chemical and magnetic equivalence, Chemical shift values and correlation for protons bonded to carbon and other nuclei as in alcohols, phenols, enols, carboxylic acids, amines, amides. Spin-spin coupling, Coupling constant (J), Factors affecting J, geminal, vicinal and long range coupling (allylic and aromatic). First order spectra, Karplusequation. **^{13}C NMR spectroscopy:** Theory and comparison with proton NMR, proton coupled and decoupled spectra, off-resonance decoupling. Factors influencing carbon shifts, correlation of chemical shifts of aliphatic, olefin, alkyne, aromatic and carbonyl carbons. **Mass spectrometry:** Molecular ion peak, base peak, isotopic abundance, metastable ions. Nitrogen rule, Determination of molecular formula of organic compounds based on isotopic	

	abundance and HRMS. Fragmentation pattern in various classes of organic compounds (including compounds containing hetero atoms), McLafferty rearrangement, Retro-Diels-Alder reaction, orthoeffect. Structure determination involving individual or combined use of the above spectral techniques.	

Paper III (MS-FCH-2P3**) Practicals**
Separation of Binary mixture using micro-scale technique
1. Separation of binary mixture using physical and chemical methods.
2. Characterization of one of the components with the help of chemical analysis and confirmation of the structure with the help of derivative preparation and its physical constant.
3. Purification and determination of mass and physical constant of the second component. The following types are expected:
(i) Water soluble/water insoluble solid and water insoluble solid,
(ii) Non-volatile liquid-Non-volatile liquid (chemical separation)
(iii) Water-insoluble solid-Non-volatile liquid.
Minimum three mixtures from each type and a total of ten mixtures are expected.

Paper- IV ANALYTICAL CHEMISTRY (MS-FCH-204**)**

Sr No	Topics	No. of Lectures
UNIT- I	**Chromatography**	**12**
	Recapitulation of basic concepts in chromatography: Classification of chromatographic methods, requirements of an ideal detector, types of detectors in LC and GC, comparative account of detectors with reference to their applications (LC and GC respectively), qualitative and quantitative analysis. **[2 L]** Concept of plate and rate theories in chromatography: efficiency, resolution, selectivity and separation capability. Van Deemter equation and broadening of chromatographic peaks. Optimization of chromatographic conditions. **[4 L]** Gas Chromatography: Instrumentation of GC with special reference to sample injection systems – split/splitless, column types, solid/ liquid stationary phases, column switching techniques, temperature programming, Thermionic and mass spectrometric detector, Applications. **[2 L]** High Performance Liquid Chromatography (HPLC): Normal phase and reversed phase with special reference to types of commercially available columns (Use of C8 and C18 columns). Diode array type and fluorescence detector,Applications of HPLC .Chiral and ionchromatography. **[3L]** Introduction to HPTLC as hyphenated technique **[1L]**	
UNIT- II	**Spectroscopy**	**11**
1	**X-ray spectroscopy**: principle, instrumentation and applications of X-ray fluorescence, absorption and diffraction spectroscopy. **[3 L]**	
2	**Mass spectrometry**: recapitulation, instrumentation, ion sources for molecular studies, electron impact, field ionization, field absorption, chemical ionization and fast atom bombardment sources. Mass analyzers: Quadrupole, time of flight and ion trap. Applications**.** **[4 L]**	
3	**Neutron Activation Analysis (NAA) -** principle, instrumentation, Advantages / limitations, and applications **[4 L]**	
UNIT- III	**Surface Analytical Techniques, NMR and ESR**	**11**
1	**Surface Analytical Techniques – [4 L]** Introduction, Principle and Applications of: Scanning Electron Microscopy (SEM) Scanning Tunneling Microscopy (STM) Transmission Electron Microscopy (TEM) Electron Spectroscopy (ESCA and Auger)	
2	**NMR and ESR – [7L]** Introduction, basic principle, applications.	

	Interpretation of NMR of C_2H_5OH, H_3C-O-CH_3	
UNIT- IV	**Electroanalytical Methods**	**11**
1	**Electroanalytical Methods (Numericals are Expected)** • **Ion selective potentiometry and Polarography: [8 L]** Ion selective electrodes and their applications (solid state, precipitate, liquid – liquid, enzyme and gas sensing electrodes), **Polarography:** Ilkovic equation, derivation starting with Cottrell equation, effect of complex formation on the polarographic waves, Introduction Differential pulse and cyclic voltammeter • **Electrogravimetry**: Introduction, principle, instrumentation, factors affecting the nature of the deposit, applications**. [2 L]** • **Coulometry:** Introduction, principle, instrumentation, coulometry at controlled potential and controlled current **[1 L]**	

Paper IV (MS-FCH-2P4**) Practicals**
1) To determine percentage purity of sodium carbonate in washing soda pH metrically.
2) To determine amount of Ti(III) and Fe(II) in a mixture by titration with Ce(IV) potentiometrically.
3) To determine the percentage purity of a sample (glycine/sodium benzoate/primary amine) by titration with perchloric acid in a non aqueous medium using glass calomel system potentiometrically.
4) To determine the amount of nitrite present in the given water sample colorimetrically.
5) To determine the amount of Fe(II) and Fe(III) in a mixture using 1,10-phenanthroline spectrophotometrically.
6) Simultaneous determination of Cr(VI) and Mn(VII) in a mixture spectrophotometrically.
7) To determine the percentage composition of HCl and H2SO4 on weight basis in a mixture of two by conductometric titration with NaOH and BaCl2.
8) To determine amount of potassium in the given sample of fertilizers using flame photometer by standard addition method.

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