Elective papers for IV Semester (Any Two)
1. MCH-601: Organotransition Metn' Chemistry
2. MCH-602: Polymers
3. MCH-604: Heterocyclic Chemistry
4. MCH-605: Chemistry of Natural Products
5. MCH-607: Physical–Organic Chemistry

M.Sc. CHEMISTRY – IV sem. Exam June-2014

- SCHEME -

<table>
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<th>Paper</th>
<th>Course No.</th>
<th>Course</th>
<th>Hrs</th>
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<td>Paper XVI</td>
<td>MCH-504</td>
<td>Application of Spectroscopy (Organic Chemistry)</td>
<td>60</td>
<td>100</td>
<td>85+15</td>
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<tr>
<td>Paper XVII</td>
<td>MCH-505</td>
<td>Solid State Chemistry</td>
<td>60</td>
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Grand Total Marks M.Sc. 2800
SEMESTER IV

Paper-XVI
MCH-504: APPLICATION OF SPECTROSCOPY
(Organic 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 & mercaptos), chemical
exchange, effect of deuteration, complex spiespin 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-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 carbonyl carbon), coupling constants. Two dimension NMR
spectroscopy-COSY, NOESY, DEPT, IONEPT, APT and INADEQUATE techniques.
Unit V
Mass Spectrometry
Introduction ion production E1, 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
and S. Craddock, ELBS.
15. Infrared and Raman Spectral : Inorganic and Coordination Compounds K.
Nakamoto, Wiley.
Lippard, Wiley.
19. NMR, NQR, EPR and Mossbauer Spectroscopy in Inorganic Chemistry, V.
Parish, Ellis Haywood.
Bassler adn T.C. Morrill, John Wiley.
McGraw-Hill.

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

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 sulphure 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

Unit IV

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-V

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. Minimata Disease, Sevoso (Italy), London smog.

Books Suggested

5. Introduction to atmospheric Chemistry, P.V. Hobbs, Cambridge.
MCH-601: ORGANOTRANSITION METAL CHEMISTRY

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

Compounds of Transition Metal-Carbon multiple bonds
Alkylidenes, alkylidyynes, low valent carbenes and carbenes-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, arenene 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:

Unit-I

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.
MCH-604: Heterocyclic Chemistry

Unit-I

Nomenclature of Heterocycles
Replacement and systematic nomenclature (Hantzsch-Widman system) for monocyclic 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

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, bezofurans 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 quinolizinium 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. Eischer and S. Hauptmann, Thieme.
MCH-605: Chemistry of Natural Products

Unit I

Terpenoids and Carotenoids
Calification, nomenclature, occurrence, isolation, general methods of structure
determination, isoprene rule. Structure determination, stereochemistry, biosynthesis and
synthesis of the following representative molecules: Citral, Geraniol, a-Terpenol,
Menthol, Farnesol, Zingiberene, Santonin, Phytol, Abietic acid and β-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, (+)-Cocaine, Nicotine, Atropa, Quinine and Morphine.

Unit III

Steroids
Occurrence, nomenclature, basic skeleton, Diel's 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, Myricetin, Quercetin 3-glucoside, Vitexin,
Diadzein, Auricetin, Cyanidin-7-arabinoside, Cyanidin, Hirsidetin, Biosynthesis of
flavonoids: Acetate pathway and Shikimic acid pathway.

Prophyram
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, Ataur Rahman and M.L. Choudhary,
MCI-607: Physical Organic Chemistry

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

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, s1 and sR scales.
M.Sc. IV SEMISTER
PRACTICAL

(Duration: 6-8 hrs in each branch)
Practical examination shall be conducted separately for each branch.

INORGANIC CHEMISTRY
Preparation
Spectrophotometric determinations/ Flame photometric determinations
Record
Viva voice

M.M.[66]
12
36
08
10

Preparation :
Preparation of selected inorganic compounds and their studies by IR, electronic spectra and magnetic susceptibility measurements. Handling of air and moisture sensitive compounds involving vacuum lines. Selection can be made from the following:

2. Atomic absorption analysis of Mg and Ca.
4. Sodium tetrathionate Na$_2$S$_4$O$_6$.

7. Cis and Trans $[\text{Co(en)}_2\text{Cl}_2]^+$. 

8. Determination of Cr (III) complex. $[\text{Cr(H}_2\text{O)}_6]\text{NO}_3\text{3H}_2\text{O}$. Inorg. Synth., 1972, 13, 184.


10. Preparation of $[\text{Co(phenathroline-5,6 quinone) }]$.

**Spectrophotometric Determination**

a) Manganese/Chromium in steel sample.
b) Nickel by extractive spectrophotometric method.
c) Fluoride/nitrite/phosphate.
d) Copper-Ethylene diamine complex: Slope-ratio method

**Flame Photometric Determination**

a) Sodium and Potassium when present together
b) Lithium/calcium/barium/strontium
c) Cadmium and magnesium in tap water
Extraction of Organic Compounds from Natural Sources

1. Isolation of caffeine from tea leaves.
2. Isolation of casein from milk (the students are required to try some typical color reactions of protein).
3. Isolation of lactose from milk (purity of sugar should be checked by LC and PC and Rf values reported).
4. Isolation of nicotine dipiorate from tobacco.
5. Isolation of piperine from black pepper.
6. Isolation of lycopene from tomato.
7. Isolation of b-carotene from carrots.
8. Isolation of eugenol from clove.
9. Isolation of (+) limonine from clove.

Spectroscopy

Identification of organic compounds by the analysis of their spectral data (UV, IR, PMR, CMR & MS) Spectrophotometric (UV/VIS) Estimations

1. Amino acids
2. Proteins
3. Carbohydrates
4. Ascorbic acid
5. Aspirin
6. Caffeine

**PHYSICAL CHEMISTRY**

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<td>Polarography</td>
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<td>Record</td>
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<tr>
<td>Viva voice</td>
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**Thermodynamics**

i. Determination of partial molar volume of solute (e.g. KCl) and solvent in a binary mixture

ii. Determination of the temperature dependence of the solubility of a compound in two solvents having similar intramolecular in tetrations (benzoic acid in water and in DMSO water mixture and calculate the partial molar heat of solution).

**Polarography**

i. Identification and estimation of metal ions such as Cd$^{2+}$, Pb$^{2+}$, Zn$^{2+}$ and I$^{-}$ etc. polarographically.

ii. Study of metal ligand complex polarographically (using Lingane’s Method).