

Shri Vishwanath P. G. College Kalan, Sultanpur

(Affiliated)

DR. RAM MANOHAR LOHIA AVADH UNIVERSITY, AYODHYA

Structure of Syllabus for the Program: M.Sc.

Subject: Chemistry



Course Code		Course Title	Credits	T/P	Evaluation	
					CIE	ETE
A	B	C	D	E	F	G
SEMESTER I (YEAR I)						
B020701T	CORE	Spectroscopy-I	5	T	25	75
B020702T	CORE	Symmetry & Molecular Vibrations	5	T	25	75
B020703T	CORE	Organic Reaction Mechanism	5	T	25	75
B020704T	FIRST ELECTIVE (Select any one)	Chemical Kinetics & Thermodynamics	5	T	25	75
B020705T		Surface & Solid-State Chemistry	5	T	25	75
B020706P	SECOND ELECTIVE (Select any one)	Chemistry Laboratory Course-I A	5	P	50	50
B020707P		Chemistry Laboratory Course-I B	5	P	50	50
SEMESTER II (YEAR I)						
B020801T	CORE	Chemistry of Main Group Elements	5	T	25	75
B020802T	CORE	Stereochemistry & Spectroscopy-II	5	T	25	75
B020803T	CORE	Advanced Quantum Mechanics	5	T	25	75
B020804T	THIRD ELECTIVE (Select any one)	Research Aptitude	5	T	25	75
B020805T		Environmental Science	5	T	25	75

B020806P	FOURTH ELECTIVE (Select any one)	Chemistry Laboratory Course-II A	5	P	50	50
B020807P		Chemistry Laboratory Course-II B	5	P	50	50
SEMESTER III (YEAR II)						
B020901T	CORE	Coordination & Bioinorganic Chemistry	5	T	25	75
B020902T	CORE	Pericyclic, Photochemistry & Rearrangement Reactions	5	T	25	75
B020903T	CORE	Electrochemistry	5	T	25	75
B020904T	FIFTH ELECTIVE (Select any one)	Natural Products	5	T	25	75
B020905T		Medicinal Chemistry	5	T	25	75
B020906P	SIXTH ELECTIVE (Select any one)	Chemistry Laboratory Course-III A	5	P	50	50
B020907P		Chemistry Laboratory Course-III B	5	P	50	50
SEMESTER IV (YEAR II)						
B021001T	CORE	Organotransition Metal Chemistry	5	T	25	75
B021002T	CORE	Organic Synthesis	5	T	25	75
B021003T	SEVENTH ELECTIVE (Select any one)	Analytical Chemistry	5	T	25	75
B021004T		Polymer Chemistry	5	T	25	75
B021001P	RESEARCH PROJECT/ DISSERTATI ON	Practical Based Major Research Project / Dissertation	10	P	50	50

Semester I

Theoretical Paper-I

B020701T: Spectroscopy-I

Unit I

UV-Visible Spectroscopy: Different type of electronic transitions, Lambert-Beer's law, Chromophores, Auxochromes, Solvent effect, Red shift and blue shift, Woodward's rule for conjugated cyclic and acyclic dienes and α , β – unsaturated carbonyl compounds, Absorption in aromatic compounds (substituted benzene, naphthalene and anthracene), Problems related to UV-Visible Spectroscopy.

Unit II

Infrared Spectroscopy & Raman Spectroscopy: Linear harmonic oscillator, Vibrational energies of diatomic molecules, zero-point energy, force constant and bond strength, anharmonicity, Morse potential, Vibration– rotation spectroscopy, P, Q, R branches, Breakdown of Oppenheimer approximation, vibration of polyatomic molecules, selection rules, Group frequencies, Overtones, hot bands, factors affecting the bond positions and intensities for IR region, Problems related to Infrared Spectroscopy; *Raman Spectroscopy:* Classical and quantum theories of Raman effects, Pure rotational, Vibrational and Vibrational-rotational Raman spectra, Selection rule, Mutual exclusion principle, Resonance Raman spectroscopy, CARS.

Unit III

Microwave Spectroscopy: Classification of molecules, rigid rotor model, effect of isotopic substitution on the transition frequency, intensities, non-rigid rotor. Stark effect, nuclear and electron spin interaction and effect of external field applications.

Unit IV

Mossbauer Spectroscopy: Basic Principles, spectral parameters and spectrum display. Application of the technique to the studies of (a) bonding and structures of Fe^{+2} and Fe^{+3} compounds including those of intermediate spin, (b) Sn^{+2} and Sn^{+4} compounds – nature of M-L bond, coordination number, structure and (c) detection of oxidation state and in equivalent MB atoms.

Unit V

Diffraction Techniques: *X-ray Diffraction:* General Features of diffraction, Powder X-ray diffraction, Single crystal X-ray diffraction. The technique, structure factor, phase problem, brief description of time resolved X-rays diffraction techniques; *Electron Diffraction:* Scattering intensity vs scattering angle, Wierl equation, Measurement technique, Elucidation of structure of simple gas phase molecules, Low energy electron diffraction structure of surfaces; *Neutron Diffraction:* Brief introduction, difference with X-rays diffractions.

Recommended Books:

1. Fundamentals of Molecular Spectroscopy, 4th Ed. Mc Graw-Hill, C.N. Banwell.
2. Basic Principles of spectroscopy, Mc Graw –Hill, R. Chang
3. Modern Spectroscopy, J. M. Hollas, John Wiley.
4. Inorganic Electronic Spectroscopy, A. B. P. Lever, Elsevier.
5. Magnetochemistry, R. L. Carlin, Springer Verlag
6. K. Veera Reddy, Symmetry and Spectroscopy of Molecules, New Age.
7. Inorganic Chemistry, D. E. Shriver, P. W. Atkins and C. H. L. Langford, Oxford
8. Advanced Inorganic Chemistry, F. A. Cotton and G. Wilkinson, John Wiley.
9. Inorganic Chemistry, J. E. Huheey, Ellen A. Keiter, Richard L. Keiter, Addison Wesley Longman (Singapore) Pvt. Ltd.

Theoretical Paper-II

B020702T: Symmetry & Molecular Vibration

Unit I

Symmetry & Point Groups: Symmetry elements, Symmetry operations. Symmetry points group, Identification of molecular points group, Molecules of low symmetry, high symmetry and special symmetry (C_n , S_n , D_n , C_{nv} , D_{nh} only).

Unit II

Group, Subgroups, Classes and Matrices Representation: Definition, multiplication tables, group generating elements, subgroup, classes, derivation of matrices (C_n , σ , i , S_n), Direct product, Group multiplication basis, matrix representation, Character of an operation, orthogonality projection and shift operators, character table, orthogonality theorem, irreducible representation, Transformation matrices, structure of character table, determination of symmetry species for translations and rotations, construction of character table (C_{2v} , C_{3v}).

Unit III

Valence Bond Theory: Formation of hybrid orbitals of XY_3 (planar), XY_4 . (tetrahedral & square planar), Symmetry of orbital, orbital symmetry properties, Projection to get symmetry orbital, projection operations, basis functions and hybrid orbitals with example.

Unit IV

Normal Coordinate Analysis: Cartesian coordinate and internal coordinate methods applied to C_{2v} (symmetric XY_2 , ZXY_2), C_{3v} (XY_3), T_d . (XY_4) and O_h (XY_6) systems.

Unit V

Molecular Vibrations: Internal and symmetry coordinates, SALC's, Symmetric normal vibrations, mixing of linear coordinates in normal modes, determination of symmetry types of normal modes, analysis of vibration of 1, 2 dichloroethylene, IR and Raman activity of some typical molecules (C_{2v} , C_{3v} , C_{4v} , D_{2h} , D_{3h} , D_{4h} point group).

Recommended Books:

1. McWeeny, "Symmetry - An Introduction to Group Theory", Pergamon Press.
2. Lowell H. Hall "Group Theory and Symmetry in Chemistry", McGraw Hill Book Company, New York, 1969
3. K. Veera Reddy, "Symmetry and Spectroscopy of Molecules", New Age International Limited Publisher, New Delhi.
4. D.M. Bishop, "Group theory and Chemistry" Dover Publications.
5. F.A. Cotton, "Chemical Applications of Group Theory", John Wiley, 1971.
6. M. Hamaresh, "Group theory and its Applications to Physical Problems" Addison- Wisley
7. Symmetry and Group theory: Some chemical applications, Ramashankar and Suresh Ameta, Himanshu Publications, Udaipur, Delhi.

Theoretical Paper-III

B020703T: Organic Reaction Mechanism

Unit I

Principle of Reaction Mechanism: Potential energy diagram, Transition states and intermediates, methods of determining reaction mechanism, Labelling and kinetics isotopic effect and its importance in the determination of reaction mechanism, Hammond's postulate, Curtin Hammett principle, structural effects on reactivity, Hammett equation and linear free energy relation (LFER), substituent and reaction constants, Taft equation.

Unit II

Substitution Reaction: *Aliphatic Nucleophilic Substitution:* SN^1 , SN^2 , SN^i , $SN^{1'}$, $SN^{2'}$, $SN^{i'}$, mixed SN^1 and SN^2 , role of substrate's structure, nucleophile, leaving group and solvent on SN reaction, ambidentate nucleophile, Regioselectivity, competition between SN^1 and SN^2 , Nucleophilic substitution in bridged system phenonium ion, norbornyl system, Neighbouring group participation (Ph, π , σ , N, S, negatively charged oxygen), anchimeric assistance; *Aliphatic Electrophilic Substitution:* SE^1 and SE^2 , SE accompanied by double bond shifts, Effect of substrate, leaving group and solvent polarity on reactivity, *Aromatic Nucleophilic Substitution:* Aromatic SN^1 and SN^2 , addition-elimination and elimination-addition (benzyne) mechanism, effect of substrate structure, nucleophile, leaving group on ArSN reaction, *Aromatic Electrophilic Substitution:* General view, energy profile, Arenium ion mechanism (ArSE), o/p ratio.

Unit III

Free Radical Reactions: Types, generation, structures, radical effect, substitution mechanism at an aromatic substrate at a bridgehead, reactivity in the attacking radicals, effect of solvent on reactivity, Allylic halogenation (NBS), oxidation of aldehydes, autooxidation, Alkynes coupling and arylation of aromatic compounds by diazonium salts, Sandmeyer reaction, Hunsdiecker reaction.

Unit IV

Elimination Reaction: E^1 , E^2 , $E1cB$, Factors (substrate structure, attacking base, leaving group, medium) affecting these reactions, stereochemistry, orientation of the double bond (Saytzeff vs Hofmann elimination), Mechanism and orientation of pyrolytic syn elimination, Competition between substitution and elimination reactions.

Unit V

Addition Reaction: *C=C bond addition:* Mechanism, stereochemistry, electrophilic, nucleophilic, free radical addition, addition of halogen acid, 1,2-dihydroxylation, epoxidation, hydroboration, oxymercuration-demercuration, hydrogenation of double bond, triple bond, aromatic ring. cyclopropanation, Simmon-Smith cyclopropanation, epoxidation, Sharpless asymmetric epoxidation, corey epoxidation, *Carbon hetero atom multiple bond addition:* C=O bonds, cram rule, condensation reactions involving Claisen, Benzoin, Perkin, Knoevenagel, Darzen, Reformatsky and Cannizzaro reaction, Mechanism of hydrolysis of ester and amide, Ammonolysis of ester.

Recommended Books:

1. Organic Chemistry, J. Clayden, N. Greeves, S. Warren and P. Wothers (Oxford Press.)
2. Advanced Organic Chemistry, A. F. A. Carey and R. J. Sundberg, 5th Ed. Springer (2007)
3. Advanced Organic Chemistry, J. March, 6th Ed.
4. Mechanism and structure in Organic Chemistry – E. S. Gould (Holt, Rinehart and Winston)
5. Guidebook to Mechanism in Organic Chemistry, Orient Longman, Sykes, P. A New Delhi.

Theoretical Paper-IV

(Optional)

B020704T: Chemical Kinetics & Thermodynamics

Unit I

Chemical Kinetics: Methods of determining rate laws, mechanism of photochemical ($H_2 + Br_2$, $H_2 + Cl_2$), chain stopped (H_2 equation + Br_2 , decomposition of CH_3CHO , decomposition of C_6H_6), oscillatory reaction, collision theory, steric factor, Absolute reaction rate theory, comparison of result with Eyring and Arrhenius equation, steady state kinetics, kinetic and thermodynamic control of reactions, ionic reactions, kinetic salt effect, homogeneous catalysis, kinetics of enzyme reactions, heterogeneous catalysis, Fast reactions, luminescence and electron transfer process, flow technique, Relaxation method, flash photolysis, magnetic resonance method.

Unit II

Chemical Equilibrium: Free energy, entropy of mixing, partial molar quantities (free energy, volume, heat contents), Gibbs Duhem equation, Equilibrium constants, Van't Hoff equation, Fugacity and its determinations.

Unit III

Ideal and Non-ideal Solution: Excess function, activities, hydration number, activities in electrolytic solution, mean ionic activity coefficient, determination of activity, Phase rule, Phase diagram of one, two and three component systems.

Unit IV

Non-Equilibrium Thermodynamics: Postulates, methodologies, linear laws, Gibbs equation, Onsager reciprocal theory;

Unit V

Statistical Thermodynamics: Thermodynamic probability and entropy, concept of distribution, most probable distribution, Ensemble averaging, Maxwell-Boltzmann distribution, postulates of canonical, grand canonical, microcanonical ensemble, Bose-Einstein and Fermi-Dirac statistics, partition function, translational, rotational, vibrational and electronic partition function for diatomic molecules, calculation of thermodynamic functions and equilibrium constant, theories of specific heat for solids, application of partition function.

Recommended Books:

1. P. W. Atkins, Physical Chemistry, Oxford University Press, New York.
2. S. Glasston, Physical Chemistry, Nostrand
3. K. L. Kapoor, Advance Physical Chemistry (Vol-1,2,3,4), Mac Millan, India
4. Puri, Sharma, Pathania, Advance Physical Chemistry.
5. M.C. Gupta, Statistical Thermodynamics, Second Edition, New Age International Limited Publisher.
6. Statistical Thermodynamics, Second Edition, New Age International Limited Publisher, India by M.C. Gupta.

Practical

B020706P: Chemistry Lab Course-IA

Credit 05

10h/Week

Course Objectives: The objective of this course to provide advanced insight about the qualitative analysis of inorganic mixture containing one rare element of first & second group and organic mixtures, chromatographic separations, chemical kinetics, thermochemistry and phase equilibria.

INORGANIC CHEMISTRY

Qualitative analysis: Qualitative analysis of an inorganic mixture of seven radicals including one rare element of first & second group (TI, W, Se, Mo, and Te). Semi- micro analysis is to be done. Mixture can have insoluble substances, interfering anions and combination of anions.

Chromatography: Chromatographic separation of first and second group metal ion of the following combinations:

- i. Pb^{2+} , Ag^+ , Hg_2^{2+}
- ii. Pb^{2+} , Cd^{2+} , Cu^{2+}
- iii. Bi^{3+} , Cd^{2+} , Hg^{2+}

ORGANIC CHEMISTRY

Qualitative Analysis: Separation, purification and identification of components of binary organic mixture (both solids, one solid & one liquid). Systematic analysis of each component laying emphasis on solubility, element detection, melting point, boiling point determination, ignition test, unsaturation test, functional group test, specific test and preparation of suitable derivative.


Chromatography: Separation, identification and determination of Rf value of the components present in the binary mixture of amino acids by paper chromatographic methods.

PHYSICAL CHEMISTRY

Chemical Kinetics:

- i. Kinetics of ester (methyl acetate) hydrolysis in presence of acid.
- ii. Determine the velocity constant and order of reaction for hydrolysis of ethyl acetate by sodium hydroxide at given temperature (saponification of an ester).
- iii. Kinetics of acetone and I_2
- iv. Kinetics of KBrO_3/KI
- v. Kinetics of $\text{Na}_2\text{S}_2\text{O}_8/\text{HCl}$

Thermochemistry/Phase Equilibria:

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- i. Determination of the solubility of benzoic acid in water at different temperatures and calculate the heat of solution.
- ii. Determination of the solubility of a salt (KCl, KNO₃) at different temperatures and calculate the heat of solution.
- iii. Construct the phase diagram for three component Ethanol, benzene and water system.
- iv. Construct the phase diagram for three component chloroform, acetic acid and water system.
- v. Construct the phase diagram for two component system.

System of Marking:-

Time: 12h

Inorganic: 33

Organic: 34

Physical: 33

Recommended Books:

1. Experimental Inorganic Chemistry by Mounir A, Malati, Horwood series in Chemical Science (Horwood publishing Chichester) 1999.
2. Practical Inorganic Chemistry, G. Marrand, B.W. Rockett, Van Nostrand.
3. Practical Physical Chemistry, A.M. James and F.E. Prichard, Longman.
4. Findley's Practical Physical Chemistry revised, B.P. Levitt, Longman.
5. Experimental Physical Chemistry, R.C. Das and Bebera, Tata Mc Grawhill.
6. Senior Practical Physical Chemistry, B.D. Khosla and V.S. Barg (R. Chand and Co., Delhi)
7. Experimental Physical Chemistry by D.P. Shoemaker Mc Grawhill, 7th Edition 2003.
8. Experiments in Chemistry, D.V. Jahagirdar, Himalaya Publishing House.
9. Practical Physical Chemistry, B. Vishwanathan and P.S. Raghwan, Viva Books.
10. General Chemistry Experiments, Anil J Elias, University Press (2002)
11. Experimental Physical Chemistry, V.D. Athawale, ParulMathur, New Age International (P) Limited.
12. Systematic Experiment in chemistry, ArunSethi, New Age International (P) Limited.
13. The systematic Identification of Organic Compounds, R.L. Shringer and D.Y. Curlin.

Semester II

Theoretical Paper-I

B020801T: Chemistry of Main Group Elements

Unit I

Stereochemistry of Bonding Among Main Group Elements: VSEPR theory stereochemical rules and explanation of the shapes of molecules and ions of nontransition element with 2-7 valence shell electron pairs. Walsh diagram (Tri and penta atomic molecules) $d\pi-p\pi$ bonds, Bent rule, Energetics of hybridization.

Unit-II

Compounds of Main Group Elements: Preparation, Structure, Bonding and Technical Applications of Polyether complexes of alkali and alkaline earth metals; Polyphosphazenes and Thiazyl & its polymers, tetrasulfur dinitride.

Unit-III

Structure and Bonding in Ions of Some Main Group Elements: Structure and bonding of borane anions, higher boranes, carboranes, classification and structures of silicates.

Unit-IV


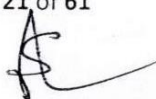

Carbides & Polyanions: Synthesis and structure of Carbides & polyions of Ge, Sn, Pb, Sb, Bi and Hg.

Unit-V

Hapticity & Organometallics: Definition and classification of organometallic compounds on the basis of hapticity and polarity of metal-carbon bond; Preparation, Properties, Structure and Applications of alkyl and aryls of Lithium, Beryllium, Aluminum, Mercury and Tin.

Recommended Books:

1. Advance Inorganic Chemistry, 6th Edition, Cotton and Wilkinson.
2. Inorganic Chemistry, 4th Edition, Principles of Structure and Reactivity by J.F. Huheey, E.A. Keiter and R.L. Keiter, 1993
3. Chemistry of Elements by N.N. Greenwood and A. Ernshaw, Butterworths 1997.



Theoretical Paper-II

B020802T: Stereochemistry & Spectroscopy -II

Unit I

Stereochemistry: Stereochemistry with chiral centre: chirality, Polychiral centre molecules, Threo-erythro isomers, stereoisomerism with axial/ planar chirality and Helicity, Principle of axial and planar chirality, optical isomerism in the absence of chiral carbon (biphenyl, allenes, spiranes), optical activity due to intermolecular overcrowding, chirality due to helical shape, Absolute configuration (R/S, E/Z), Stereochemistry of compounds having S, N, P atoms, Geometrical isomerism of compounds having C=N, N=N bonds; *Topocity and Prostereoisomeriam:* Homotopic, enantiotopic and diastereotopic atoms, groups and faces, nomenclature and symbols; *Atropisomerism:* Conformational analysis of acyclic system, Interconversion of Fischer, Newmann and Sawhorse projection, its effect on activity (SN^1 , SN^2 , E^1 , E^2) configuration, conformation and stability of cycloalkanes, mono and disubstituted cyclohexane, cyclohexenones, decalin, decalol.

Unit II

Proton Magnetic Resonance Spectroscopy: Spinning nuclei, nuclear spin, nuclear resonance, saturation, chemical shift, chemical shift measurement, factors affecting the chemical shift, anisotropic effect, shielding mechanism, spin - spin coupling, coupling constant, chemical exchange, effect of deuteration, factor influencing coupling constant 'J', Karplus curve-variation of coupling constant with dihedral angle, Spin decoupling, simple, virtual and complex coupling, chemical and magnetic equivalence, first and non -first order spectra, analysis of AB, AMX and ABX system, simplification of complex spectra, contact shift reagents, solvent effects. NOE, hindered rotation and rate process, NMR studies of ^{19}F , ^{31}P , instrumentation, FT NMR & its advantages, DEPT, 2DNMR: COSY, NOESY, HETCOR, application of 1H NMR spectra in structural determination of simple organic molecules, use of NMR in medical.

Unit III

Carbon Magnetic Resonance Spectroscopy: Introduction, peak assignment, chemical shift, ^{13}C - 1H coupling, off resonance, decoupling, deuterium, fluorine and phosphorous coupling, DEPT, 2DNMR: COSY, NOESY, HETCOR, application to simple organic molecules (aliphatic, olefinic, alkyne, aromatic, heteroaromatic and carbonyl carbon).

Unit IV

ESR Spectroscopy: Basic principles, zero field splitting and Kramer's degeneracy, factors affecting 'g' value, Isotropic and anisotropic hyperfine coupling constants, Application to organic free radicals - methyl free radical, naphthalene and benzene free radicals, CIDNP.

Unit V

Mass Spectrometry: Measurement technique (EI, CI, FD and FAB), Ion production, factors affecting fragmentation, group metastable peak, Ion analysis, Molecular base and molecular ion, Ion abundance, factors affecting Ion abundance, Mc Lafferty rearrangements, retro Diels Alder fragmentation, Nitrogen rule, determination of molecular composition, fragmentation patterns of organic compounds, common functional group with reference to their structure determination, Interpretation of mass spectra, High resolution mass spectrometry.

Recommended Books:

1. Stereochemistry of Organic Compounds, Nasipuri, New Age International (P) Limited.
2. Stereochemistry of Carbon Compounds, E. L. Eliel and S. H. Wilen
3. Spectrometric Identification of Organic Compounds, Silverstein and Webster, John Wiley, New York.
4. Organic Spectroscopy, P. S. Kalsi, New Age International (P) Limited.
5. Introduction to Spectroscopy, Pavia, Lampman, Kriz, Vyvyan, Cengage Learning.
6. Organic Spectroscopy, I Fleming, McGraw-Hill Inc., US.
7. Organic Spectroscopy, W. Kemp, Macmillan, London.

Theoretical Paper-III

B020803T: Advanced Quantum Mechanics

Unit I

Symmetry Properties and Quantum Mechanics: Invariability of Schrodinger Equation for a molecule with respect to symmetry operations and its consequences. Construction of molecular orbitals of ammonia and pie molecular orbitals of naphthalene, the direct product representation and its application in the derivation of selection rules for electronic, vibrational and Raman spectra.

Unit II

Huckel MOT of Conjugated Systems and its Applications: Calculation of energy levels and delocalization energy of butadiene, cyclic conjugated systems: cyclopropenyl, cyclobutadiene, cyclopentadienyl, benzene, brief idea about delocalization energies of tropylium radical and cyclooctatetraene, concept of aromaticity and antiaromaticity, Huckel treatment of linear polyenes.

Unit-III

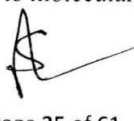
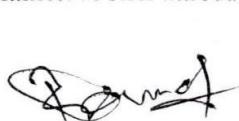
Semi-Empirical and Ab-Intio SCF Theories: Hartee-Fock Self consistent (SCF) method, Semi empirical SCF theory (CDNO, INDO & MNDO), Slater and Gaussian type orbitals, Configurational interaction and electron correlation, Moellar-Plasset perturbation methods.

Unit-IV

Introduction to Density Functional Theory: Concept of basis sets, exchange- correlation energy, The Hohenberg variational theorem and Kohn- Sham orbitals, The Local Density Approximation (LDA) and Generalized Gradient Approximation (GGA). Density Functional theory and its significance.

Unit-V

Molecular Mechanics: A brief introduction to molecular mechanics.



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Recommended Books:

1. Quantum Chemistry by Donald A. Macquarrie
2. Physical Chemistry by T. Engel and P. Reid
3. Introductory Quantum Chemistry by A. K. Chandra
4. Quantum Chemistry by R. K. Prasad
5. Molecular Quantum Mechanics by Atkins and Friedman
6. Quantum Chemistry by Ira N. Levine, Prentice Hall of India, New Delhi 1995
7. Chemical Application of Group Theory by F. A. Cotton

Theoretical Paper-IV

(Optional)

B020805T: Environmental Science

Unit I

Basics of Environment: Introduction, Composition of atmosphere, Vertical temperature, heat budget of the earth atmospheric system, vertical stability atmosphere. Biogeochemical cycles of C, N, P, S and O, bio distribution of elements.

Unit II

Atmosphere: Regions, chemical composition of atmosphere, Particles, ions & radicals and their formation, Chemical & photochemical reaction in atmosphere, smog formation, oxides of N,C,S,O and their effect, pollution by chemicals, petroleum, minerals, ozone layer, ozone layer depletion, chlorofluoro hydrocarbons, Green House effect, acid rain, Global warming, Analytical methods for measuring air pollutants, continuous monitoring instruments.

Unit III

Hydrosphere: Chemical composition of water bodies *viz.* lakes, streams, rivers, and wet lands, Hydrological cycle, Recycle of waste water, Sewage treatment; *Water pollution:* Inorganic, Organic, Pesticide, Agricultural, Industrial and Sewage, detergents, oil spills and oil pollutants, Water quality parameters-dissolved oxygen, biochemical oxygen demands, solids metals, content of chloride, sulphate, phosphate, nitrate and micro-organisms water quality standards, Analytical methods for measuring DO, BOD and COD, residual chloride and chlorine demand, Purification and treatment of water.

Unit IV

Soil: Composition, micro and macro nutrients, Pollution- fertilizers, pesticides, plastics and metals, waste treatment.

Unit V

Industrial Pollution: Cement, sugar, distillery, drug, paper and pulp, thermal power plants, nuclear power plants, metallurgy, polymers, drugs etc. Radionuclide analysis, Disposal of Wastes and their management; *Environmental Toxicology:* Toxic chemicals in the environment, Chemical solution to environment, Principles of decomposition, biodegradability, better industrial process.

Recommended Books:

1. Manahan, Stanley E. Fundamentals of Environmental Chemistry Boca Raton: CRC Press, LLC, 2001.
2. Sonja Krause, Herbert M. Clark, James P. Ferris, Robert L. Strong Chemistry of the Environment, Elsevier Science & Technology Books, 2002.
3. Eugene R. Weiner Applications of Environmental Chemistry 2000 CRC Press, LLC.
4. By Clair, N. Sawyer, Perry L. Mc Carty, Gene F. Parking Chemistry for environmental engineering and Science (5th edition) McGraw Hill Professional.

Practical

B020806P : Chemistry Lab Course-II A

Credits-5

10h/Week

Course Objectives: The objective of this course to provide advanced insight about the quantitative estimations (one volumetrically and other gravimetrically) of the metals present in inorganic mixtures, inorganic and organic preparations, chromatographic separations of sugars, and experiments related to physical chemistry viz. Solubility & distribution coefficient, optical methods (colorimetry, refractometry and polarimetry).

INORGANIC CHEMISTRY

Quantitative Analysis: Estimation of two metal ions (one gravimetric and other volumetric) from the following mixtures:

- i. Ni^{2+} and Cu^{2+}
- ii. Pb^{2+} and Cu^{2+}
- iii. Ba^{2+} and Cu^{2+}
- iv. Ag^+ and Cu^{2+}

Inorganic Preparation:

Check the purity of the synthesized compounds by TLC and report the percentage of yield.

- i. $\text{K}_3[\text{Cr}(\text{C}_2\text{O}_4)_3] \cdot 3\text{H}_2\text{O}$
- ii. $[\text{Co}(\text{NH}_3)_4 \cdot \text{CO}_3]\text{NO}_3$
- iii. $\text{NH}_4[\text{Cr}(\text{SCN})_4(\text{NH}_3)_2]\text{H}_2\text{O}$
- iv. $(\text{NH}_4)_2[\text{PbCl}_6]$
- v. $\text{Hg}[\text{Co}(\text{SCN})_4]$
- vi. $\text{Ni}(\text{DMG})_2$

ORGANIC CHEMISTRY

Organic Synthesis:

Two steps synthesis involving following reactions and check the purity of the synthesized compounds by TLC and report the percentage of yield:-

- i. Acetylation
- ii. Hydrolysis
- iii. Oxidation
- iv. Aromatic electrophilic substitution
- v. Condensation
- vi. Sandmeyer reaction

Chromatography: Separation and identification of the sugars present in the organic mixture by paper chromatographic methods and determination of R_f value.

PHYSICAL CHEMISTRY

Solubility & Distribution Coefficient:

- i. To draw the solubility curve for water-acetic acid-chloroform system.
- ii. Determination of the distribution coefficient of acetic acid between benzene and water.
- iii. Determination of the distribution coefficient of iodine between carbon tetrachloride and water.
- iv. Determination of the dimerization constant of benzoic acid in benzene medium by partition method.
- v. Solubility of an organic acid in water at room temperature.

Optical Methods (Colorimetry, Refractometry and Polarimetry):

- i. To verify Lambert's Beer Law colorimetrically.
- ii. Determine the rate constant for inversion of cane sugar using a polarimeter.
- iii. Determination of the molar refractivity of methyl alcohol, acetic acid, ethyl acetate and carbon tetrachloride and calculate the refraction equivalents of carbon, hydrogen and chloride atoms.

System of Marking:-

Time: 12h

Inorganic: 33

Organic: 34

Physical: 33

Recommended Books:

1. Vogel's Text book of Quantitative Analysis revised, J. Bessett, R.C. Denney, G.H. Jellery and J. Mendhan ELBS.
2. Microscale Inorganic Chemistry, Z. Scafran, R.M. Pike and M.M. Singh Wiley.
3. Practical Inorganic Chemistry, G. Mairand, B.W. Rockett, Van Nostrand.
4. Vogel's Textbook of Practical Organic Chemistry, A.R. Tatchell, John Wiley.
5. Systematic Experiment in chemistry, Arun Sethi, New Age International (P) Limited.
6. Practical Physical Chemistry, A.M. James and F.E. Prichard, Longman.
7. Findley's Practical Physical Chemistry revised, B.P. Levitt, Longman.
8. Experimental Physical Chemistry, R.C. Das and Bebera, Tata Mc Grawhill.

SEMSETER - III

Theoretical Paper-I

B020901T: Coordination & Bioinorganic Chemistry

Unit I

Basics of Energy Level in Atoms: Electronic configuration, coupling of orbital angular momenta, coupling of spin angular momenta, spin orbital coupling, energy terms, Determining the ground state terms -Hund's rules. Determination of term symbol for a closed subshell, Hole formulation, Derivation of terms for a d^2 configuration. Inter electron repulsion parameter. Variation of Racah B and C parameters in different transition series. Spin orbit coupling parameters.

Unit-II

Free Ions in Crystal Fields: Effect of weak crystal field on free ion terms in octahedral, square planar and tetrahedral symmetries. Orgel diagrams, mixing of terms, Medium and strong field approximation in Oh point group, transition from weak to strong field and correlation diagram for only d^2 case, non-crossing rule, Tanabe Sugano diagrams.

Unit-III

Electronic Spectra of Complexes: Laporte orbital, selection rules, spin selection rules, Splitting of electronic energy level and spectroscopic states, Interpretation of the spectra of $[M(H_2O)_6]^{n+}$ in aqueous medium, calculation of Dq, B and β parameters, Jahn Teller distortion and its effect on electronic spectra.

Unit-IV

Metal-Ligand Bonding & Magnetic Properties of Complexes: Effects of crystal field splitting, Limitations of CFT, Nephelauxetic series, molecular orbital energy level diagram of octahedral, tetrahedral and square planer complexes; *Magnetic Properties of Complexes:* Dia, para, ferro and anti-ferromagnetism, Quenching of orbital angular momentum by ligand and magnetic properties of A, E and T terms.

Unit-V

Metalloenzymes: Function, structure, bonding and stereochemistry of the active site of *Natural dioxygen carriers:* Haemoglobin, myoglobin, hemerythrin, hemocyanin; *Electron Transport:* Iron sulphur protein- Rubredoxin, Ferredoxin, Cytochromes (types a, band c); *Redox enzymes:* Mo containing: Nitrogenase, Xanthine oxidase, Sulphite oxidase, Nitrate reductase, Fe containing: Cyt c oxidase, Catalases Peroxidases; Cu containing: Superoxide dismutase (SOD), Bovine superoxide dismutase (BOD), Ascorbic acid oxidase, Zn containing: Carboxypeptidase A & B, Carbonic anhydrase, Urease, Co containing: Vitamin B₁₂, Vitamin B₁, Methyl cobalamime, Biomethylation.

Recommended Books:

1. Advanced Inorganic Chemistry, F. A. Cotton and G. Wilkinson, John Wiley
2. Inorganic Chemistry, J. E. Huheey, Ellen A. Keiter, Richard L. Keiter, Addison Wesley Longman (Singapore) Pvt. Ltd.
3. Chemistry of the Elements, N. N. Greenwood and A. Earnshaw, Pergamon.
4. Organometallic Chemistry: A Unified Approach, R. C. Mehrotra and A. K. Singh, New Age
5. Principles of Organometallic Chemistry, G. E. Coates, M. L. H. Green, P. Powell and K,
6. Principles of Bioinorganic Chemistry, S. J. Lippard and J. M. Berg, University Science Books
7. Bioinorganic Chemistry, I. Bertini, H. B. Gray, S. J. Lippard and J. S. Valentine, University Science Books.
8. Bioorganic, Bioinorganic and Supramolecular Chemistry, P.S. Kalsi, New Age International (P) Limited.

Theoretical Paper-II

B020902T: Pericyclic, Photochemistry & Rearrangement Reactions

Unit I

Pericyclic Reactions: Basic concepts, classifications, characteristics, conservation of MO symmetry, FO of ethylene, 1-3 butadiene, 1,3,5-hexatriene, allyl system, Woodward, Hoffmann rule for correlation diagram, FMO & PMO approach to study of *Electrocyclic reactions* of linear conjugated $4n$, $4n+2$, allyl system; *Cycloaddition reaction* of [2+2], [4+2] system, [2+2] addition of ketene, 1, 3-dipolar cycloaddition; *Sigmatropic*: [1,3], [1,5], [3,3], [5, 5] group transfer reaction, suprafacial, antarafacial shift of H, Sigmatropic shift involving carbon moieties, Claisen, Cope rearrangement, Fluxional tautomerism, Aza cope rearrangement, Ene reaction, Chelotropic reaction, Prototropic reaction.

Unit II

Photochemistry: Electronically excited states, spin multiplicity, Jablonski diagram, ISC; *Photochemistry of alkenes*: Geometrical isomerization, cyclisation, dimerization, di- π methane rearrangement, H abstraction addition, acetylene dimerization, photochemistry of diene, 1,3-butadiene, [2+2] addition leading to cage structure; *Photochemistry of Carbonyls*: Reduction, Norrish I cleavage of acyclic, cyclic, α , β and γ unsaturated carbonyl compounds, photochemistry of Norrish II cleavage, Paterno Buchi reaction, intra and inter molecular H abstraction, rearrangement of α , β unsaturated ketones, cyclohexadienones, photoenolization, photocycloaddition of ketones with unsaturated compound, photodimerisation of (enones), α , β unsaturated ketones, rearrangement of enones, dienones photochemistry of p- benzoquinones.

Unit III

Photochemistry of Aromatics: Ring isomerization, excited state of benzene and its 1,2 & 1, 3 shifts, photo Fries rearrangement (of anilide), cyclisation reactions, Skeletal isomerism, Dewar Prismane isomerization of disubstituted benzene, photo substitution reaction of benzene, photolysis of nitride ester.

Unit IV

Rearrangements: *Photochemical Rearrangements*: Sommet Hauser, Hofmann-Loffler Freytag, Barton, Fries; *Molecular Rearrangements*: General mechanistic considerations, nature of migration, migratory aptitude, memory effects, a detailed study of the following rearrangements- Wagner-Meerwein, Demjanov ring expansion, Diene-phenol, Benzil-Benzilic acid, Wolf, Lossen, Beckman, Stevens, Wittig, Neber, Arndt-Eistert synthesis, Amino ketone, benzidine, Shapiro reaction.

Unit V

Selective Name Reactions: Stark enamine, Chichibabin, Birch reduction, Heck, Suzuki, Mukaiyama, Woodward & Prevost hydroxylation, Peterson synthesis.

Recommended books:

1. Textbook of Pericyclic Reaction, Concept and Application, K.C. Majumdar and P. Biswas, Scientific International Pvt. Ltd.
2. Organic Photochemistry: A visual approach, Jan Kopecky, VCH publishers (1992).
3. Organic Photochemistry, O. Kan, McGraw-Hill Inc., US.
4. Organic Chemistry, J. Clayden, N. Greeves, S. Warren and P. Wothers, Oxford.
5. Fundamentals of Photochemistry, K. K. Rohatagi, New Age International (P) Limited.
6. Photochemistry and Pericyclic Reactions, Jagdamba Singh and Jaya Singh, New Age
7. Principles of Molecular Photochemistry, Nicholas J. Turro, V. Ramamurthy J. C., Viva Books. International (P) Limited.
8. Organic photochemistry, J. Coxon and B. Halten, Cambridge University Press.
9. Essential of Molecular Chemistry, A. Gilbert and J. Baggot, Blackwe II.
10. Molecular photochemistry, N. J. Turro, W. A. Benjamin.
11. Introductory Photochemistry, A. Cox and T. Camp, McGraw-Hill
12. Photochemistry, R. P. Kundalland, A. Gilbert, Thomson Nelson.

Theoretical Paper-III

B020903T : Electrochemistry

Unit I

Electrokinetic Phenomenon: Electrokinetic Effects, Electrokinetic potential/Zeta potentials, Determination of zeta potential, influence of ions on electrokinetic phenomena, Quantitative treatments of Electro-Osmosis, Electrophoretic and Streaming potential, sedimentation potential, The electrical double layer, Theoretical and quantitative treatment of electrokinetic phenomena, Mobility and Bound hydrogen ion.

Unit II

Electrolytic Conductance, Transference and Interface: Debye Huckel theory of strong electrolyte (DHO eqn.), Debye Falkenhagen effect, Wein effect the ionic association, effect of ionic strength on rate of ionic reactions, activity coefficient, ionic strength, its effect on reaction rate, Debye Huckel theory of mean activity coefficient of strong electrolyte (DHLL); *Electrolyte interface:* Bjerrum theory of ion association in electrolyte solutions, Lippmann equation, determination of surface excess, structure of electrified interface, The Helmholtz –Perin Theory & Guoy–Chapman diffuse charge model of double layer, Stern Modification in the Gouy-Chapman Theory.; *Electrode:* The equilibrium exchange current density, Butler Volmer Equation, Tafel plot, high field and low field approximation, Electrodeposition and electropolymerization, *Irreversible electrode process:* Overvoltage, corrosion (mechanism, corrosion current, corrosion potential, electrochemical corrosion theory, estimation of corrosion rates prevention methods, polarization resistance, electrodeposition. Polarization Resistance

Unit III

Electrochemical Cell Reactions: Galvanic cells, half reactions and reversible electrodes, single electrode potential, thermodynamics of reversible electrodes and cells, Nernst equation, Standard Electrode potential, Electrochemical series, EMF of Galvanic cells; *Fuel Cells and Batteries:* Fuel cell and its theory, different types of fuel cell, Solid oxide fuel cells (SOFC), Polymer electrolyte fuel cell (PEM), Direct Electrolyte Fuel Cell (DEFC); *Super Capacitors:* Theory, Measurements and importance; *theories of Batteries:* Solid state batteries.

Unit IV

Polarography and Voltammetry: Principle of polarography, variations of the conventional polarographic methods, Pulse Polarography, AC polarography, square wave polarography, Anodic stripping and Cyclic voltammetry, Qualitative and quantitative application of polarography, Determination of stoichiometry and formation constants of complexes, Amperometric titrations and advantages.

Unit V

Conductors and Semiconductors: General principles of semi conductivity and semiconductors, Temperature dependence of electrical resistances, Coherent Length, Piezoelectric effect, Piezoelectric and pyroelectric materials, Fullerenes-Doped conductors, Brief idea of Electrochemistry of molten electrolytes and non-aqueous solvents.

Recommended Books:

1. Modern Electrochemistry, Vol.1&2, J.M. Bockris and A.K.N Reddy, Plenum.
2. Introduction to electrochemistry, S. Glasston, VanNostrand.
3. Electro-Analytical Chemistry, J. J. Lingane, Willey Inter science.
4. Polarography, D.R. Crow, J. V. Westwood, Methuen and Co.
5. Principle of Polarography, J. Heyrovsky, P. Zuman and L. Kuta
6. Solid state Electrochemistry, Haldil, Academic Press.
7. Electrochemistry of solids, H. Rickett, Springer Book.
8. Ions, Electrodes and Membranes, J. Koryta, Willey and Sons.

Theoretical Paper-IV (Optional)

B010904T: Atomic & Molecular Spectroscopy

Unit I

Alkaloids: General methods of structure elucidation, classification based on N-heterocyclic ring, Degradation, *Stereochemistry and synthesis*: Nicotine, Quinine, Morphine (Retrosynthesis also), Ephedrine, Reserpine (Retrosynthesis also).

Unit II

Terpenoids and Carotenoids: Classification, General methods of structure elucidation, isoprene rule; *structure, stereochemistry, synthesis*: Camphor (Retrosynthesis also), Abietic acid, Squalene, Citral, α -Terpenol, Menthol, Farnesol, Santonin, β -Carotene, Longifolene (Retrosynthesis also).

Unit III

Steroids: Basic skeleton, Diels' hydrocarbon and stereochemistry, structural determination and synthesis of cholesterol, testosterone, estrone and progesterone.

Unit IV

Prostaglandin: Occurrence, nomenclature, classification, physiological effects and synthesis of PGE₂ and PGF_{2a}.

Unit V

Proteins: Amino acids, polypeptide, structure of protein.

Nucleic acids: General structure of RNA and DNA.

Biosynthesis: Acetate hypothesis, poly- β -keto acid, meta orientation of hydroxyl group in naturally occurring phenols, biogenesis of fatty acids, mevalonic acid from acetyl coenzyme A, biosynthesis of mono, sesqui, di, tri terpenes, shikimic acid pathway for biosynthesis of aromatic ring, general biosynthesis of alkaloids.

Recommended Books:

1. Organic Chemistry, I.L. Finar Vol. I and II, ELBS.
2. Natural Products: Chemistry and Biological, J. Mann. R.S. Davidson, J.B. Hobbs, D.V. Bantrophe and J.B. Harborne, Longman, Essex.
3. Chemistry, Biological and Pharmacological Properties of Medicinal Plants from the Americas, Ed. Kurt Hostettmann. M.P. Gupta and A. Marston, Harwood Academic publishers.
4. Stereoselective Synthesis: A Practical Approach, M. Nogradi, VCH.
5. Rodds Chemistry of Carbon Compounds, Ed. S. Coffey, Elsevier.

Practical

B020906P : Chemistry Laboratory Course -III A

Credits-5

10h/Week

Course Objectives: The objective of this course to provide advanced insight about the inorganic preparations in aqueous and organic medium, colorimetry, spectrophotometry, flame photometry, qualitative analysis of ternary organic mixtures and three steps organic synthesis, interpretation of the spectral data of organic & inorganic compounds and experiments related to physical chemistry viz. potentiometry and conductometry.

INORGANIC CHEMISTRY

Inorganic preparation in aqueous and organic medium:

- i. Preparation of $K_3[Fe(C_2O_4)_3].3H_2O$
- ii. Preparation and separation of cis and trans $-[Co(en)Cl_2]$
- iii. Preparation of $CuCl_2$ DMSO and Copper glycine complex.
- iv. Preparation of Ph_3P and its complexes.
- v. Preparation of ferrocene.
- vi. Preparation of $Mn(gly)_3$

Spectroscopy: Record the spectra (UV, IR & Mass) and analyze the spectral data of the synthesized inorganic complex compounds.

Colorimetry and Spectrophotometry:

- i. Estimation of the metals in solution V, Mo, and Fe Colorimetry /Spectrophotometry.
- ii. Colorimetric and Spectrophotometric analysis: Determination of iron, copper, ammonium, phosphate, fluoride and nitrite ions.
- iii. To verify Lambert's Beer Law colorimetrically/ spectrophotometrically of inorganic compounds.

Flame Photometry:

- i. Estimation of magnesium and calcium in tap water
- ii. Estimation of calcium in calcium salt solution

ORGANIC CHEMISTRY

Qualitative Analysis: Separation purification and identification of components of ternary organic mixtures (all liquids, two liquids & one solid, all solids). Each component should not contain more than two functional groups. The student should check the purity by TLC, systematic analysis of each component leading to their final identification laying emphasis on solubility, element detection, melting point, boiling point determination, ignition test, unsaturation test, functional group test and preparation of suitable derivative.

Organic Synthesis: Three step synthesis of organic compounds.

Spectroscopy: Record the spectra (UV, IR, ^1H NMR, ^{13}C -NMR and Mass) and analyze the spectral data of synthesized organic compounds.

PHYSICAL CHEMISTRY

Potentiometry:

- i. Determination of the solubility of a sparingly soluble salt in water by EMF method.
- ii. Titration of ferrous ammonium sulphate against $\text{K}_2\text{Cr}_2\text{O}_7$ (or KMnO_4) potentiometrically and determine the formal redox potential of Fe^{2+} - Fe^{3+} system.
- iii. Find out the normality of the given HCl solution by titrating it potentiometrically with N/15 NaOH solution.

Conductometry:

- i. Determination of the strength of strong acid conductometrically by using strong alkali solution.
- ii. Determination of the strength of weak acid conductometrically by using strong alkali solution.
- iii. Determination of cell constant of the conductivity meter with the help of KCl solution.

System of Marking:-

Time: 12h

Inorganic: 33

Organic: 34

Physical: 33

Recommended Book:

1. Experimental Inorganic Chemistry by Mounir A, Malati, Horwood series in Chemical Science (Horwood publishing Chichester) 1999.
2. Inorganic Experiments, J. Derexwoolings VCH
3. Practical Inorganic Chemistry, G. Marrand, B.W. Rockett, Van Nostrand.
4. Synthesis and characterization of Inorganic compounds, W.L. Jolly, Prentice Hall
5. The systematic Identification of Organic Compounds, R.L. Shringer and D.Y. Curlin.
6. Handbook of Organic Analysis Qualitative and Quantitative, H. Clark, Adward Ar.
7. Vogel's Textbook of Practical Organic Chemistry, A.R. Tatchell, John Wiley.
8. Systematic Qualitative Organic Analysis, H. Middeton, AdwardArnoid.
9. Practical Physical Chemistry, A.M. James and F.E. Prichand, Longman.
10. Findley's Practical Physical Chemistry revised, B.P. Levitt, Longman.
11. Experimental Physical Chemistry, R.C. Das and Bebera, Tata Mc Grawhill.
12. Senior Practical Physical Chemistry, B.D. Khosla and V.S. Barg (R. Chand and Co., Delhi)
13. Experimental Physical Chemistry by D.P. Shoemaker Mc Grawhill, 7th Edition 2003.
14. Systematic Experiment in chemistry, Arun Sethi, New Age International (P) Limited.
15. Practical Physical Chemistry, B. Vishwanathan and P. S. Raghwan, Viva Books.

Semester IV

Theoretical Paper-I

B021001T: Organotransition Metal Chemistry

Unit I

Metal Carbonyls: Preparation, Structure and reactions/ properties of mononuclear and polynuclear metal carbonyls, Nature of M-CO bonding. Vibrational spectra of metal carbonyl, Principal reaction types, Verities of CO bridging; *Metal nitrosyls:* bonding, structure, Metal carbonyl-metal nitrosyl complex: Carbonyl metal hydride. vibrational spectra of metal carbonyls for structural elucidation.

Unit II

Organometallics: Nomenclature, general characteristics, Major types of transition metal to carbon bonds, Preparation stability and important reaction of transition metal alkyl and aryls; *Inorganic π -Acid ligands:* O, N, tertiary phosphine and arsines as ligands ; *Complexes of σ -donor ligands:* General methods of preparation, properties, nature of bonding and structural features of Transition metal alkenyls, alkynyls and carbines, carbines & Pi Complexes of unsaturated molecules: alkenes, alkynes, allyl, dienes, dienyl cyclopentadienyl, thenyl (arenes) complexes, Important reactions related to nucleophilic and electrophilic attack on ligands, reactions, with special reference to organic synthesis; *Transition Metal compounds with M-H bond:* Metal hydrides (Classical, non-classical), synthesis and important reactions; *Metal alkoxides:* Preparation, Properties, Structure, Industrial application.

Unit III

Organometallic Catalyst: General ideal of important catalytic steps, ligands coordination, and dissociation, and elimination, nucleophilic attack on coordinated ligands & coordinated molecular oxygen, Template synthesis, Oxidative addition, Reductive elimination and migration (insertion) reactions; *Homogeneous Catalysis:* Hydrogenation of alkenes using Wilkinson's catalyst, Hydroformylation of alkenes using Co and Rh catalysts, Carbonylation of methanol to acetic acid (Monsanto process), Oxidation of alkenes (Wacker process).

Unit IV

Metal Clusters & Micro-Macrocylic Complex: M-M multiple bonds containing binuclear, trinuclear, tetranuclear and octahedral clusters, synthesis and bonding in clusters, metal carbonyl halides, Chalcogenide clusters; Types of macrocyclic ligands, design and synthesis by coordination template effect, di and polynuclear macrocyclic complexes, Application of macrocyclic complexes.

Unit V

Fluxional Organometallic Compounds: Fluxionality and dynamic equilibria in compounds such as η^2 -olefine, α allyl and dienyl complexes; *Organometallic Compounds of Lanthanides and Actinides:* Methods of preparation, properties and structural features.

Recommended Books:

1. Advanced Inorganic Chemistry, F. A. Cotton and G. Wilkinson, John Wiley
2. Inorganic Chemistry, J. E. Huheey, Ellen A. Keiter, Richard L. Keiter, Addison Wesley Longman (Singapore) Pvt. Ltd.
3. Chemistry of the Elements, N. N. Greenwood and A. Earnshaw, Pergamon.
4. Organometallic Chemistry: A Unified Approach, R. C. Mehrotra and A. K. Singh, New Age
5. Principles of Organometallic Chemistry, G. E. Coates, M. L. H. Green, P. Powell and K. Wade, Chapman and Hall, London.
6. Comprehensive Organometallic Chemistry, Ed. E.W. Abel, Abel, F.G.A. Stone and G. Wilkinson, Pergamon.

Theoretical Paper-II

B011002T: Organic Synthesis

Unit I

Oxidation & Reduction: Different oxidative processes, Hydrocarbon alkenes, aromatic ring, saturated C-H groups (activated and inactivated) Alcohols, diols, aldehydes, ketones, carboxylic acids, amines, hydrazine, sulphide; *Reduction:* Different reductive process, Hydrocarbon-alkanes, alkenes, alkynes, aromatic rings, carbonyls-aldehyde, ketones, acids, acid derivatives, epoxides, hydrogenolysis.

Unit II

Reagents: LiAlH_4 , NaBH_4 , SnBu_3H , $\text{RhCl}(\text{PPh})_3$, $\text{IC}_6\text{H}_5(\text{OAc})_2$, SeO_2 , RuO_4 , OsO_4 , RCO_3H , HIO_4 , $\text{Pb}(\text{OAc})_4$, CH_2N_2 , NBS, R_2CuLi , LDA, DCC, 1,3-dithiane (reactivity umpolung), Me_3Si , Baker's yeast, organophosphorus compounds, ylides (S, N, P), Phase transfer catalyst, quaternary ammonium and phosphonium salts, crown ethers, Merrifield resins, DDQ, Jone's reagent, $\text{Ti}(\text{NO}_3)_3$, DIBAL, B_2H_6 , di-isoamylborane, 9-BBN.

Unit III

Asymmetric Synthesis: Stereospecific, stereoselective synthesis, Enzymatic and catalytic nexus, Enantioselective synthesis with chiral non racemic and catalysts, hydroboration with chiral boranes (IpcBH_2). $(\text{Apc})_2\text{BH}$, carbonyl group reductions and chiral complex hydride (BINAL-H). Chiral oxazaberlidines, Diastereoselective synthesis, Asymmetric synthesis involving chiral, auxiliary chiral reagent and chiral catalysis, methods of resolution, enantiomeric excess i.e., quasi racemate and optical purity.

Unit IV

Retrosynthetic Analysis: Synthons, synthetic equivalent, one group C-X and two group C-X disconnection, Disconnection (C-C, C-S, C-O) bonds, FGI, Chemoselectivity, Cyclisation reactions, synthetic strategy for formation of C-C, C-N, C-X bonds. Reversal of polarity, Amine synthesis, multistep synthesis; *Protection:* Principles, deprotection of alcohols, thiols, 1,2 and 1,3-diols, amines, carbonyls and carboxyl groups in organic synthesis.

Unit V

Synthesis of Some Complex Molecules and Green Chemistry: Application of the above in the synthesis of following compounds: Camphor, Longifolene, Cortisone, Reserpine, Vitamin D, Juvabione, Aphidicolin and Fredericamysin A; *Green Chemistry:* Basic Principle, Microwave assisted organic synthesis, Combinatorial chemistry.

Recommended Books:

1. H.O. House, Synthetic Organic Chemistry, Benjamin-Cummings Publishing Co.
2. Organic Chemistry J. Clayden, N. Greeves, S. Warren and P. Wothers, Oxford Press.
3. Organic Synthesis, Pragati Edition, Jagdamba Singh and L.D.S Yadav.
4. Some modern methods of organic synthesis, W. Carruthers, Cambridge University Press.
5. Organic Reactions and Their Mechanisms, P. S. Kalsi, New Age Science.
6. Workbook for Organic Synthesis, Stuart Warren, John Wiley & Sons.
7. Graham Solomon, T.W., Fryhle, C.B. & Snyder, S.A. Organic Chemistry, John Wiley & Sons.
8. Ram V. J.; Sethi, A.; Nath, M.; Pratap, R.; (2019), The Chemistry of Heterocycles (Nomenclature and Chemistry of three to five membered Heterocycles), Elsevier publication.
9. Ram V. J.; Sethi, A.; Nath, M.; Pratap, R.; (2019), The Chemistry of Heterocycles (Chemistry of six to eight membered N, O, S, P and Se heterocycles), Elsevier publication.

Practical-I

B021001P : Practical Based Major Research Project/ Dissertation

Credits 10

Course Objectives: The objective of this course is to develop interest of students towards major research project/ dissertation and to elevate their understanding towards experimental aspect of some targeted fields of Chemistry. Analytical ability of the students is to be developed and to train the students to work in any research group by motivating them to execute research in the area of their interest in chemical sciences.

Course Outcomes:

- CO-1. After completing this major research project/dissertation, students will learn to work independently.
- CO-2. Students will be able to plan and strategize a scientific problem, and implement it within a reasonable time frame.
- CO-3. Students will be able to know the library search and to interpret the spectral data independently.
- CO-4. Students will be able to critically examine research articles, and will improve their scientific writing as well as communication skills.
- CO-5. Students will be able to present their finding by using OHP/PPT.

For major research project work/dissertation, the area of the work would be decided by the advisor/mentor/HOD. On completion of the major research project work/dissertation, students have to submit the work in the form of a dissertation followed by oral presentation in the presence of faculty members and finally it will be evaluated by internal and external examiners followed by conducting viva voce examination.

Abha Bishnoi

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Bansal

Bansal
03.09.22
Narhar Singh

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