MCH-601: ORGANOTRANSITION METAL CHEMISTRY

Unit-I
Alkyls and Aryls of Transition Metals
Type, routes of synthesis, stability and decomposition pathways organocupper in organic synthesis.

Compounds of Transition Metal-Carbon multiple bonds
Alkylidenes, alkylidyienes, low valent carbenes and carbines-synthesis, nature of bond, structural characteristics, nuleophilic and electrophilic reactions on the ligands, role in organic synthesis.

Unit –II
Transition Metal π-Complexes
Transition metal π -Complexes with unsaturated organic molecules, alkenes, alkynes, allyl, diene, dienyl, arene and trienyl complexes, preparation, properties, nature of bonding and structural features. Important reactions relating to nucleophilic and electrophilic attack on ligands and to organic synthesis.

Unit –III
Transition metal compounds with bonds to hydrogen, boron, silicon
Transition metal compounds with bonds to hydrogen, boron, silicon

Unit –IV
Homogeneous Catalysis
Stoichiometric reaction for catalysis, homogeneous catalytic hydrogenation. Zeigler-Natta Polymerization of olefins, catalytic reactions involving carbon monoxide such as hydrocarbonylation of olefins (oxo-reaction), oxopalladation reaction, acetic acid synthesis.

Unit-V
Fluxional Organometallic Compounds
Flexionality and dynamic equilibrium in compounds such as acyclic alkenes, σ-bonded cyclic alkenes, π- bonded cyclic alkenes, metal carbonyls.

BOOKS SUGGESTED:
Basics

Unit-II
Polymer Characterization


Unit-III
Analysis and testing of polymers

Unit-IV
Inorganic Polymers
A general survey and scope of Inorganic Polymers special characteristics, classification, homo and hetero atomic polymers.

Structure, Properties and Applications of

a. Polymers based on boron-borazines, boranes and carboranes.

b. Polymers based on Silicon, silicone's polymetalloxanes and polymetallosiloxanes, silazanes.

Unit V
Structure, Properties and Application of

a. Polymers based on Phosphorous-Phosphazenes, Polyphosphates
b. Polymers based on Sulphure-Tetrasulphur tetranitride and related compounds.
c. Co-ordination and metal chelate polymers.

Books Suggested
5. Inorganic Rings and Cages : D.A. Armitage.
SEMESTER IV

Paper-XVI

MCH-504: APPLICATION OF SPECTROSCOPY
(Chemistry)

Unit-I

Ultraviolet and Visible spectroscopy
Various electronic transitions (185-800 nm) Beer-Lambert law, effect of solvent on
electronic transitions, ultraviolet bands for carbonyl compounds, unsaturated carbonyl
compounds, dienes, conjugated polyenes, Fieser Woodward rules for conjugated dienes
and carbonyl compounds, ultraviolet spectra of aromatic compounds. Steric effect in
biphenyls.

Unit II

Infrared Spectroscopy
Characteristic vibrational frequencies of alkanes, alkenes, alkynes, aromatic compounds,
alcohols, ether's, phenols and amines. Detailed study of vibrational frequencies of
carbonyl compounds (ketone's, aldehyde's, esters, amides, acids, anhydride's, lactones,
lactams and conjugated carbonyl compounds). Effect of hydrogen bonding and solvent
effect on vibrational frequencies, overtones, combination bands and fermi resonance.

Optical Rotatory Dispersion (ORD) and Circular Dichromium (CD)
Definition, deduction of absolute configuration, octant rule for ketones.

Unit-III

Nuclear Magnetic Resonance Spectroscopy
General introduction and definition, chemical shift, spin-spin interaction, shielding
mechanism, mechanism of measurement, chemical shift values and correlation for
protons bonded to carbon (aliphatic, olefinic, aldehydic and aromatic) and other nuclei
(alcohols, phenols, enols, carboxylic acids, amines, amides & mercapto), chemical
exchange, effect of deuteration, complex spin-spin interaction between two, three, four
and five nuclei (first order spectra), Stereochemistry, hindered rotation, Karplus curve-
variation of coupling constant with disordered angle. Simplification of complex
spectra of nuclear magnetic double resonance, NMR shift reagents, solvent effects. Fourier
transform technique, nuclear overhauser effect (NOE).

Unit-IV

Carbon-13 NMR Spectroscopy
General considerations, chemical shift (aliphatic olefinic, alkyne, aromatic,
heteroaromatic and carboxyl carbon), coupling constants. Two dimension NMR
spectroscopy-COSY, NOESY, DEPT, IONEPT, APT and INADEQUATE techniques.
Unit V
Mass Spectrometry
Introduction ion production EI, CI FD, ESI and FAB, factors affecting fragmentation, ion analysis, ion abundance Mass spectral fragmentation of organic compounds, common functional groups, molecular ion peak, metastable peak. Me Lafferty rearrangement. Nitrogen rule. High resolution mass spectrometry. Example of mass spectral fragmentation of organic compounds with respect to their structure determination.

Book Suggested


Paper XVII
MCH-505: SOLID STATE CHEMISTRY

Unit I

Solid State Reactions
General principles, experimental procedure, co-precipitation as a precursory to solid state reactions, kinetics of solid state reactions.

Unit II
Crystal Defects and Non-Stoichiometry
Perfect and imperfect crystals, intrinsic and extrinsic defects-point defects, line and plane defects, vacancies-Schottky detects and Frenkel defects. Thermodynamics of Schottky and Frenkel defect formation, colour centres, non-stoichiometry and defects.
Unit III

Electronic Properties and Band Theory
Metal, s insulators and semiconductors, electronic structure of solids band theory band structure of metals, insulators and semiconductors, Intrinsic and extrinsic semiconductors, doping semiconductors, p-n junctions, superconductors. Optical properties-Application of optical and electron microscopy, Magnetic Properties-Classification of materials: Effect of temperature calculation of magnetic moment, mechanism of ferro and anti ferromagnetic ordering super exchange.

Unit IV

Organic Solids
Electrically conducting solids, organic charge transfer complex, organic metals, new superconductors.

Unit IV

Liquid Crystals:
Types of liquid crystals: Nematic, Smectic, Ferroelectric, Antiferroelectric, Various theories of LC, Liquid crystal display, New materials.

Books Suggested.


Paper XVIII

MCH-506 : ENVIRONMENTAL CHEMISTRY

Unit-I

Atmosphere

Atmospheric Chemistry
Sources of trace atmospheric constituents: nitrogen oxides, sulphure dioxide and other sulphur compounds, carbon oxides, chlorofluorocarbons and other halogen compounds, methane and other hydrocarbons.

Tropospheric Photochemistry
Mechanism of Photochemical decomposition of NO2 and formation of ozone. Formation of oxygen atoms, hydroxyl, hydroperoxy and organic radicals and hydrogen peroxide. Reactions of hydroxyl radicals with methane and other organic compounds. Reaction of
OH radicals with SO2 and NO2. Formation of Nitrate radical and its reactions. Photochemical smog meteorological conditions and chemistry of its formation.

Unit-II

Air Pollution
Air pollutants and their classifications. Aerosols-sources, size distribution and effect on visibility, climate and health.

Acid Rain
Definition, Acid rain precursors and their aqueous and gas phase atmospheric Oxidation reactions. Damaging effects on aquatic life, plants, buildings and health. Monitoring of SO2 and NOx. Acid rain control strategies.

Stratospheric Ozone Depletion
Mechanism of Ozone formation, Mechanism of catalytic Ozone depletion, Discovery of Antarctic Ozone hole and Role of chemistry and meteorology. Control Strategies.

Green House Effect
Terrestrial and solar radiation Spectra, Major green house gases and their sources and Global warming potentials. Climate change and consequences.

Urban Air Pollution
Exhaust emissions, damaging effects of carbon monoxide. Monitoring of CO. Control strategies.

Unit-III

Aquatic Chemistry and Water Pollution

Environmental Toxicology
Toxic heavy metals : Mercury, lead, arsenic and cadmium. Causes of toxicity.
Bioaccumulation, sources of heavy metals. Chemical speciation of Hg, Pb, As, and Cd. Biochemical and damaging effects.

Toxic Organic Compound : Pesticides, classification, properties and uses of organochlorine and ionospheres pesticides detection and damaging effects.

Polychlorinated biphenyls : Properties, use and environmental continuation and effects.

Polynuclear Aromatic Hydrocarbons : Source, structures and as pollutants.

Unit IV

Soil and Environmental Disasters
Soil composition, micro and macronutrients, soil pollution by fertilizers, plastic an metals. Methods of re-mediation of soil. Bhopal gas tragedy, Chernobyl, three mile island. Minimtata Disease, Sevoso (Italy), London smog.

Books Suggested

MCH-604: Heterocyclic Chemistry

Unit-I

Nomenclature of Heterocycles
Replacement and systematic nomenclature (Hantzsch-Widman system) for monocylic fused and bridged heterocycles.

Aromatic Heterocycles
General chemical behaviour of aromatic heterocycles, classification (structural type), criteria of aromaticity (bond lengths, ring current and chemical shifts in 1H NMR-spectra. Empirical resonance energy, delocalization energy and Dewar resonance energy, diamagnetic susceptibility exaltations). Heteroaromatic reactivity and tautomerism in aromatic heterocycles.

Unit-II

Non-aromatic Heterocycles
Strain-bond angle and torsional strains and their consequences in small ring heterocycles. Conformation of six-membered heterocycles with reference to molecular geometry, barrier to ring inversion, pyramidal inversion and 1,3-diaxial interaction. Atereo-electronic effects anomeric and related effects. Attractive interactions-hydrogen bonding and intermolecular nucleophilic lectrophilic interactions. Heterocyclic Synthesis
Principles of heterocyclic synthesis involving cyclization reactions and cycloaddition reactions.

Unit-III

Small Ring Heterocycles
Three-membered and four-membered heterocycles-synthesis and reactions of aziridines, oxiranes, thiranes, azetidines, oxetanes and thietanes.

Benzo-Fused Five-Membered Heterocycles
Synthesis and reactions including medicinal applications of benzopyrroles, benzofurans and benzothiophenes.
Unit IV

Meso-ionic Heterocycles
General classification, chemistry of some important meso-ionic heterocycles of type A and B and their applications.

Six-Membered Heterocycles with one Heteroatom
Synthesis and reactions of pyrylium salts and pyrones and their comparison with pyridinium & thiopyrylium salts and phridones. Synthesis and reactions of quionlizinium and benzopyrylium salts, coumarins and chromones.

Unit V

Six Membered Heterocycles with Two or More Heteroatoms Synthesis and reactions of diazones, triazines, tetrazines and thiazines. Seven- and Large-Membered Heterocycles Synthesis and reactions of azepines, oxepines, thiepines, diazepines thiazepines, azocines, diazocines, dioxocines and dithiocines.

Heterocyclic Systems Containing P, As, Sb and B
Heterocyclic rings containing phosphorus: Introduction, nomenclature, synthesis and characteristics of 5- and 6-membered ring systems phosphorinaes, phosphorines, phospholanes and phospholes. Heterocyclic rings containing As and Sb: Introduction, synthesis and characteristics of 5- and 6-membered ring system. Heterocyclic rings containing B: Introduction, synthesis reactivity and spectral characteristics of 3-5- and 6-membered ring system.

Books Suggested:

2. The Chemistry of Heterocycles, T. Eicher and S. Hauptmann, Thieme.
Unit I
Terpenoids and Carotenoids
Calcifications, nomenclature, occurrence, isolation, general methods of structure
determination, isoprene rule. Structure determination, stereochemistry, biosynthesis and
synthesis of the following representative molecules: Citral, Geraniol a-Terpeneol,
Menthol, Farnesol, Zingiberene, Santonin, Phytol, Abietic acid and b-Carotene.

Unit II
Alkaloids
Definition, nomenclature and physiological action, occurrence, isolation, general methods
of structure elucidation, degradation, classification based on nitrogen heterocyclic ring,
role of alkaloids in plants. Structure, stereochemistry, synthesis and biosynthesis of the
following: Ephedrine, (+)-Coniine, Nicotine, Atropine, Quinine and Morphine.

Unit III
Steroids
Occurrence, nomenclature, basic skeleton, Diels hydrocarbon and stereochemistry,
Isolation, Structure determination and synthesis of Cholesterol, Bile acids, Androsterone,
Testosterone, Estrone, Progesterone, Aldosterone, Biosynthesis of Steroids.

Unit IV
Plant Pigments
Occurrence, nomenclature and general methods of structure determination. Isolation and
synthesis of Apigenin, Luteolin Quercetin, Myrctein, Quercetin 3-glucoside, Vitexin,
Diodzein, Aureusin, Cyanidin-7-arabinoside, Cyanidin, Hirsutidin, Biosynthesis of
flavonoids: Acetate pathway and Shikimic acid pathway.

Prophyrins
Structure and synthesis of Haemoglobin and Chlorophyll.

Unit V
Prostaglandins
Occurrence, nomenclature, classification, biogenesis and physiological effects. Synthesis
of PGE2 and PGF2a.

Pyrethroids and Rotenones
Synthesis and reactions of Pyrethroids and Rotenones. (For structure elucidation,
emphasis is to be placed on the use of spectral parameters wherever possible).

Books Suggested
1. Natural Products: Chemistry and Biological Significance, J. Mann, R.S.
2. Organic Chemistry: Vol. 2 1L. Finar, ELBS
5. Chemistry, Biological and Pharmacological Properties of Medicinal Plants from
   the Americas, Ed. Kurt Hostettmann, M.P. Gupta and A. Marston. harwood
   Academic Publishers.
7. New Trends in Natural Product chemistry, Ataaur Rahman and M.L. Choudhary,
Unit-I

Concepts in Molecular Orbital (MO) and Valence Bond (VB) Theory
Introduction to Hückel molecular orbital (MO) method as a mean to explain modern theoretical methods. Advanced techniques in PMO and FMO theory. Molecular mechanics, semi-empirical methods and ab initio and density functional methods. Scope and limitations off several computational programmes.

Unit-II

Quantitative MO theory: Hückel molecular orbital (HMO) - method as applied to ethene, allyl and butadiene. Qualitative MO theory ionisation potential. Electron affinities. MO energy levels. Orbital symmetry. Orbital interaction diagrams. MO of simple organ systems such as ethene, allyl, butadiene, methane and methyl group. Conjugation and hyper-conjugation. Aromaticity.

Unit-III

Principles of Reactivity
Theory of isotope effects. Primary and secondary kinetic isotope effects. Heavy atom isotope effects. Tunneling effect. Solvent effects.

Structural Effects on Reactivity
Linear free energy relationships (LFER). The Hammett equation, substituent constants, theories of substituent effects. Interpretation of s-values. Reaction constants. Deviations from Hammett equation. Dualparameter correlations, inductive substituent constant. The Taft model, σ1 and σR scales.
Unit-IV

Acids, Bases, Electrophiles, Nucleophiles and Catalysis


Steric and Conformation Properties
Various type of steric strain and their influence on reactivity. Steric acceleration.

Unit-V

Nucleophilic and Electrophilic Reactivity
Structural and electronic effects on SN1 and SN2 reactivity. Solvent effect Kinetic isotope effects. Intromolecular assistance. Electron transfer nature of SN2 reaction.
Nucleophilicity and SN2 reactivity based on curved crossing mode. Relationship between polar and electron transfer reactions. SRN1 mechanism. Electrophilic reactivity, general mechanism. Kinetic of SE2 Ar reaction. Structural effects on rates and selectivity. Curve-crossing approach to electrophilic reactivity.

Supramolecular Chemistry
Properties of covalent bonds-bond length, inter-bond angles, force constant, bond and molecular dipole moments. Molecular and bond polarizability, bond dissociation energy, entropy. intermolecular forces, hydrophobic effects. Electrostatic, induction, dispersion and resonance energy, magnetic interactions, magnitude of interaction energy, forces between macroscopic bodies, medium effects. Hydrogen bond.

Book Suggested:

4. Introduction to Theoretical Organic Chemistry and Molecular Modeling.