M.Sc. CHEMISTRY

ANALYTICAL CHEMISTRY SPECIALISATION

SYLLABUS OF III & IV SEMESTERS

REVISED AS PER NEW (CB) SYLLABUS

FOR STUDENTS ADMITTED FROM THE YEAR 2016 ONWARDS

M.Sc. CHEMISTRY (ANALYTICAL CHEMISTRY SPECIALISATION)
Syllabus for III and IV Semesters
(for the batches admitted in academic year 2016 & later under CBCS pattern)
[Under Restructured CBCS Scheme]
Grand total marks and credits (all 4 semesters) 2400 marks – 96 credits
(Approved in the P.G. BOS meeting held on 01-07-2017)

Semester - III (ANALYTICAL CHEMISTRY)
[Under CBCS Scheme]
(for the batches admitted in academic year 2016 & later under CBCS pattern)

	Hrs/week	Internal assessment	Semester exam	Total	Credits
CH(AC)301T (core)	4	20 marks	80 marks	100 marks	4
CH(AC)302T (core)	4	20 marks	80 marks	100 marks	4
CH(AC)303T (Elective)	4	20 marks	80 marks	100 marks	4
CH(AC)304T (Elective)	4	20 marks	80 marks	100 marks	4
CH(AC)351P (LAB-I)	9			100 marks	4
CH(AC)352P (LAB-II)	9		100 marks	4	
Total				**600 marks**	**24**

Semester - IV (ANALYTICAL CHEMISTRY)

	Hrs/week	Internal assessment	Semester exam	Total	Credits
CH(AC)401T (core)	4	20 marks	80 marks	100 marks	4
CH(AC)402T (core)	4	20 marks	80 marks	100 marks	4
CH(AC)403T (Elective)	4	20 marks	80 marks	100 marks	4
CH(AC)404T (Elective)	4	20 marks	80 marks	100 marks	4
CH(AC)451P (LAB-I)	9			100 marks	4
CH(AC)452P (LAB-II)	9		100 marks	4	
Total				**600 marks**	**24**

Grand total marks and credits (all 4 semesters) 2400 marks - 96 credits

M.Sc.ANALYTICAL CHEMISTRY

Semester III

Paper I :CH (AC) 301T: CORE :
Sampling, Data handling, Classical and Atomic spectral methods of analysis
AC-1:Sampling & Data handling
AC-2:Titrimetric & Gravimetric analysis
AC-3:Thermal & Radiochemical methods of analysis
AC-4:Atomic Spectroscopy

Paper II:CH (AC) 302T:CORE :
Spectroscopic methods of Analysis-I
AC-5: Multinuclear NMR
AC-6: Advanced NMR
AC-7: Electron Spin Resonance Spectroscopy
AC-8: Mossbauer and NQR

Paper III:CH (AC) 303T: ELECTIVE IIIa:
Miscellaneous Methods of Analysis
AC- 9 :Surface Analysis Methods
AC-10: Diffraction Methods, X-Ray Absorption and X-Ray Fluorescence
AC-11 : Electroanalytical Methods
AC-12 :Micromeritics, Dissolution and disintegration

Paper III:CH (AC) 303T: ELECTIVE IIIb:
Bonding, Group Theory and its Applications
AC-09: Group Theory, Normal mode analysis and Specral activity
AC-10: MOT of Metal Complexes
AC-11: Electronic Spectroscopy of Metal Complexes
AC-12: IR and Raman Spectroscop

Paper IV:CH (AC) 304T: ELECTIVE IVa:
Applied Aalysis
AC-13: Industrial Analysis
AC-14:Analysis of Air and Water Pollutants
AC-15:Clinical and Pharmaceutical analysis
AC-16:Food and Agricultural analysis

Paper-IV: CH(IC) 304T: ELECTIVE IVb
Nuclear Chemistry, Zeolites, Solid State, and
Surface Chemistry
AC-13: Nuclear Chemistry
AC-14: Zeolites and Molecular Sieves
AC-15: Solid State Chemistry
AC-16: Surface Chemistry & Superconductors

LABORATORY COURSE
Paper CH (AC) 351P: Titrimetry, Solvent extraction,Chromatography and Water analysis.

Paper CH (AC) 352P: Colorimetry, Spectrophotometry

Semester IV

Paper I:CH (AC) 401T: CORE :Spectroscopic Methods of Analysis-II
AC-17: U.V. visible spectroscopy,
AC-18: IR & Raman spectroscopy
AC-19: Optical Methods
AC-20:Fluorimetry, Phosphorimetry,Nephelometry and Turidimetry

Paper II:CH (AC) 402T:CORE Separation Methods
AC-21:Solvent extractions
AC-22:Chromatography
AC-23:Mass spectrometry & Hyphenated techniques
AC-24:Electrophoresis

Paper III:CH (AC) 403T:ELECTIVE IIIa: Laboratory Management
AC-25:Automation in laboratory
AC-26:LIMS & Computer aided analysis
AC-27:Laboratory Management & Standard reference materials
AC-28:Accreditation of Laboratories, Quality management

Paper IV:CH(AC) 403T: ELECTIVE IIIbApplied analysis and Green Analytical Chemistry
AC-25: Enzyme catalysis- Analytical applications
AC-26:Forensic Chemical Analysis
AC-27: Limit tests
AC-28:Green Analytical Chemistry

Paper IV:CH (AC)404 T:Ida Quality Assurance and Accreditation
AC-29: Quality Assurance – I
AC-30: Quality Assurance – II
AC-31: Quality Assurance – III
AC-32: Quality Accreditation

Paper IV:CH (AC)404 T:IDb
Inorganic Material Chemistry
AC-29:Composite Materials
AC-30:Liquid Crystals
AC-31:Explosives and Propellants
AC-32:Fuels and Combustion

Paper CH (AC) 451P: Electro analytical techniques:

Paper CH (AC) 452P: Spectroscopy and Evaluation of Physical Parameters Of Tablets

M.Sc. ANALYTICAL CHEMISTRY SPECIALIZATION

Syllabus for III and IV Semesters

III Semester Syllabus

Paper- I: CH (AC) 301T: CORE :Sampling, Data handling, Classical and Atomic spectral methods ofanalysis

AC – 01 Sampling & Data handling

AC – 02 Titrimetric & Gravimetric analysis

AC – 03 Thermal & Radiochemical methods of analysis

AC – 04 Atomic Spectroscopy

AC – 01 Sampling & Data handling 15 Hrs

Classification of Analytical Methods. Types of samples, Preparation of sample for analysis, effect of sampling uncertainties, sample treatment, moisture in sample, decomposition of organic & inorganic compounds, procedure of sampling of solids, liquids and gases.

Errors and Evaluation:-Accuracy, precision, sensitivity, detection limits, significant figures, rounding off. Types of errors – determinate and indeterminate errors. Ways of expressing accuracy, absolute and relative errors. Significant figures and propagation of errors. Confidence limit, Test of significance – the F-test and T-test. The statistical Q-test for rejection of a result, statistics for small data sets. Linear least squares method. The correlation coefficient. Calculation for the above parameters.

AC – 02 Titrimetric and Gravimetric Analyses 15 Hrs

Redox titrations: Formal and Standard potentials in various media, standardization, Oxidizing systems: Mn(VII), Ce(IV), Cr(VI). V(V). Reducing systems: V(II), Ti(III), Sn(II), Fe(II) in H_3PO_4. Detection of end point in redox titrations – selection of suitable indicator.

Complexometric titrations: Introduction, stability constants of EDTA complexes, titration curves, types of EDTA titrations with examples. Standard EDTA solutions, some practical considerations during EDTA titrations. Titration of mixtures (Mg^{2+}&Ca^{2+}; Pb^{2+}&Ca^{2+}; Mn^{2+}&Mg^{2+}), selectivity, masking and demasking agents. Metal ion indicators: General properties, theory of the use of metal ion indicators, use of Murexide, Eriochrome black- T, Calcon, Xylenol orange, Methyl thymol blue, Fast sulphon black- F.

Gravimetric Analysis: Theory, principles, precipitation reagents (DMG, Oxine), Determination of Nickel as dimethylglyoximate, Aluminium as 8-hydroxyquinolate & Chloride as silver chloride.

AC – 03 Thermal and Radiochemical methods of Analysis 15 Hrs

Thermal methods of analysis: Thermogravimetry, Differential Thermal Analysis and Differential Scanning Calorimetry, instrumentation. Methodology of TG, DTA and DSC.Application of TG to study of oxalates and chromates. Determination of Glass transition, Heat capacity determination, Characterization of polymer blends. Problems based on decomposition path way and % composition. Evolved gas analysis.

Thermometric titrimetry – theory, instrumentation, applications.

Radiochemical methods of analysis: Radioactive tracer techniques and its applications, isotope dilution analysis, neutron activation analysis, radiometric titrations: principle, theory, applications and problems.

AC – 04 Atomic Spectroscopy 15 Hrs

Atomic Absorption Spectroscopy (AAS): Principles of AAS, Instrumentation – flame AAS and furnace AAS, resonance line sources, sensitivity and detection limits in AAS, interferences –chemical and spectral, evaluation methods in AAS and applications in qualitative and quantitative analysis.

Atomic Emission Spectroscopy (AES): Principle of AES, Instrumentation, Interferences, evaluation methods, Application in quantitative analysis.

Inductively Coupled Plasma- Atomic Emission Spectroscopy (ICP-AES): Limitations of AES, Principles of plasma spectroscopy, plasma as an excitation source. Inductively coupled plasma source, ICP-AES – Instrumentation. Applications of ICP-AES.Comparison with AAS.

Suggested Books

1. Principles of Instrumental Analysis - Skoog, Holler, Nieman, 5th ed., Harcourt CollegePublishers, 1998.
2. Analytical Chemistry – Gary D. Christian, 6th ed., John Wiley and sons. Inc., New York1994.
3. Instrumental methods of Analysis - Willard, Merit, Dean, 6th ed., CBS Publishers &distributors, 1986.
4. Hand Book for Instrumental Techniques for Analytical Chemistry, Ed. Frank Settle,Prentice Hall, New Jersey, USA, 1997.
5. Vogel's Text book of Quantitative Analysis – GJ Jeffery, J Bassett et al, 5th ed.,Longmann, ELBS Publications, 2000.
6. Principles and practice of Analytical Chemistry, F.W.Fifield & D Kealey, 5th Ed.Blackwell Science, 2000.
7. Quantitative Chemical Analysis, Daniel C. Harris, 6th Ed. WH Freeman & Co. NewYork,2003.
8. Analytical Chemistry An Introduction, Crouch, 7th Ed. Saunders CollegePublishing,2000.
9. Organic Analytical Chemistry theory and practice, Jag Mohan, Narosa Publications,2003.
10. Pharmaceutical analysis,. Watson
11. Electronic Absorpption Spectroscopy and related techniques, D.N.Satyanarayana, University Press, 2001.

Paper-II: CH (AC) 302T: CORE :Spectroscopic methods of Analysis-I
AC – 05 Multinuclear NMR
AC – 06 Advanced NMR
AC – 07 Electron Spin Resonance Spectroscopy
AC – 08 Mossbauer and NQR

AC – 05 Multinuclear NMR

^{13}C nmr spectroscopy: CW and PFT techniques. Types of 13C nmr spectra: undecoupled, proton- decoupled, single frequency off-resonance decoupled (SFORD) and selectively decoupled spectra. ^{13}C chemical shifts, factors affecting the chemical shifts

Chemical equivalence and magnetic equivalence. Virtual Coupling and its importance in study of Metal Complexes $[Pd\{P(CH_3)_3\}_2I_2]$. Spin Dilute Systems-Satellites in Pt(II) Complexes cis-$[Pt(PEt_3)_2Cl_2]$, $Sn(CH_3)_4$. NMR Time Scale and its use in studying Stereo chemical Non –rigidity (PF_5, $[Rh(PR_3)_5]^+$, $[Rh\{Cp\}_2(CO)_2]$) -ΔR, the Ring Contribution to ^{31}P Chemical Shifts –Metal and Chelate size on ΔR. Applications of ^1H, ^{13}C, ^{19}F, ^{31}P and ^{15}N to simple inorganic and Coordination Compounds - 1)^{1}H-NMR: $PtHCl(PEt_3)_2$, $Pt(NH_3)_3(CH_3)_3$, BH_4^-, NH_4^+, CH_3CN, [^{6}h- C_7H_8 $Mo(CO)_3$], [^{7}h-$C_7H_7Mo(CO)_3]^+$, B_2H_6; $^{29}SiH_3SiH_3$, 2)^{19}F: BF_4^-, H_2PF_3; 3)^{31}P: $Mo(CO)_3(PPh_3)_3$, [Rh $(PPh_3)_3Cl$] ,trans-$[PtCl_4(PEt_3)_2]$, $^{31}PF_2H(^{15}NH_2)_2$ 4) 13C; [^{4}h C_8H_8 $Ru(CO)_3$], $Fe(CO)_5$, $Fe_2(CO)_9$, $Fe_3(CO)_{12}$, $FeICp(CO)_2$, $Cl(CH_2)_3Si(OCH_3)_3$, [$^{13}C^{15}N$ $Co(DH)_2$Pyridine]. $^{13}C\{^1H\}$ NMR spectrum of σ-bonded C_6H_5 ligand

AC – 06 Advanced NMR Spectroscopy:- Spin-Lattice (T_1) and Spin-Spin Relaxation (T_2). pin Echo Polarization Transfer – Spin Echo Measurements. ^{13}C-NMR spectral editing techniques: Attached proton test (APT spectra) by Gated Spin Echo, Cross polarization, INEPT spectra, DEPT spectra (Distortionless enhancement by polarization transfer) (eg $Cl(CH_2)_3Si(OCH_3)_3$). INADEQUATE spectra (Incredible Natural Abundance Double Quantum Transfer Experiment).

Two Dimensional NMR: Basic principles, Types of 2-D NMR ;i)J- resolved spectroscopy a)homo and b)Heteronuclear J- resolved spectroscopy ii) Correlation spectroscopy ; Homo nuclear shift correlation spectroscopy (COSY) and Hetero nuclear shift correlation spectroscopy (HETCOR) iii) NOESY(Nuclear Overhauser Enhancement Spectroscopy). HOESY (two dimensional heteronuclear NOE). Advantages of 2-D NMR

AC – 07 Electron Spin Resonance Spectroscopy

Principle- Selection Rules – Instrumentation- Microwave source(energy bands). Application of ESR to the study of simple free radicals: methyl (CH_3)., amine (NH_2)., diphenyl picryl hydrazyl, cyclopentadienyl (C_5H_5)., hydroxy methyl(CH_2OH).radicals. Zero-Field Splitting (ZFS) - Effective Spin - Orbitally Non-degenerate and Degenerate States. ESR Spectra of d^1-d^9 Transition Metal Complexes with examples. Interpretation of g in cubic ,axial and rhombohedral geometries. Factors affecting g values. Calculation of g values with simple examples. Intensities of ‘g$\parallel$ and g$\perp$ peaks . Evidence for Metal-Ligand Bond

Covalency- Cu(II)- Bis –Salicylaldimine. $[(NH_3)_5\ Co\ O_2\ Co\ (NH_3)_5]^{5+}$, Cu(II)- diethyldithio phosphinate, Vanadyl dithio phsphinate, Copper(II) tetraphenyl porphyrin, Co(II)-phthalocyanine, $K_2[IrCl_6]$. Interpretation of 'g' and 'A' values from esr spectral data in- i) MnF_6^{4-}, ii) CoF_6^{4-}, and CrF_6^{3-}. ESR spectra of dinuclear Cu (II) complexes.

AC – 08 Mossbauer and Nuclear Quadrupole Resonance Spectroscopy

Mossbauer Spectroscopy:Principle, Experimental Considerations and Presentation of the Spectrum - Isomer Shifts – Quadrupole splitting and Magnetic hyperfine splitting - Selection Rules.

Applications

Iron Compounds: Low-spin and High-spin Fe(II) and Fe(III) Complexes - π-bonding Effects in Iron complexes - Study of High-spin Low-spin Cross-over c) Diamagnetic and Covalent Compounds - Structural aspects of Iron Carbonyls and Iron-Sulfur Proteins

Tin Compounds: Tin Halides and Organotin Compounds.

Iodine Compounds: Isomer Shifts of ^{127}I and ^{129}I – Applications to Alkali metal iodides and Molecular Iodine. .

Nuclear Quadrupole Resonance Spectroscopy : Principle, nuclear quadrupole resonance experiment, structural information from NQR spectra, Interpretation of nuclear quadrupole coupling constants.

SUGGESTED BOOKS

1. Structural Methods in Inorganic Chemistry, E. A. V. Ebsworth, D. W. H. Rankin and S. Craddock, ELBS.
2. Physical Methods in Chemistry, R. S. Drago, W.B. Saunders Co., 1977.
3. Physical Methods for Chemists, Russell S. Drago Second edition, Saunders College Publishing, 1992.
4. Principles of Mossbauer spectroscopy, T. C. Gibb, Chapman and Hall, London, 1976.
5. Mossbauer Spectroscopy, N. N. Greenwood and T. C. Gibb, Chapman and Hall, London, 1971.
6. Principles of Instrumental Analysis, Skoog, Holler and Nieman.
7. Instrumental Techniques for Analytical Chemistry, Frank Settle.
8. Principles of Analytical Chemistry, M. Valcarcel.
9. Physical Methods in Advanced Inorganic Chemistry, Hill and Day
10. Magneto Chemistry, Dutta & Shyamal
11. Oxford Chemistry Primers, Vol 62

Paper-III CH (AC) 303T: ELECTIVE IIIa: Miscellaneous Methods of Analysis

AC – 09 Surface Analysis Methods
AC – 10 Diffraction Methods, X-Ray Absorption and X-Ray Fluorescence
AC –11 Electroanalytical Methods
AC – 12 Micromeritics, Dissolution and disintegration

AC-09Surface Analysis Methods 15 Hrs

Introduction, types of surface measurements.

Photon Probe Tecnhniques: X-Ray Photoelectron spectroscopy - Principle, Instrumentation, applications.

Electron Probe Techniques: Scanning electron microscopy (SEM) – Principle, Instrumentation, applications. Electron Probe X-ray analysis (EPXMA) - Principle, Instrumentation, applications. Auger electron spectroscopy (AES) - Principle, Instrumentation, applications.

Ion Probe Techniques: Rutherford backscattering spectrometry (RBS) - Principle, Instrumentation, applications. Secondary ion mass spectrometry (SIMS) – Fundamental aspects of sputtering, Principle, Instrumentation (static & dynamic), applications

Scanning probe microscopy Techniques: Scanning Tunneling Microscopy – Principle, Instrumentation, applications. Atomic Force Microscopy - Principle, Instrumentation, applications.

AC-10 : Diffraction Methods, X-Ray Absorption and X-Ray Fluorescence 15 Hrs

X – ray Diffraction : X –rays and their generation – choice of radiation; Miller indices, Braggs equation, Experimental methods – Powder and single crystal methods, Indexing the reflections, Systematic absences, Electron density studies by X – rays – Platinum phthalocyanine complex, Silyl acetate, Tetraalkyl biphosphate; Advantages and limitations of X – ray Diffraction.

Electron Diffraction by gases: Principles, Applications to Silyl monothioacetate and Germyl monothioacetate and $HgCl_2$ molecules, Advantages and Limitations

Neutron Diffraction: Principle, Application in Hydrogen bonding studies, Advantages and limitations.

X-ray absorption method: Principle, radiographic non-dispersive x-ray Absorptiometers

X-ray fluorescence method: Instrumentation, qualitative and quantitative applications of XRF– advantages and limitations.

AC-11: Electro Analytical Methods 15 Hrs

pH-metry: Accuracy of direct potentiometer measurements. The Glass pH electrode – Theory, construction, standard buffers, accuracy of pH measurements, measurements with the pH – meter, pH titration of unknown soda ash.

Electrogravimetry: Basic principles of electrogravimetry, Instrumentation, electrogravimetry determination with constant applied voltage and at constant current. Applications of electrogravimetry. Problems based on effect of concentration on electrode potentials, calculation of theoretical cathode potential at the start of deposition, effect of pH in electrolytic separations.

Coulometry: Basic principles, Types of coulometers, constant current coulometric analysis, coulometric titrations – principle, circuit and cell for coulometry, Application to neutralization, Redox, precipitation, complexometric titrations, Advantages of coulometric

titrations and errors. Controlled potential coulometry – Technique & applications of inorganic & organic compounds.

High Frequency Titrations
Introduction, Theory, Instrumentation, Applications, Advantages and disadvantages

AC-12:Micromeritics,Dissolution and disintegration 15 Hrs
Particle size analysis- concepts of particle size, size distribution, mean size of particulate system, methods of particle size analysis (sieving, microscopic method, sedimentation methods, electrical sensing zone method, optical sensing zone and light diffraction method). Dissolution: Drug absorption, theories of drug dissolution – Diffusion layer model, Danckwert's model & interfacial barrier model. Dissolution tests for tablets and capsules (basket apparatus, paddle apparatus, flow through cell apparatus).Disintegration tests for tablets, capsules and enteric coated tablets.

Suggested Books
1. Structural methods in Inorganic Chemistry - E.A.V. Ebsworth, et al., ELBS Publications, 1988.
2. Physical Methods in Chemistry - R.S. Drago, W.B. Saunders Co, 1977.
3. Instrumental Methods & Chemical Analysis – Galen Ewing, 5th ed., McGraw-Hill Publishing Company Ltd., 1985.
4. Analytical Chemistry - Gary D. Christian, 6th ed. John Wiley and sons. Inc, New York, 1994.
5. Principles of Instrumental Analysis – Skoog, Holler, Nieman, 5th ed., Harcourt College Publishers, 1998
6. Principles and practice of Analytical Chemistry, F.W.Fifield & D Kealey, 5th Ed. Blackwell Science, 2000.
7. Quantitative Chemical Analysis, Daniel C. Harris, 6th Ed. WH Freeman & Co. NewYork, 2003.

CH(AC)303T: ELECTIVE IIIb :Bonding, Group Theory and its Applications

AC-09: Group Theory, Normal mode analysis and Spectral Activity
AC-10: MOT of Metal Complexes
AC-11: Electronic Spectroscopy of Metal Complexes
AC-12: IR and Raman Spectroscopy

AC-09: Group Theory, Normal Mode Analysis and Spectral Activity

Properties of a Group-Closure rule, Identity rule, associative rule, inverse rule, Abelian and Non-abelian groups. Classes of Symmetry Elements of a Group: Similarity transformation, properties of conjugate elements, rules of Classes, Classes of C_{2v}, C_{2h} and C_{3v}. Matrix Representation of Symmetry Elements: Simple Matrices, Matrix addition, subtraction and multiplication, Block-Factorization. Matrix Representation of *E, C_n, S_n*, i and σElements and C_{2v}, C_{3v}, C_{2h}, C_{4v} & D_{2h}.Great Orhogonality Theorem: Reducible and Irreducible Representations, Properties of Irreducible Representations, Construction of Character Tables for C_{2v}, C_{2h} and C_{3v}. Mulliken Symbolism for Irreducible Representations - Standard Reduction Formula – Direct Products.

Use of Character tables for IR & Raman spectroscopy, symmetry based selection rules for for IR and Raman activity. Standard reduction formula. Type and Symmetry of Normal Modes and IR and Raman activity of molecules: Cartesian coordinate method of analysis for C_{2v} (eg H_2O/SO_2, SF_4, ClF_3, Cis-N_2F_2), C_3V ($NH_3/SO_3^{2-}/PCl_3$, $POCl_3$), C_{2h} (trans-N_2F_2), D_{3h} (CO_3^{2-}/BF_3), Td($SO_4^{2-}/PO_4^{3-}/ClO_4^-/NH_4^+$), Oh ($SF_6$). Internal coordinate method of analysis for C_{2v}(H_2O), C_3V (NH_3), Td (SO_4^{2-}). Internal Coordinates and Redundancy (Qualitative concept).

AC-10: Molecular Orbital Theory of Metal Complexes

Symmetry Classification of Metal and Ligand Orbitals in Cubic and Non-Cubic Environments: Octahedral, Tetrahedral, Square Planar, Square Pyramidal, Trigonal Bipyramidal Geometries – Concept of Ligand Group Orbitals – Construction of Molecular Orbital Energy Level Diagrams for Octahedral, Tetrahedral and Square Planar Metal Complexes with Sigma (σ) and Pi (π) Bonding Contribution from the Ligands.

AC-11: Electronic Spectroscopy of Metal Complexes

Classification of Electronic Spectra for Metal Complexes, Selection Rules: Electric Dipole Transitions, Magnetic Dipole Transitions, Orbital Selection Rules, Spin Selection Rules, Relaxation in Selection Rules. Nature of Electronic Spectral Bands: Band Widths, Band Intensities. Factors Influencing Band Shapes: Jahn-Teller Effect, Spectrochemical Series, Nephelauxetic Effect. Orgel Diagrams for d^1-d^9 Configurations, Crystal Field Spectra of O_h and T_d Metal Complexes of 3d Metals. Charge Transfer Spectra. Strong Field Configurations: The Method of Descending Symmetry, Correlation Diagrams and Tanabe-Sugano Diagrams for d^2 and d^8 Configurations. Calculation of 10Dq Values, Racah Parameter (B) and Nephelauxetic Ratio (β) .

AC-12: Infrared and Raman Spectroscopy

Conditions for Infrared and Raman Spectroscopies – Structure Fitting. Determination of Coordination Sites and Linkage Isomers(NO_2^-, SCN^-), Assigning Denticity of Ligands (SO_4^{2-}, CO_3^{2-}), Prediction of Diagnostic Fundamentals in Isomers of Metal Complexes and Distinguishing Isomers of Metal Complexes. Effect of Coordination on Ligand Vibrations: Examples involving Mono, Bi and/or Polydentate Ligands of Oxygen, Sulfur, Nitrogen, Phosphorous, Carbon and Halogen Donors (NH_3, H_2O, Glycine, PPh_3, 2,2,-Bipy, 1,10-Phen, Carbonyl and halides). Raman effect and molecular structure- CO, HCN, CO_2, N_2O, H_2O.

Principles of Resonance Raman Spectroscopy.Application of Resonance Raman Spectroscopy to Structural Elucidation of the active Sites of Heme and Non-Heme Oxygen Carriers.

SUGGESTED BOOKS

1. *Symmetry and Spectroscopy of Molecules*, K. Veera Reddy, Second Edition, New Age International (P) Limited Publishers (2009)
2. *Chemical Applications of Group Theory,* F. A. Cotton, 3rd edition, Wiley NY (1990)
3. *Symmetry and Group Theory In Chemistry*, Mark Ladd, Harwood Publishers, London (2000)
4. *Symmetry Through the Eyes of a Chemist,* I. Hargittai and M. Hargittai, 2nd Edition, Plenum Press, NY (1995)
5. *Molecular Symmetry and Group Theory,* Robert L. Carter, John Wiley & Sons (1998)
6. *Group Theory for Chemists,* G. Davidson, Macmillan Physical Science Series (1991)
7. *Molecular Symmetry,* Schoenland
8. *Electronic Spectroscopy,* A. B. P. Lever
9. *Introduction to Ligand fields,* B. N. Figgis
10. *Infrared and Raman Spectroscopy of Inorganic and Coordination Compounds,* K. Nakamoto
11. *Infrared spectroscopy of Inorganic Compound,* Bellamy.

Paper -IV CH(AC) 304T: ELECTIVE IVa:Applied Analysis
AC –13 Industrial Analysis
AC –14Analysis of Air and Water Pollutants
AC – 15 Clinical and Pharmaceutical analysis
AC – 16 Food and Agricultural analysis

AC –13 Industrial Analysis 15 Hrs

Analysis of Ferroalloys: Analysis of steel - Molybdenum, Phosphorous. Analysis ofFerromanganese, Ferrovanadium. **Analysis of non- Ferrous alloys**: Analysis of Tin, Zinc andCopper in Brass, Bronze. Analysis of Tin and lead in Solder.**Analysis of Cement**: Composition of Portland cement, estimation of Aluminium oxide andFerrous oxide. Determination of Alumina in Cement by Polarography.**Analysis of Oils & Fats:** Theory, Melting point of fats, Chemical Characteristics:Saponification value, Iodine value, Thiocyanogen value, ketone or perfume rancidity. Analysisof fatty acid composition in oil by GLC, Oxidation levels of fats by TLC.**Soaps & Detergents:** Composition of Soaps. Determination of low level Surfactants,determination of Germicides in soaps and detergents by photometric method, analysis ofphosphates by paper chromatography, determination of detergent alkylates by MassSpectrometry.**Paints& Pigments**: Constituents of Paints, Analysis of Tio_2 in Titanium dioxide pigments byXRD. Determination of Zn, Pb in Paint pigments by Polarographic method. Analysis ofpolyesters, acrylics by Gel permeation chromatography.

AC-14 : Analysis of Air and Water Pollutants 15 Hrs

Analysis of Air Pollutants: Air quality standards, sampling, analysis of air pollutants-SO_2 (UV_Vis, IR), H_2S (Spectrophotometry and Non-dispersive IR Spectrophotometry), NO-NOx (Chemiluminescence technique, Colorimetric technique- Saltzman method), CO & CO_2 (IR, AAS & GC), Hydrocarbons (GC, GC-MS), Aromatic hydrocarbons in automobile exhaust, petrol, air, O_3 (Chemiluminiscence & Spectrophotometry), particulate matter analysis.

Analysis of Water Pollutants: Objectives of analysis, sampling, preservation and pre-concentration methods, physical analysis - colour, odour, temperature, pH, EC, redox potential, total desolved solids (turbidimetry), Chemical analysis of anions – CN-, Cl-, F-, NO_2^-, NO_3^- (spectrophotometry), SO_4^{2-}, PO_4^{3-}. Determination of BOD, COD, TOC & DO.
Analysis of Toxic Metals: Hg, As, Pb, Cd, Be, Al, Cr (Atomic Absorption Spectroscopy and Spectrophotometry)

AC-15 : Clinical and Pharmaceutical Analysis 15 Hrs

Clinical Analysis: Determination of (1) Serum Calcium (2) Serum/Plasma Bicarbonate (Titrimetry). (3) Serum sodium and potassium (Flamephotometry). Determination of Serum Chloride (Coulometry) - Determination of (1) Cholesterol (2) Total Protein (3) Blood Urea in Serum (4) Amylase (5) Aspartate Amino Transferase (AST) and Alanine Amino Transferase (ALT) (by Spectrophotometry). Determination of (1) Thyroxin and (2) Thyroid-Stimulating Hormone (TSH)(by RIA Method)

Pharmaceutical analysis: Determination of Diclofenac (non-aqueous titration), Calcium in Vitamin D and Calcium formulations (Complexometry), Sulphanilamide (potentiometry), Pethidine hydrochloride (UV-Vis), Frusemide (UV-Vis), Aspirin,paracetamol and codein in APC tablets (NMR), Phenobarbitone in tablets (IR), pivolic acid in dipivefrin eye drops(GC),

Assay of hydrocortisone cream. (HPLC). Impurity profiling of Propranolol (GC-MS), famotidine (LC-MS).

AC -16:Food and Agricultural Analysis 15 Hrs

Food Analysis: Analysis of Chemical Additives in foods : Division of colour additives, Chromatographic identification of colours, and quantitative estimation of added dyes in foods (Titanium Trichloride Method) - chemical preservatives and synthetic sweetening agents (Organic-ether extractable and Non-ether extractable) - Analysis of SO_2 & Sodium Benzoate (Chemical Methods), Sorbic Acid (Chromatography) - Types of Antioxidants used in Foods, Analysis of Butylated Hydroxy Toluene (BHT) (Spectrophotometry).

Agricultural Analysis: Analysis of soils for available Major Nutrients - Estimation of available Nitrogen (Kjeldahl Method), Phosphorus (Olsen's Method and Bray and Kurtz Method), and Exchangeable Calcium & Magnesium (by EDTA). Soil analysis for Micronutrients - Estimation of Available Zinc, Copper, Manganese and Iron (AAS) - Analysis of Pesticide Residues - Determination of Methyl Parathion Residues in food grains & vegetables (Solvent Extraction and Titrimetry) - Determination of Organochlorine pesticides by Gas Chromatography (Cypermethrin) - Determination of Malathion and DDT Residues in food grains (Spectrophotometry).

SUGGESTED BOOKS

1. Analytical Chemistry, Gary Christian, VI Ed, John Wiley & Sons Inc, New York
2. Fundamentals of Analytcal Chemistry, Skoog & West
3. Pharmaceutical Drug Analysis, Ashtoshkar
4. Vogel's Text Book of Quantitative Chemical Analysis, 6th Ed, Pearson Education Ltd
5. Environmental Pollution Analysis, S M Khopkar, Wiley Eastern Ltd 1995
6. Environmental Analytical Chemistry, F W Fifield, P J Haines, Blackie Academic& Professional.
7. Environmental Chemistry, B K Sharma, Goel Publishing House, Meerut.
8. Handbook of Analysis and quality control for fruit and vegetable products, S Ranganna, Tata Mc Graw Hill Publishers Ltd, 1986
9. Introduction to chemical analysis of foods, S Suzanna & Nielsen, CBS Publishers & Distributors
10. Practical pharmaceutical Chemistry, a H Beckett and J B Stenlake, III Ed, Vol I and Vol II, CBS Publishers & Distributors,1997
11. Pharmaceutical Analysis, David G Watson,Churchill Livingstone Harcourt Brace and Company Ltd, 1999
12. Handbook of analysis of drugs, Nagavi
13. Medical Laboratory Technology – Mukherjee , Tata Mc Graw Ltd 1988.
14. Medical Laboratory Technology – Ramnik Sood , Jaypee Brothers Ltd 1999.
15. Text Book of Clinical Chemistry V Edn Carl.A. Burtis Edward R. Ashwood Saunders Harcourt India 2001.

Paper -IV CH(AC) 304T: ELECTIVE IVb: Nuclear Chemistry, Zeolites, Solid State and Surface Chemistry

AC-13: Nuclear Chemistry
AC-14: Zeolites and Molecular Sieves
AC-15: Solid State Chemistry
AC-16: Surface Chemistry & Superconductors

AC-13: Nuclear Chemistry

Introduction: The atomic nucleus-elementary particles, quarks, classification of nuclides based on Z and N values, nuclear stability, nuclear potential, binding energy.

Nuclear structure: Shell model-salient features, forms of the nuclear potential, magic numbers, filling of orbitals, nuclear configuration, Liquid drop model, Fermi gas model, Collective model and Optical model.

Nuclear reactors :- General aspects of reactor design, thermal, fast and intermediate reactors, reactor fuel materials, reactor moderators and reflects, coolants, control materials, shield, regeneration and breeding of fissile matter, types of research reactors.

Nuclear reactions, fission and fusion, radio-analytical

Radioactivity, radioactive decay kinetics, Parent-daughter decay-growth relationship-secular and transient equilibria, theories of α, β-, β+ and γ-decay, internal conversion, Auger effect. Radio isotopes & its applications.

AC-14: Zeolites and Molecular Sieves

Introduction to porous materials:

Classification into micro-, meso- and macro porous materials, the origin of pores and its significance, distinction from condensed materials.

Zeolites:

Definition, natural and synthetic zeolite or aluminosilicates, the primary and secondary building blocks, final framework structures, Lowensteins rule, sodalite and other structures, Nomenclature: Atlas of zeolite; structural distinctions, Novel zeolites, examplels of small, medium, large and extra large pore zeolites; general properties and application of molecular sieves.

Characterization of zeolite:

XRD, SEM and other techniques; spectral techniques: FT-IR and solid-state NMR; sorption capacity, surface area by BET method, pore volume and pore structure, the origin of Brönsted and lewis acidity in zeolites, the number and the strength, techniques for the estimation of acidity: adsorption of bases and IR spectra, temperature programmed desorption of bases.

AC-15: Solid State Chemistry

Electronic structure of solids and band theory, Fermi level, K Space and Brillouin Zones.

Structure of ionic Crystals & Compounds: Ionic Crystals with stoichiometry MX, Ionic Crystals with stoichiometry MX2, spinel structure, perovskite structure. AB [nickel arsenide (NiAs)], AB2 [fluorite (CaF2) and anti-fluorite structures, rutile (TiO2) structure and layer structure [cadmium chloride and iodide (CdCl2, CdI2)].

Crystal Defects and non-stoichiometry:

Classification of Defects: subatomic, atomic and lattice defects in solids; Thermodynamics of vacancy in metals; Thermodynamics of Schottky defects in ionic solids ; Thermodynamics of Frenkel defects in silver halides; Calculation of number of defects and average energy

required for defect, Other examples of defect structure; Non-stoichiometry and its classifications.
Preparative method of solids:
Introduction, Ceramic method, microwave synthesis, Precursor method, Hydrothermal method, Chemical vapour deposition (CVD) Method, Chemical vapour Transport, Choosing a method for solids.
Crystal Growth: law governing nucleation; Growth of nuclei; Reaction between two solids; Improving the reactivity of solids; Zone refining method; Crystal growth.

AC-16: Surface Chemistry & Superconductors
Surface Chemistry:
Mechanism of catalytic reactions on the surfaces – diffusion of reactants to the surfaces, adsorption of reactants, reaction within the adsorbed layer, desorption of the products, diffusion of the products away from the surface; The mechanism of chemisorption on metals – The formation of chemisorptions layer, the character and nature of the chemisorption bond, the mechanism of chemisorptions for some gases; Nature of adsorbates on surfaces.
Superconductors:
Discovery of super conductors, Meissner effect, Type I and II conductors, Leavitation, BCS theory and Cooper pairs, High Tc Super Conductors, applications of super conductors.

SUGGESTED BOOKS
1. Essentials of nuclear chemistry, 4th edition; H. J. Arniker, NAIL publishers (1995); Chapters 1, 3 and 4.
2. Nuclear and Radioactive chemistry; Friedlander, Kennedy and Miller; Chapters 8 and 9.
3. Introduction to zeolite science and practice, H. Van Bekkum, E. M. Flanigen, P. A. Jacobs and J. C. Jansen (Elseviver Pub. Amsterdam, 2001)
4. Breck.D.w. Zeolites molecular sieves- Structure, chemistry and use. John Wiley & Sons N.Y. (1974).
5. Solid-State Chemistry an Introduction (2nd Edition) – Lasley Smart and Elaine Moore (Chapman & Hall 1996)
6. Solid State Chemistry- D.K.Chakraborty (New Age International Pvt.Ltd.New Delhi, 2000)
7. Introduction to Soilds-L.V.Azaroff (tata McGraw Hill Publication Ltd. New York)
8. Principles of the Solid State-H.V.Keer (Wiley Eastern Ltd.New Delhi, 1994)
9. Solid state Chemistry –N.B.Hannay (Prentice Hall, New Jersey, 1967)
10. Superconductivity, Joi, Khachan & Stephen Bio Science, -----
11. Chemisorption, B. M. W. Trapnell, Butterworths Scientific Publications, London, 1955.
12. Adsorption on solids, VladimirPonec, Zlatko Knor, Slavoj Cerny, Butterworth & Co – publishers, 1974.
13. Catalysis: Principle and Applications, B. Viswanathan, S. Sivasanker, A. V. Ramaswamy, Narosa Publishing House, 2002.

LABORATORY COURSE

Paper CH (AC) 351P: Titrimetry, Solvent extraction,Chromatography and Water analysis.

I. Titrimetry:

1. Determination of Ca^{2+}, Mg^{2+}, CO_3^{2-}& HCO_3^- in soil sample.
2. Determination of Calcium in Vitamin-D and Calcium tablelts
3. Determination of Fe & Ca in Cement
4. Determination of Saponification value and Iodine value of an oil sample

II. Solvent extraction:

1. Determination of Pb using Dithiazone

III. Chromatography (Demonstration):

1. Separation of Co & Ni in Cellulose column
2. Separation of amino acids in a mixture by TLC using Ninhydrin
3. Separation of additives in Ink by GC.
4. Separation of synthetic corticosteroids in by HPLC.

IV. Water analysis:

1. Determination of residual Chlorine in water by Iodometry
2. Determination of Dissolved Oxygen.
3. Determination of COD.
4. Determination of BOD.
5. Determination of residual Chlorine in water by Iodometry

Paper CH (AC) 352P: Colorimetry, Spectrophotometry

I. COLORIMETRY:

1. Determination of blood sugar
2. Determination of blood cholesterol
3. Determination of Paracetamol
4. Determination of Ampicillin
5. Estimation of Ascorbic acid

II. SPECTROPHOTOMETRY:

1. Determination of Manganese in steel
2. Determination of Phosphorous in human serum
3. Determination of Creatinine in a sample
4. Determination of pKa of an organic Indicator (Methyl Orange)
5. Simultaneous determination of Cr and Mn in an admixture
6. Spectrophotometric Titration of Fe(II) with o-Phen
7. Determination of composition of Complex by Job's Method and Mole ratio Method of Cu(II)-EDTA complex

SUGGESTED BOOKS

1. Chemistry Experiments for Instrumental Methods, Donald T Sawyer William
2. R.Hememan etal John Wiley & Sons 1984.
3. Analytical Chemistry by Gary D.Christian 6th Edition
4. John Wiley&Sons Inc New York 1994.
5. A Text Book of Quantitative Inorganic Analysis by A.I. Vogel 3rEdition

Elbs Publication 1969.
6. a)Vogel's Text Book Of Quantitative Inorganic Analysis Jeffery etal 4th edition Elbs Publications 1988.
   b)Vogel's Text Book of Quantitative Chemical Analysis, 6th edition. Pearson Education Ltd2002.
7. Analytical Chemistry Thoery and Practice by R.M. Verma 3rd Edn.CBS Publishers & Distrbutors1994.
8. Comprehensive Experimental Chemistry by V.K. Ahluwalia etal New Age Publications1997.
9. Laboratory hand Book of Instrumental Drug Analysis.by B.G. Nagavi 2nd edn. 1996
10. Practical Pharmaceutical Chemistry, A.H. Beckett and J.B. Stenlake 4thedn. CBS
11. publishers, 2001
12. Separation methods, MN Sastri, 2nd edn, Himalaya Publishing House1996
13. Hand book of analysis and quality control for fruit and vegetable products. S. Ranganna,
14. 2nd edn, Tata MCGraw-Hill Publishing Company, 2002.
15. Gas Chromatography, Rajbir Singh, 1st edn, Mittal Publications, 2002

IV SEMESTER

Paper-I: CH (AC) 401T CORE: Spectroscopic methods of Analysis-II

AC – 17: U.V. visible spectroscopy,
AC –18 :IR & Raman spectroscopy
AC – 19:Optical Methods
AC – 20: Fluorimetry, Phosphorimetry,Nephelometry and Turidimetry

AC – 17: UV and visible spectroscopy 15 Hrs

UV and visible spectroscopy: Beer Lamberts law, Real limitations to Beer's law,instrumentation for colorimetry and spectrophotometry – Numerical problems based on Beer'slaw, simultaneous & differential spectrophotometry. First derivative spectrophotometry.Classification of Electronic Spectra for Metal Complexes, Selection Rules: Electric Dipole Transitions, Magnetic Dipole Transitions, Orbital Selection Rules, Spin Selection Rules, Relaxation in Selection Rules. Nature of Electronic Spectral Bands: Band Widths, Band Intensities. Factors Influencing Band Shapes: Jahn-Teller Effect, Spectrochemical Series, Nephelauxetic Effect. Orgel Diagrams for d^1-d^9 Configurations, Crystal Field Spectra of O_h and T_d Metal Complexes of 3d Metals – Calculation of 10Dq Values, Racah Parameter (B) and Nephelauxetic Ratio (β) – Charge Transfer Spectra.

AC – 18 : IR & Raman spectroscopy

IR Spectroscopy: Principle,Instrumentation, sample handling, Fourier transform infrared spectroscopy- Principle, instrumentation & its advantages. IR in quantitative analysis. Applications of IR spectroscopy: structure analysis of organic compounds, inorganic molecules-Sulphato, Carbonato, Nitrato & metal chelates - Acetylacetanato Complexes. Analysis of petroleum hydrocarbons, oil and grease contents by EPA method, Quantitative analysis of multi-component mixtures.

Raman Spectroscopy: Theory, Instrumentation, sample handling,Illumination diagnosis and structureanalysis, polarization measurements, quantitative analysis, laser applications,Resonance Raman spectroscopy-Principle, theory and its applications.

AC – 19Optical Methods 15 Hrs

Refractometry: Theory, instrumentation, specific and molecular refraction, Abbe, Pulfrich and immersiton types, applications

Polarimetry: Theoritical considerations – Plane polarized light, optical activity, specific and molecular rotations. Iinstrumentation,, applications.

Optical rotator dispersion and Circular dichorism: Optical rotation, circular birefringence, circular dichroism and Cotton effect, Octet Rule, Experimental Techniques, Applications : quantitative analysis,determination of absolute configuration, conformational studies and equilibrium studies. Use of CD in the conformational studies of metal complexes, DNA and DNA-metal complexes.

AC –20: Fluorimetry, Phosphorimetry,Nephelometry and Turbidimetry 15 Hrs

Fluorimetry and Phosphorimetry: Theory of Fluorescence and Phosphorescence- Excited states producingFluorescence and Phosphorescence. Rates of absorption and emission. Deactivation processes,Variables affecting Fluorescence and Phosphorescence. Types of Photoluminescence spectra forPhenanthrene. Instrumentation – Components of Fluorimeter,

Spectroflourimeters andPhosphorimeters. Applications of Fluorimetry- Determination of Inorganic Cations,Fluorimetric reagents. Fluorimetric determination of organic species – Thiamine, AneurineHydrochloride, Plolycyclic aromatic hydrocarbons. Phosphorimetry-Determination of Aspirinin blood serum. Chemiluminescence- Origin, measurements. Analytical applications-Atmospheric pollutants (Oxides of Nitrogen and Sulphur compounds, Ozone). Detection in GasChromatography, High Performance Liquid Chromatography and Capillary Electrophoresis.Detection of Enzyme reaction products. Immunoassay and Nucleic acid assays.

Nephelometry and Turbidimetry: Principles and instrumentation for Nephelometry and Turbidimetry, Applications

Suggested Books

1. Principles of Instrumental Analysis– Skoog, Holler, Nieman, 5th ed., HarcourtCollege Publishers, 1998.
2. Introduction to Ligand Fields – Figgis, Wiley Eastern Ltd, 1966.
3. Inorganic Electronic Spectroscopy – A.B.P. Lever, Elsevier Publishing Company,London, 1968.
4. Chemical Analysis – A. K. Srivatsava & Jain, 3rd ed., S,Chand & Company Ltd.,1977.
5. Hand Book for Instrumental Techniques for Analytical Chemistry, Ed. FrankSettle. Prentice hall, New Jersey, USA, 1997.
6. Analytical Chemistry – Gary D. Christian, 6th ed, John Wiley and sons. Inc., NewYork, 1994.
7. Introduction to Inductively Coupled Plasma Emission Spectroscopy - GL Moore,Elsevier Science publishers, New York, 1989.
8. Analytical Chemistry – Skoog & West, 6th ed, W.B. Saunders, 1998.
9. Infrared and Raman Spectra of Inorganic and Coordination Compounds, KazuoNakamoto, 5th ed., John Wiley & Sons, 1995.
10. Vogel's Text book of Quantitative Analysis – J. Mendham et al, 6th ed., PearsonEducation Ltd, 2002.
11. Instrumental methods of Analysis - Willard, 6th ed., CBS Publishers &distributors, 1986.
12. Analytical Chemisstry Instrumental techniques, Maninder Singh, DominentPublishers, New Delhi, 2002.

Paper-II: CH (AC) 402T: CORE: Separation Methods
AC - 21: Solvent extractions
AC –22: Chromatography
AC –23:Mass spectrometry & Hyphenated techniques
AC –24:Electrophoresis

AC-21: Solvent extractions 15 Hrs

The distribution coefficient, distribution ratio, relation between KD& D, the percent extracted.

Solvent extraction of metals – ion association complexes, metal chelates, effect of pH and reagent concentration, extraction process, separation efficiency of metal chelates, analytical separations – multiple counter current distribution, solid phase extraction, solvent extraction of flow injection analysis. Super critical fluid extraction.

Organic reagents in Inorganic analysis :- Theoretical basis for the use of organic reagents in inorganic analysis. Extraction of metal ions by the use of organic reagents – acetylacetone,

thionyl-trifluoroacetone, tri-n-octyl phosphine oxide. Applications to extractions of metal ions by chelating agent (Dithiazone, 8-hydroxy quinoline and cupferron) Determination of salts of organic acids and bases, determination of alkaloids in crude drugs.

AC –22: Chromatography 15 Hrs

HPTLC: Principle, Technique, advantages over TLC

Gas Chromatography (GC) – Theory, Data acquisition and processing Applications - Derivatization techniques. Monitoring of ethylene dibrombide (EDB) residue in Indian Black pepper by GC using electron capture detector. Analysis of petroleum products. Headspace analysis of tobacco. Preparative gas chromatography

High Performance Liquid Chromatography (HPLC) – Theory, and separationmodes,Applications with respect to separation of enantiomers, Organic and inorganic systems.

Supercritical fluid chromatography (SFC) – Instrumentation of SFC, stationary and mobile phases used in SFC, Detectors, Advantages of SFC. Technique and applications of SFC.

Size Exclusion Chromatagraphy: Principle of Gel Chromatography, Filtration Chromatography, Instrumentation, retention behaviour, resolution, selection of gel type – applications . Ion Exclusion – Principle and applications.

Ultra Performance Liquid Chromatography: Principle, Instrumentation

AC-23:Mass Spectrometry & Hyphenated techniques 15 Hrs

Advanced Mass spectrometry

Quadruple analysers, Ion traps. Time of flight mass spectrometry.

Mass Spectrometry / Mass Spectrometry Tandem Mass Spectrometry. Ion cyclotron resonance spectrometers and Ion traps for MS/MS.

Quantitative mass spectrometry: Introduction, principle, calibration and internal standards.

Hyphenated techniques:

GC-MS: Principle, instrumentation, Interfaces, Mass analyzer, Mass chromatogram,Applications. Analysis of metabolite of drug Imipramine

GC-FT-IR: Principle, Instrumentation and Applications

LC-MS: Principle,Instrumentation, Interfaces and Applications.

LC-MS-MS : Principle,Instrumentation, Interfaces and Applications.

ICP-MS: Instrumentation, principles, Quantitative analysis and applications.

AC-24: Electrophoresis

Introduction, Definition

Paper Electrohoresis: Principle, Experimental Requirements, Technique, Factors governing the migration of ions, Applications

Capillary Electrophoresis: Electro osmotic flow, migration in CE,instrumentation, control of separation, applications

Gel Electrophoresis: Principle, technique, applications

Immunoelectrophoresis: Principle, technique, applications

Suggested Books

1. Separation Methods - M. N. Sastri, 1st ed., Himalaya Publishers, 1991.
2. Principles of Instrumental Analysis – Skoog, Holler, Nieman, 5th ed., Harcourt College Publishers, 1998.29
3. Analytical Chemistry - Gary D.Christian, 6th ed, John Wiley and sons. Inc., New York, sixth edition, 1994.

4. Mass spectrometry for Chemists and Biochemists, Robert A.W. Johnstone and Macolm. E. Rose, 2th ed Cambridge University Press 1996.
5. Structural methods in Inorganic chemistry - E.A.V. Ebsworth, et al ELBS Publications,1988

6. Introduction to analytical Gas Chromatography, Raymond PW Scott,2nd Ed. Marcel Dekker, Inc. New York,1988.
7. Techniques and practice of Chromatography, Raymond PW Scott, Marcel Dekker, Inc. New York,1995.
8. Liquid Chromatography-Mass Spectrometry Principles & Applications, WMA Neissen & JV Greef, Marcel Dekker, Inc. New York,1992.

Paper-III CH (AC) 403T: ELECTIVE IIIa: Laboratory Management
AC – 25 Automation in laboratory
AC – 26 LIMS & Computer aided analysis
AC – 27 Laboratory Management & Standard reference materials
AC – 28 Accreditation of Laboratories, Quality management

AC- 25 Automation in Laboratory. 15 Hrs

Introduction, classification of Analytical methods, Types of Instrumental methods, Instrumentsfor analysis. Analog & Digital signals, Planning for laboratory automation. An overview ofautomatic instruments & instrumentation.
Flow Injection Analysis, Discrete Automatic systems.
Good laboratory practices: Instrumental standardization, optimization of procedures.

AC-26 LIMS and Computer aided Analysis 15 Hrs

Laboratory Information Management System: Laboratories as information producers,properties of good information, Laboratory information management system, conclusions.**Computer aided analysis:** Computer-instrument interaction, computer organization-Hardware -Basic Digital circuit components, Microprocessors and Microcomputers, Computer Software -Software control of the computer-instrument interfaces. Automated laboratory – Automatedinstruments (AAS), Applications of computers, Computer Networks.

AC- 27 Laboratory Management & Standard reference materials 15 Hrs

Introduction – Administration, Geographical location of the laboratory, relationship with theindustrial exploratory and regulatory work and the analytical laboratory. Disciplines representedin the Laboratory. Educational requirements of the laboratory personnel. Work load statistics ofthe laboratory coordination between routine work and research cell. Regular academic researchwork, opportunities for training. Internal organization of the laboratory. Architectural issues,laboratory infrastructure of equipment and instrumentation.

Standard reference materials

Standards of Analysis, Analytical standards, reference materials, High purity substances,working and secondary standards.

AC- 28 Accreditation of Laboratories, Quality Management 15 hrs

Accreditation of Laboratories: International organization for standardization, Nationalaccreditation board for testing and calibration laboratories. Scope of accreditation.
Analytical Methods: choosing the methods- standard methods, official methods, literaturemethods. Validation of new methods - comparison of analytical methods.

Quality systems, the operational aspects required to deliver a quality system (Traceability,quality control, quality assurance, quality management and quality manual) calibration and testmethods.
Total Quality Management (TQM) – Essentials of TQM: Quality Planning, Quality control,Quality Audit, Quality surveillance, Quality assurance, Quality circles.
Analytical methods of validation:Characteristics of Analytical procedures – Accuracy, precision, linearity, Range specificity,Detection limit, Quantitation limit, robustness process validation, Types of process validation –prospective, concurrent and retrospective process validation.

Suggested Books

1. Principles of Instrumental Analysis - Skoog. Holler, Nieman, 5th ed., Harcourt College Publishers, 1998.
2. Model for Quality assurance in design/development production, installation and servicing, ISO 9001.
3. Journal of Validation technology, Vol.-III and IV, 1997.
4. Instrumental Methods of Analysis - Willard, Merit, Dean, 6th ed., CBS Publishers & distributors, 1986.
5. Hand Book for Instrumental Techniques for Analytical Chemistry, Ed. Frank Settle, Prentice Hall, New Jersey, USA, 1997.
6. Handbook of Quality Assurance for the analytical chemistry laboratory, James P. Dux, Van Nostrand Reinhold, New York, 1986.
7. Quality in Totality – Parag Diwan, Deep & Deep Publications, 1st ed., 2000.
8. QA manual – DH Shah, Business Horizons, 1st ed., 2000.

PAPER – III: CH (AC) 403T:IIIb : Applied analysis and Green Analytical Chemistry
AC-25 Enzyme catalysis- Analytical applications
AC-26Forensic Chemical Analysis
AC-27 Limit tests
AC-28 Green Analytical Chemistry

AC-25:Enzyme catalysis- Analytical applications
Basic principles, Catalysis – measurement of catalytic reactions, Nonspecificity of catalysts, types of reactions catalyzed. Enzyme catalysis, enzyme kinetics, properties of enzymes, enzyme inhibitors and activators, enzyme specificity, Determination of enzymes and enzyme substrates. Example of enzymatic analysis: Dehydrogenase reactions, Substrate determinations: Glucose, Uric acid. Immobilized enzymes. Evaluation methods.
AC-26:Forensic Chemical Analysis:
Contact traces – Analysis of soil, fiber and paint evidence in forensic work.
Analysis of narcotic drugs and psychotropic substances (opiates, cannabinoids, barbiturates,benzodiazepines, amphetamimes with one example each and LSD) by colour/micro crystal tests,chromatographic methods (TLC, GC, and LC) and spectroscopic methods (UV-Vis, IR, MS andGC-MS).Analysis of explosives and explosion residues(Low explosive residues – cations and anions;High explosive residues – RDX) by spot tests, chromatographic methods (TLC, GC AND GCMS)and spectroscopic methods (UV-Vis, IR, MS and GC-MS).
Analytical toxicology – extraction techniques for dugs and pesticides – analytical techniques inforensic toxicology for alcohols, drugs and pesticides involving spot tests (TLC, GC & LCMS). Interpretation of analytical data – court testimony.
AC -27: Limit tests
Limit tests for insoluble matter, limit tests of soluble matter, limits of moisture, volatile matter, residual matter, residual solvents, limits of nonvolatile matter, limits of residue on ignition, limits of loss on ignition, limits on ash value. Limit tests for metallic impurities: lead, arsenic, iron: Limit tests for acid radical impurities, chlorides, sulfates, arsenate, carbonate, cyanide, oxalate, phosphate. Limit tests for nonmetallic impurities: Boron, free Halogens, Selenium.
AC- 28:Green Analytical Chemistry 15 Hrs
Green Analytical Chemistry: Concepts and trends
"Greening" Sample Treatment: Reduced and solvent- free sample preparation methodologies, alternative solvents, energy saving procedures.
Green Instrumental Analysis: Assessment of analytical methods for "Greenness", greening flow injection analysis, chemical sensors, liquid green chromatography.

Suggested Books
1.Analytical Chemistry - Gary D. Christian, 6th ed. John Wiley and sons. Inc, New York,1994.
2. Kinetics methods of analysis – Marck & Rekniz Vol25
3. Practical Pharmaceutical Chemistry, A.H. Beckett et al, 3rd ed. – Vol. 1 & Vol. 2 CBS Publishers & distributors, 1986.

4. Green Analytical Chemistry: Theory & Practice, Miguel De La Guardia, Sergio Armenta, Elsevier
5.Green Analytical Chemistry, Mihkel Koel, Mihkel Kaljurand, RSC Publishing

PAPER – IV: CH (AC) 404T: IDa: Quality Assurance and Accreditation
AC-29 Quality Assurance – I
AC-30 Quality Assurance – II
AC-31 Quality Assurance – III
AC-32 Quality Accreditation

AC -29: Quality Assurance – I 15 Hrs

Introduction to Quality Control and quality assurance: Concepts and significance.

Quality control and statistical techniques: Quality control charts, the X-quality control chart,the R-quality control chart and its interpretation, spiked sample control charts, use of blindsamples in quality control, use of proficiency evaluations in quality control.

Calibration and maintenance of Instruments / Equipment: Instrument calibration – linearcalibration curves, equipment calibration, frequency of calibration, calibration of commonlaboratory instrument and equipment (Analytical balances, volumetric glassware, ovens,furnaces, UV / Visible spectrophotometer, pH meter, conductivity meter, IR spectrophotometers,AAS, GC, HPLC etc.,). Maintenance of instruments and equipment.

AC-30: Quality Assurance – II 15 Hrs

Documentation for quality assurance: Raw Data - Type of notebooks, control of notebookdistribution and data entry. General Reagents and volumetric reagents. Sampling – samplingmethods, sample labeling, sample log-in/register. Sample analysis, reporting, recording andpersonal training. Instrument calibration and maintenance. Analytical report. Personnel, training,records - professional personnel, technician personnel. Filing quality assurance documentation.

Good laboratory practices and personnel, Quality Programme, Instrument andOrganisationcalibration, Customer Satisfaction.

AC -31: Quality Assurance – III 15 Hrs

Computers and quality assurance: Sample handling. Data Acquisition. Quality control data and calculations. Computer generated analytical reports. Security considerations. Hardware andsoftware.

Establishing a Quality Assurance program: Management commitment. Define the qualityassurance program. Writing standard operating procedures. Topics for standard operatingprocedures. Consolidating the programme. Monitoring the program – monitoring qualityassurance data, reporting quality assurance problems. Writing the quality assurance manuals.

AC -32: Quality Accreditation: 15 Hrs

Laboratory Accreditation: Need for laboratory accreditation. International aspects oflaboratory accreditation and in India. Criteria for laboratory accreditation. Benefits of laboratoryaccreditation,

Evolution and significance of Quality Management, Background to ISO 9000, comparison between ISO-9001,ISO-9002 & ISO-9003., ISO 9000-2000 series of standards onquality

managament system, - evolution of series of standards, introduction to ISO organization,Registration / certification - benefits of QMS certification. Structure of ISO 9000-2000 family ofstandards. Advantages of ISO 9000-2000. Requirements of ISO 9001-2000 QMS andapplications, Steps for effective implementations. Significance of ISO - 9001,9002,9003 &9004.
Requirements of ISO9000/IS14001. Concepts of OHSMS (BS 8800) Quality Managament Principles in QMS, QMS documentation, Quality Manual, Quality policy, conformities and Non-confirmities.

Suggested Books:

1. Handbook of Quality Assurance for the analytical chemistry laboratory, James P. Dux, Van
Nostrand Reinhold, New York, 1986.
2. Applying ISO-9000 Quality Management Systems, International Trade Centre Publishing, UNCTAD/WTO. Geneva, Switzerland, Indian Edition Printed by D.L.Shah Trust.
3. How to practice GLP, PP Sharma, Vandana Publications, 2000, New Delhi
4. Training manuals on ISO 9000 / 2000 PQM, Girdhar J Gyani, Raj Publishing House, 2001
5. Quality Assurance in Analytical Chemistry, B.W. Wenclawiak, Springer,India, 2004.

PAPER – IV: CH (AC) 404T: IDb: Inorganic Material Chemistry
AC- 29:Composite Materials
AC- 30: Liquid Crystals
AC-31: Explosives and Propellants
AC-32: Fuels and Combustion

AC-29: Composite Materials

Introduction, Advantageous Properties of the Composites, Constituents of Composites, Types of Composites – Fibre-reinforced composites (Glass, carbon, Armid, Alumina reinforced composites), Particulate composites, Layered composites, Processing of Fibre-reinforced Composites, Micromechanics of Fibre and Particle Reinforced Composites, Fabrication of the Composites.
Refractories: Characteristics and Classification of Refractories, Properties of Refractories, Manufacture of Refractories, Common Refractories Bricks – Silica Bricks, Alumina Bricks, Magnesite Bricks, Dolomite Bricks, Carbon Bricks and Chromite Bricks.
Ceramics: Plasticity of Clays, Whitewares or White-Pottery, Manufacture of White-Pottery, Glazing, Methods of glazing, Earthenwares and Stonewares.

AC-30: Liquid Crystals

Introduction, Types of Mesophases, Characterization of Liquid Crystals, Physical Properties of Liquid Crystals, Structure of Liquid Crystal forming compounds, Classification of Liquid Crystals-Thermotropic Liquid Crystals and Lyotropic Liquid Crystals, Chemical Properties of Liquid Crystals, Applications with special reference to Display systems, Applications and Importance of Lyotropic Liquid Crystals, Future of Liquid Crystals.

AC-31: Explosives and Propellants

Explosives: Introduction, Classification of Explosives, Primary Explosives, Low Explosives, High Explosives, Precautions During Storage of Explosives, Blasting Fuses, Manufacture of Important Explosives-Lead azide, Diazonitrophenol (DDNP), Trinitrotoluene (TNT), Nitroglycerine (NG) or Glycerol trinitrate (GTN), Pentaerythrital tetranitrate (PETN) and RDX; Recent uses of Explosives

Propellants: Rocket Propellants - Introduction, Principle of Rocket Propulsion, Classifications of Propellants-Solid propellants, Composite propellants, Liquid Propellants, Mono-propellants, Bi-propellants; Differences between Solid propellants and Liquid Propellants

AC-32: Fuels and Combustion

Introduction, Classification of Fuels, Calorific Value, Characteristics of a Good Fuel, Theoretical Calculation of Calorific value of a Fuel, Coal, Classification of Coal by Rank, Analysis of Coal – Proximate analysis and Ultimate analysis, Metallurgical Coke, Types of Carbonization of Coal – Low-temperature and high temperature carbonization, Manufacture of Metallurgical Coke by Beehive oven process, Petroleum, classification of petroleum, Refining of crude oil, Cracking – Thermal cracking, Catalytic cracking- Moving-bed catalytic cracking, LPG as a Fuel, Natural Gas, Producer Gas, Water Gas (or Blue Gas), Non-Conventional Sources of Energy-Solar energy, Solar cells and Uses of solar cells.
Combustion: Combustion, Mass Analysis from Volume Analysis and Vice Versa, Analysis of Flue Gas

SUGGESTED BOOKS

1. “Liquid Crystals, Nature’s delicate phase of matter”, Peter J Collings, Princeton University Press, 2002
2. “Liquid Crystals: Fundamentals”, Shri Singh, World Scientific Publishing Company; 1st edition (November 7, 2002)
3. “Science of Engineering Materials”, C.M. Srivastava and C. Srinivasan, Wiley-Eastern Ltd.
(1991).
4. “Engineering Chemistry”, Jain P C and Monica Jain, 15th Edition, Dhanpat Rai Publishing Company Ltd, New Delhi, India, 2005.
5. A Text book of Engineering Chemistry”, Shashi Chawla” Dhanpat Rai Publishing Company (P) Ltd., New Delhi, India, 2007.
6. Textbook of Engineering Chemistry, C Parameswara Murthy, C V Agarwal, Andra Naidu, BS Publications, Hyderabad, India.
7. “A Textbook of Engineering Chemistry”, Dr. Y. Bharathi Kumari and Dr. Jyotsna Cherukuri, VGS Publications, First Edison, India, 2009

LABORATORY COURSE

Paper CH (AC) 451P: Electro analytical techniques:

I. POTENTIOMETRY:
1.Determination of Ferrous using $K_2Cr_2O_7$
2.Determination of iron in iron wire using $KMnO_4$
3. Determination of a mixture of Ferrous and Vanadyl using Ceric ammonium nitrate
4. Determination of silver in silver metal
5. Assay of sulphanilamide in samples
Use of ion selective electrodes:
6.Determination of mixture of halides using Ag ion electrode

II. pH METRY:
1. Strong acid Vs strong base titration
2. Mixture of acids Vs strong base
3.Determination of mixture of carbonates and bicarbonates
4. Determination of Dissociation constants of Histidine monohydrochloride
5. Determination of binary stability constants of Cu(II) – Histidine complexes

III.POLAROGRAPHY:
1. Polarographic determination of Cu & Zn in brass

IV. CONDUCTOMETRY:
1. Mixture of acids Vs strong base titration
2. Mixture of bases Vs strong acid titration
3. K_2SO_4 Vs $BaCl_2$ titration.
4. Determination of the composition of Cu(II) oxine complex
5. Determination of Quinine dihydrochloride with NaOH
6. Determination of Aspirin with KOH

Paper CH (AC) 452P: Spectroscopic Techniques , Spectral problems and Evaluation of Physical Parameters Of Tablets

I. FLAME PHOTOMETRY:
1. Determination of i)Na, ii)K, iii)Ca, iv)Li

II. FLUORIMETRY
1. Determination of Vitamin – B_1 (Thiamine)
2. Determination of Vitamin – B_2 (Riboflavin)
3. Determination of Quinine sulphate.

III. ATOMIC ABSOPTION SPECTROSCOPY
1.Determination of i) Fe, ii) Zn, iii) Cu, iv) Pb.

IV. Structural elucidation based on spectral data from UV – Vis, IR, NMR and Mass Spectrometry

V. EVALUATION OF SOME PHYSICAL PARAMETERS OF TABLETS:
1. Dissolution profile of Ampicillin.
2. Disintegration test for Ibuprofen (coated tablet).
3. Determination of friability of Paracetamol tablet.

SUGGESTED BOOKS

1.Chemistry Experiments for Instrumental Methods, Donald T Sawyer William R.Hememan etal John Wiley & Sons 1984.
2.Analytical Chemistry by Gary D.Christian 6th Edition John Wiley&Sons Inc New York 1994.
3.A Text Book of Quantitative Inorganic Analysis by A.I. Vogel 3rEdition Elbs Publication 1969.
4.Vogel's Text Book Of Quantitative Inorganic Analysis Jeffery etal 4th edition Elbs Publications 1988.
5.Vogel's Text Book of Quantitative Chemical Analysis, 6th edition. Pearson Education Ltd 2002.
6.Analytical Chemistry Thoery and Practice by R.M. Verma 3rd Edn.CBS Publishers & Distrbutors1994.
7.Comprehensive Experimental Chemistry by V.K. Ahluwalia etal New Age Publications 1997.
8.Laboratory hand Book of Instrumental Drug Analysis by B.G. Nagavi 2nd edn. 1996
9.A Text Book of Quantitative Inorganic Analysis by A.I.Vogel 3rd Edition, ELBS Publication 1969.
10.Determination and use of Stability Constants – Martell and Motekaitis VCH Publishers INC 1988.
11.Metal Complexes in Aqueous Solutions A.E.Martell and R.D. Handcock, Plenum Press, New York – 1996.
12.Experiments in Chemistry, D.V. Jahagirdar, 2nd edn, Himalaya Publishing House, 2003
13.Practical Pharmaceutical Chemistry, A.H. Beckett and J.B. Stenlake 4thedn. CBS publishers, 2001

M.Sc. CHEMISTRY

INORGANIC CHEMISTRY SPECIALISATION
SYLLABUS OF III & IV SEMESTERS
REVISED AS PER NEW (CB) SYLLABUS

FOR STUDENTS ADMITTED FROM THE YEAR 2016 ONWARDS

Osmania University

M.Sc. Chemistry (Inorganic Chemistry)III and IV Semesters Programme

(For the batch admitted during the academic year 2016-2017 under the CBCS pattern)

[Under Restructured CBCS Scheme]

	III Semester			
	Course	**Hours**	**Credits**	**Marks**
CORE	**Paper-I: CH(IC)301T: Bonding, Group Theory and its Applications** IC-09: Group Theory, Normal mode analysis and Spectral Activity IC-10: MOT of Metal Complexes IC-11: Electronic Spectroscopy of Metal Complexes IC-12: IR and Raman Spectroscopy	4	4	100
CORE:	**Paper-II: CH(IC) 302T: Organo Metallic Chemistry of Transition Metal Complexes** IC-13: Mono,Di and Trihapto Complexes IC-14: Tetra, Penta, Hexa, Hepta and Octahapto Complexes IC-15: Catalytic Role of OTMC-I IC-16: Catalytic Role of OTMC-II	4	4	100
ELECTIVE IIIa	**Paper-III: CH(IC) 303T: Analytical Techniques-I** IC-17: Data Handling IC-18: AAS, AES, ICP-AES IC-19: Diffraction Methods IC-20: Advanced Mass spectrometry	4	4	100
ELECTIVE IIIb	**Paper-III: CH(IC)303T: Supramolecular Chemistry, Photochemistry, Green Chemistry and Nanotechnology** IC-21: Supramolecular Chemistry IC-22: Photochemistry of Metal Complexes IC-23: Green Chemistry IC-24: Nanotechnology	4	4	100
ELECTIVE IVa	**Paper-IV:CH(IC) 304T: Analytical Techniques-II** IC-25: Thermal Methods IC-26: Surface Analysis Methods/ Microscopic analysis IC-27: Advanced Separation Techniques IC-28: Optical Methods	4	4	100
ELECTIVE IVb	**Paper-IV: CH(IC) 304T: Nuclear Chemistry, Zeolites, Solid State, and Surface Chemistry** IC-29: Nuclear Chemistry IC-30: Zeolites and Molecular Sieves IC-31: Solid State Chemistry IC-32: Surface Chemistry & Superconductors	4	4	100
LABORATORY COURSE -I	**CH (IC) 351P: Synthesis and Characterization of Metal Complexes**	9	4	100
LABORATORY COURSE –II	**CH (IC) 352P: Electro-Analytical techniques**	9	4	100

	IV Semester			
	Course	**Hours**	**Credits**	**Marks**
CORE	**Paper-I: CH(IC)401T: Molecular Spectroscopy of Inorganic Compounds** IC-33: Multinuclear NMR IC-34: Advanced NMR techniques IC-35:Applications of ESR to Metal Complexes IC-36:Mossbauer Spectroscopy and Nuclear Quadrupole Resonance Spectroscopy	4	4	100
CORE	**Paper-II: CH(IC) 402T: Bioinorganic Chemistry** IC-37: Metal ions Interactions with Nucleic acids and their constituents. IC-38: Transport of Electrons and Metal ions. IC-39: Metallo-Enzymes of Iron, Zinc and Nickel. IC-40:Metallo-Enzymes of Cobalt, Copper Molybdenumand Manganese	4	4	100
ELECTIVE IIIa	**Paper-III: CH(IC)403T: Medicinal Inorganic Chemistry, Spectroscopic Analysis of Drug/Metal Complexes and Applications of Nanomaterials** IC-41: Metal complexes in Clinical Chemistry IC-42:Metal complexes as Drugs and Anticancer agents IC-43:Spectroscopic analysis of drug/metal complexes binding to DNA IC-44: Applications of Nanomaterials	4	4	100
ELECTIVE IIIb	**Paper-III:CH(IC)403T:Analytical Techniques-III** IC-45: Electroanalytical Methods IC-46: Radiochemical Methods IC-47: Fluorimetry, Phosphorimetry, Nephelometry and Turbidimetry IC-48: Industrial Analysis	4	4	100
ELECTIVE IVa **(ID Paper)**	**Paper-IV: CH(ID) 404T: Interdisciplinary Course (Environmental and Applied Analysis)** IC-49 : Clinical and Pharmaceutical Analysis IC-50: Food and Agricultural analysis IC-51: Analysis of Air and Water Pollutants IC-52: Drinking Water and Sewage Water Treatment	4	4	100
ELECTIVE IVb **(ID Paper)**	**Paper-IV: CH(ID) 404T: Interdisciplinary Course (Inorganic Material Chemistry)** IC-49 : Composite Materials IC-50: Liquid Crystals IC-51: Explosives and Propellants IC-52: Fuels and Combustion	4	4	100
LABORATORY COURSE –I	**CH (IC) 451P: Conventional Methods of Analysis**	9	4	100
LABORATORY COURSE –II	**CH (IC) 452P: Spectroscopic Techniques**	9	4	100

M.Sc. INORGANIC CHEMISTRY SPECIALIZATION
SEMESTER-III
PAPER I

CH(IC)301T: Bonding Group Theory and its Applications

IC-09: Group Theory, Normal mode analysis and Spectral Activity
IC-10: MOT of Metal Complexes
IC-11: Electronic Spectroscopy of Metal Complexes
IC-12: IR and Raman Spectroscopy

IC-09: Group Theory, Normal Mode Analysis and Spectral Activity
Properties of a Group-Closure rule, Identity rule, associative rule, inverse rule, Abelian and Non-abelian groups. Classes of Symmetry Elements of a Group: Similarity transformation, properties of conjugate elements, salient features about Classes, Classes of C_{2V}, C_{2h} and C_{3V}. Matrix Representation of Symmetry Elements: Simple Matrices, Matrix addition, subtraction and multiplication, Block-Factorization. Matrix Representation of *E, C_n, S_n*, i and σ Elements. Great Orhogonality Theorem: Reducible and Irreducible Representations, Properties of Irreducible Representations, Construction of Character Tables for C_{2V}, C_{2h} and C_{3V}. Mulliken Symbolism for Irreducible Representations - Standard Reduction Formula.
Use of Character tables for IR & Raman spectroscopy, symmetry based selection rules for IR and Raman activity. Type and Symmetry of Normal Modes and IR and Raman activity of molecules: Cartesian coordinate method of analysis for C_{2V} (eg. H_2O, SF_4), C_3V (NH_3, $POCl_3$), C_{2h} (trans-N_2F_2), D_{3h} (BF_3), Td(SO_4^{2-}), Oh (SF_6). Internal coordinate method of analysis for C_{2V} (H_2O), C_3V (NH_3), Td (SO_4^{2-}).

IC-10: Molecular Orbital Theory of Metal Complexes: Limitations of Crystal Field Theory, Adjustments to the Crystal Field Theory to allow for covalence -Experimental evidences for Metal - Ligand orbital overlap. The Adjusted Crystal Field Theory. Introduction to Molecular Orbital Theory. Symmetry Classification of Metal and Ligand Group Orbitals in Cubic and Non-Cubic Environments: Octahedral, Tetrahedral, Square Planar, Square Pyramidal, TrigonalBipyramidal Geometries – Concept of Ligand Group Orbitals – Construction of Molecular Orbital Energy Level Diagrams -Octahedral Metal Complexes with (i) Sigma (σ), (ii) sigma(σ) &Pi (π) and (iii) sigma (σ), Pi (π) and Pi* (π*) bonding contribution from the Ligands - Tetrahedral Metal Complexes with (i) Sigma (σ) and (ii) sigma(σ) &Pi (π), and Square Planar Metal Complexes with (i) Sigma (σ) and (ii) sigma(σ) &Pi (π) bonding contribution from the ligands - Molecular orbital electron configurations and calculation of Magnetic Moments.

IC-11: Electronic Spectroscopy of Metal Complexes
Classification of Electronic Spectra for Metal Complexes, Selection Rules: Electric Dipole Transitions, Magnetic Dipole Transitions, Orbital Selection Rules, Spin Selection Rules, Relaxation in Selection Rules. Nature of Electronic Spectral Bands: Band Widths, Band Intensities. Factors Influencing Band Shapes: Jahn-Teller Effect, Spectrochemical Series, Nephelauxetic Effect. Orgel Diagrams for d^1-d^9 Configurations, Crystal Field Spectra of O_h and T_d Metal Complexes of 3d Metals. Charge Transfer Spectra. Strong Field Configurations: The Method of Descending Symmetry, Correlation Diagrams and Tanabe-Sugano Diagrams for d^2 and d^8 Configurations. Calculation of 10Dq Values, Racah Parameter (B) and Nephelauxetic Ratio (β).

IC-12: Infrared and Raman Spectroscopy
Conditions for Infrared and Raman Spectroscopies, Direct product – symmetry requirements for overtones, binary and ternary combination bands. Partial Normal mode analysis-Structure Fitting, Determination of Coordination Sites and Linkage Isomers(NO_2^- , SCN^-), Assigning Denticity of

Ligands (SO_4^{2-}, CO_3^{2-}), Prediction of Diagnostic Fundamentals in Isomers of Metal Complexes and Distinguishing Isomers of Metal Complexes. Effect of Coordination on Ligand Vibrations: Examples involving Mono, Bi and/or Polydentate Ligands of Oxygen, Nitrogen, Carbon and Halogen Donors (NH_3, H_2O, Glycine, Carbonyl and halides). Raman effect and molecular structure- CO, HCN, CO_2, N_2O, H_2O. Principles of Resonance Raman Spectroscopy. Application of Resonance Raman Spectroscopy to Structural Elucidation of the active Sites of Heme and Non-Heme Oxygen Carriers

SUGGESTED BOOKS

1. Symmetry and Spectroscopy of Molecules, K. Veera Reddy, Second Edition, New Age International (P) Limited Publishers (2009)
2. Chemical Applications of Group Theory, F. A. Cotton, 3rd edition, Wiley NY (1990)
3. Symmetry and Group Theory In Chemistry, Mark Ladd, Harwood Publishers, London (2000)
4. Symmetry Through the Eyes of a Chemist, I. Hargittai and M. Hargittai, 2nd Edition, Plenum Press, NY (1995)
5. Molecular Symmetry and Group Theory, Robert L. Carter, John Wiley & Sons (1998)
6. Group Theory for Chemists, G. Davidson, Macmillan Physical Science Series (1991)
7. Molecular Symmetry, Schoenland
8. Electronic Spectroscopy, A. B. P. Lever
9. Introduction to Ligand fields, B. N. Figgis
10. Infrared and Raman Spectroscopy of Inorganic and Coordination Compounds, K. Nakamoto
11. Infrared spectroscopy of Inorganic Compound, Bellamy.

PAPER II

CH(IC)302T: Organo Metallic Chemistry of Transition Metal Complexes

IC-13: Mono,Di and Trihapto Complexes
IC-14: Tetra, Penta, Hexa, Hepta and Octahapto Complexes
IC-15: Catalytic Role of OTMC-I
IC-16: Catalytic Role of OTMC-II

IC-13: Mono, Di and Tri hapto Complexes

Nomenclature and Classification based on the number of Coordinated Carbons (hapticity) and number of electrons donated by the Ligand. 16 and 18 electron rules. Electron countingcovalentand ionic models. η^1 – Complexes : General methods of Preparation –Bonding of Ligand to Metal :αand βInteraction and agostic interaction– Stability and decomposition pathways –η^1 Complexes –Tertiary Phosphine – Transition Metal Alkyl and Aryl Complexes of Pt – Ortho-effect – Bonding in Metal – Carbene and Carbyne Complexes. η^2 –Complexes: General methods of preparation of Metal – Alkene Complexes – Structure and Bonding in η^2 Complexes-Zeises salt – Trans Effect – Rotation of Olefin around Metal-Olefin Bond. η3 - Complexes: Metal-Allyl Complexes – General Preparative Routes – Structure and Bonding in η3 Allyl Complexes – Fluxionality.

IC-14: Tetra, Penta,Hexa,Hepta and Octahapto Complexes

η4 Complexes: Structure and Bonding in η4 Complexes –Butadiene and Cyclobutadiene Complexes. η5 – Complexes: General methods of Preparation – Bis (η5-cyclopentadienyl) metal complexes (Metallocenes) – Ferrocene: Structure and Bonding –Reactions of Ferrocene – Mechanism of Electroplilic substitution – Friedel Crafts acylation, alkylation, nitration, halogenation and Metallation Reactions.

η^6Complexes : Metal –Arene Complexes – Dibenzenechromium – Preparation, Structure and Bonding in Bis(arene)-Metal Complexes – Reactions. η^7Complexes : Preparation , Structure and Reactions of η^7 –

C_7H_7 Complexes. η^8Complexes : C_8H_8 as a Ligand – Cyclooctatetraene Complexes – Preparation, Structure and Bonding in Uranocene.

IC-15: Catalytic Role of OTMC-I

Oxidative addition and Reductive Elimination : Stereochemistry and Mechanism of Oxidative Addition – Insertion Reactions – Hydrogenation of Olefins –Transfer Hydrogenation –Hydrosilation of Olefins – Isomerisation of Olefins – Ziegler –Natta Polymerization of Olefins – Oligomerization of Butadiene Alkene Metathesis. Dupont-1,4-hexadiene synthesis.Oxidation of Olefins to Carbonyl Compounds – Oxidation of Hydrocarbons to Alcohols and Acids – Oxidation of Aldehydes, Cyclohexanol, Cyclohexanone, p-Xylene.

IC-16: Catalytic Role of OTMC- II

Reactions of Carbon monoxide and Hydrogen:Hydroformylation – Carbonylation –Syngas- Water gas shift Reaction (WGS) – Reactions of Syngas. Applications of Metal Clusters in Catalysis:Hydroformylation of Ethylene using $[HRu_3(CO)_{11}]$ – , Hydrogenation of Olefins. Use of $[Fe_4C(CO)14]$ as a model for Fischer – Tropsch process. Recent Developments in Homogenous Catalysis: Phase Transfer Catalysis (PTC) – Homogeneous Transition Metal Catalyzed Reactions under Phase Transfer Conditions: Hydrogenation. Bio Catalysis : Enzyme Analogue Catalysis: Introduction, Examples of Enzymatic Conversions, Reduction of >C=O and >C=C< bonds, Templates: Introduction, Metal Cations as Templates, Covalent molecules as Templates, External and Internal Templates – Homogeneous Catalysts and theirHeterogenization or Immobilization by Aqueous Catalysis.

SUGGESTED BOOKS

1.Organometallics-A Concise Introduction, Ch.Eischeinbroich and Salzer-VCH
2.Organotransition Metal Chemistry Fundamental Concepts and Applications, John AkioYamamato, Wiley & Sons.
3.Homogeneous Catalysis by Metal Complexes, M MTaqui Khan and A E Martel
4. Applied Homogenous Catalysis with Organo Metallic Compounds Vol I & II, Boy Cornillsand W A Herrmann – VCH
5. Organometallic Compounds, G E Coates, M C H Green, K Wade vol II
6. Advanced Inorganic Chemistry, Cotton and Wilkinson, V & VI Ed
7. Symmetry and spectroscopy, K Veera Reddy
8. Homogenous catalysis, G W Parshall, John Wiley & Sons, New York
9. Basic organometallic Chemistry, B.D. Gupta / A. J. Elias

PAPER III

CH(IC) 303T (Elective IIIa): Analytical Techniques - I

IC-17: Data Handling
IC-18: AAS, AES, ICP-AES
IC-19: Diffraction Methods
IC-20: Advanced Mass spectrometry

IC-17: Data Handling

Accuracy, Precision, Types of errors – determinate and indeterminate errors, minimization of determinate errors, statistical validation- statistical treatment of finite data (mean, median, average deviation, standard deviation, coefficient of variation and variance), significant figures – computation rules, comparison of results – student's t-test, F-test, statistical Q test for rejection of a result, confidence limit, regression analysis – method of least squares, correlation coefficient, detection limits. Calculations.

IC-18: AAS, AES, ICP-AES

Atomic Absorption Spectroscopy (AAS): Principles of AAS, Instrumentation – flame AAS and furnace AAS, resonance line sources, sensitivity and detection limits in AAS, interferences –chemical and spectral, evaluation methods in AAS and application in qualitative and quantitative analysis.

Atomic Emission Spectroscopy (AES): Principles of AES, Instrumentation, evaluation methods, Application in quantitative analysis.

Inductively Coupled Plasma - Atomic Emission Spectroscopy (ICP-AES): Limitations of AES, Principles of plasma spectroscopy, plasma as an excitation source. Inductively coupled plasma source, ICP-AES – Instrumentation. Application of ICP-AES, Comparison with AAS.

Flame Photometry: Principle, Theory, Instrumentation and Applications

IC-19: Diffraction Methods

X – ray Diffraction : X –rays and their generation – choice of radiation ; Miller indices, Braggs equation, Experimental methods – Powder and single crystal methods, Indexing the reflections, Systematic absences, Electron density studies by X – rays – Platinum phthalocyanine complex, Silyl acetate, Tetraalkylbiphosphate ; Advantages and limitations of X – ray Diffraction.

Electron Diffraction by gases :Principles , Radial distribution curves- Interpretation of results for $PBrF_2S$, PF_3S, PF_2HS, $HClO_4$, Silylmonothioacetate and Germylmonothioacetate and $HgCl_2$ molecules, Advantages and Limitations

Neutron Diffraction: Principle, Application in Hydrogen bonding studies, combined use of X – ray and Neutron diffraction studies, Advantages and limitations.

IC-20: Advanced Mass spectrometry

Mass Analyzers: Quadruple, Ion traps, Time of flight (TOF) mass analyzers

Mass Spectrometry / Mass Spectrometry: Tandem Mass Spectrometry, Instrumentation, Applications.

Hyphenated Techniques: GC-MS Principle, instrumentation, Interfaces- Direct coupling interface and open split interface. Application based on gas chromatography/mass spectrometry-Analysis of metabolite of drug Imipramine. **LC-MS-** principle, Instrumentation – Interfaces- Moving belt interface, particle beam interface, thermospray interface, Electrospray interface, atmospheric pressure chemical ionization interface.**ICP – MS** - Principle Instrumentation, and Applications.

Matrix-assisted laser desorption/ionization-Time of flight Mass spectrometry (MALDI-TOF-MS): Principle, Matrix, Sample Preparation for MALDI-MS - Dried droplet Crystallization, Thin layer method, Sandwich Crystallization, Instrumentation, Applications

SUGGESTED BOOKS

1. Analytical Chemistry, Gary Christian, VI Ed, John Wiley & Sons Inc, New York.
2. Instrumental Methods of Chemical Analysis, H. Kaur.
3. Vogel's Text Book of Quantitative Chemical Analysis, 6th Ed, Pearson EducationLtd.
4. Principles of Instrumental Analysis, Skoog, Holler and Nieman.
5. Instrumental Techniques for Analytical Chemistry, Frank Settle.
6. Principles of Analytical Chemistry, M. Valcarcel.
7. Solid State Chemistry and its Applications, *West.*
8. Introduction to Solids, Azaroff.
9. Solid State Chemistry, D.K. Chakrabarthy
10. Physical Methods in Advanced Inorganic Chemistry, Hill and Day.
11. Instrumental Methods of Analysis, Sixth edition, CBS Publishers, Willard, Merrit, Dean,and Settle.
12. Mass spectrometry for Chemists and Biochemists, Robert A.W Johnstone and Molcolm. E.Rose, second Edn.
13. Physical methods for Chemists, Russell S. Drago second edition, Saunders Collegepublishing 1992.
14. Structural methods in Inorganic Chemistry, E.A.V. Ebsworth, D.W.H Rankin and S.Craddeck, ELBS.

15. Mass Spectrometry Basics, Herbert, Christopher G.; Johnstone, Robert A.W., CRC Press.
16. Mass Spectrometry-A Textbook by Jürgen H. Gross, © Springer-Verlag Berlin Heidelberg 2004, Printed in Germany.
17. Matrix-assisted laser desorption/ionization - https://en.wikipedia.org/wiki/Matrix-assisted_laser_desorption/ionization

PAPER III

CH(IC) 303T (Elective IIIb): Supramolecular Chemistry, Photochemistry, Green Chemistry and Nanotechnology

IC-21: Supramolecular Chemistry
IC-22: Photochemistry of Metal Complexes
IC-23: Green Chemistry
IC-24: Nanotechnology

IC-21: Supramolecular Chemistry

Host – Guest chemistry: Definition and different types of host and guests with examples – types of non-covalent interactions – binding constants of host guest complex and thermo dynamics involved in it – designing principles of host.

Cation guest binding – binding between metal cations and macro cycles – chelate and cryptate effects – relationship between cavity size of host and cation radius and stability of resultant complexes – binding of macro cycles having secondary binding sites.

Anion guest binding – different hosts for anionic guests capable of binding through electro static interactions, hydrogen bonds, lewis acidic hosts – enhancement of binding strength using more than non-covalent interactions.

Neutral guest binding – binding of neutral guest using hydrogen bonding, π - π stacking, hydrophobic effect and charge transfer interactions – simultaneous binding of cation and anion guests – cascade approach, individual binding sites and zwitter ions approach –present and future applications – phase transfer agents – separation of mixtures – molecular sensors – switches and molecular machinery.

IC-22: Photochemistry of Metal Complexes

Energy, Structure, Electron Distribution and Chemical reactivity of Electronically Excited states of Coordination Compounds. Photochemistry of Cr(III) and Co(III) metal complexes . Photochemistry of $Cr(CO)6$,$Mn_2(CO)_{10}$ and $Fe(CO)_5$.

Structuredphosphorescence of Ruthenium Bipyridyl and Ortho-phenanthroline Complexes. Energy transfer Spin Correlation energy levels in the energy Transfer Systems;$[Ru(bipy)_3]^{2+}$ $[Cr(CN)_6]^{3-}$. Metal Sensitizers and Quenchers - Electron Relay. Photochemical Hydrogen production by oxidative quenching of $[Ru(bipy)_3]^{2+}$* by Methyl Viologen.

IC-23: Green Chemistry

Principles and concepts of green chemistry

Introduction, sustainable development and green chemistry, atom economy, atom economic reactions, rearrangement reactions, addition reactions, atom uneconomic reactions- substitution reactions, elimination reactions, Wittig reactions.Reducing toxicity, measuring toxicity.

Organic solvents: Environmentally benign solutions: Organic solvents and volatile organic compounds, solvent free systems, super critical fluids- supercritical carbon dioxide and supercritical water. Water as a reagent solvent, water based coatings.

Industrial case studies: A brighter shade of green – greening of acetic acid, Vitamin C synthesis –enzyme routes. Polythene manufacture-metallocene catalysis.

IC-24: Nanotechnology

Metal Nanoclusters –Introduction, Magic numbers, theoretical modeling of nanoparticles, geometric structure, electronic structure, reactivity, fluctuations, magnetic clusters, bulk to nanotransition.
Methods of synthesis: RF plasma, thermolysis, pulsed laser, chemical methods.
Carbon nanostructures- Introduction, carbon molecules, new carbon structures,
Carbon clusters- small carbon clusters, discovery of C_{60}, structure of C_{60} and its crystal, alkali doped C_{60}, superconductivity in C_{60}.
Carbon nanotubes: Fabrication, structure, electrical properties, vibrational properties, mechanical properties.
Nanophase and nanostructured materials: **Micells and Microemulsions -** Formation mechanisms of micelles and microemulsions, the critical Micelle Concentration (CMC) for surfactants, Solubilization and Formation of Microemulsions. **Synthesis of Nanoparticles from W/O Microemulsions:** Preparation of Nanoparticles of Metals, Metal Sulfides, Metal Salts, Metal oxides, Nanowires. **Synthesis of Organic Nanoparticles from O/W Microemulsions:** Styrene Latex NanoParticles, Methylmethacrylate Nanoparticles. Sol -Gel process for the fabrication of Glassy and Ceramic materials.

SUGGESTED BOOKS

1. Supramolecular Chemistry – concepts and perspectives by Jean-Marie Lehn
2. Principles and methods in Supramolecular chemistry, Hans-Jorg Schneider and A.Yatsimirsky, John Wiley and Sons
3. Analytical Chemistry of Macrocyclic and Supramolecular Compounds, S.M.Khopkar, Narosa Publishing House
4. Concepts of Inorganic PhotoChemistry A.W. Adamson and P. D. Fleschaner,Wiley.
5. Inorganic Photochemistry, Journal of Chemical Education, Vol 60. No 10, 1983.
6. Progress in Inorganic Chemistry Vol 30 ed :S.J.Lippard.
7. Coordination Chemistry Reviews Vol 39 1981,p121
8. Photochemistry of Coordination compounds V.Balzani and Carassiti,academicpresss.
9. Elements of inorganic Photochemistry G.J.Ferrendi,Wiley,
10. Structure and Bonding Vol 49 1982.
11. Separation Methods - M. N. Sastri, 1st ed., Himalaya Publishers, 1991.
12. Principles of Instrumental Analysis – Skoog, Holler, Nieman, 5th ed., Harcourt CollegePublishers, 1998.
13. Analytical Chemistry - Gary Christian, 6th ed, John Wiley and sons. Inc., New York, sixth edition, 1994.
14.Green Chemistry- An Introductory text by Mike Lancaster- RSC.
15. Green Chemistry: Theory and Practice by John C. Warner Paul T. Anastas.
16. Introduction to nanotechnology by Charles P. Poole Jr, Frank J. Owens- Wiley StudentEdition 2006.
17. Hand Book of Nanophase Materials by A.N. Gold Stein ed,Marcel Decker, New York, 1997, Chapter1
18. Clusters of Transition Atoms" by Morse, Chem. Rev 86, 1049 (1986).
19. Hand Book of Nanostructured materials by P.M. Ajayan, H.S Nalwa, ed, AcademicPress, San Diego, 2000, Vol. 5, Chapter 6.
20. Hand Book of Nanophase and Nanostructured materials, volume I: Synthesis, Zhong Lin Wang, Yi Liu,Ze Zhang.

PAPER IV

CH(IC) 304T (Elective IVa): Analytical Techniques-II

IC-25: Thermal Methods
IC-26: Surface Analysis Methods/ Microscopicanalysis
IC-27: Advanced Separation Techniques
IC-28: Optical Methods

IC-25: Thermal Methods

Thermogravimetric analysis (TGA): Principle, Instrumentation, working function of each component, applications of TGA, Study of oxalates, nitrates and chromates by TGA. Determination of carbon black in polythene.

Differential thermal analysis (DTA): Principle, Instrumentation, Methodology, applications. Differential thermogram of sulphur. TG and DTA of manganese phosphine monohydrate.

Differential scanning calorimetry (DSC): Principle, instrumentation, power compensated DSC instruments and Heat flow DSC instruments, Methodology, DSC experiment calibration and data analysis. Applications determination Glass transition temperatures and heat capacities, problems based on Thermal Techniques:

Thermometric titrations: Principle, apparatus, applications to acid base, precipitation, complexometric, redox and non-aqueous titrations.

Combined thermal instruments: Introduction to TGA/MS and TGA/FTIR, High resolution TGA, Microthermal analysis.

IC-26: Surface Analysis Methods/ Microscopic analysis

Introduction, types of surface measurements.

Photon Probe Tecnhniques: X-Ray Photoelectron spectroscopy - Principle, Instrumentation, applications.

Electron Probe Techniques: Scanning electron microscopy (SEM) – Principle, Instrumentation, applications. Transmission Electron Microscopy (TEM) - Principle, Instrumentation, applications. Energy Dispersive X-ray Spectroscopy (EDX) - Principle, Instrumentation, applications. Electron Probe X-ray analysis (EPXMA) - Principle, Instrumentation, applications. Auger electron spectroscopy (AES) - Principle, Instrumentation, applications.

Ion Probe Techniques: Rutherford backscattering spectrometry (RBS) - Principle, Instrumentation, applications. Secondary ion mass spectrometry (SIMS) – Fundamental aspects of sputtering, Principle, Instrumentation (static & dynamic), applications

Scanning probe microscopy Techniques: Scanning Tunneling Microscopy – Principle, Instrumentation, applications. Atomic Force Microscopy - Principle, Instrumentation, applications.

IC-27: Advanced Separation Techniques

Separations by extractions: Solid phase extraction- Principle, methodology, applications. Solvent extraction of flow injection analysis. Applications to extractions of metal ions by chelating agents (Dithiazone, 8-hydroxy quinoline and cupferron). Organic reagents in Inorganic analysis - Theoretical basis for the use of organic reagents in inorganic analysis. Extraction of metal ions by the use of organic reagents – acetylacetone, thionyl-trifluoroacetone, tri-n-octyl phosphine oxide.

Affinity and chiral chromatography – Principle, technique, Instrumentation and applications.

Size Exclusion Chromatography – Principles of gel – filtration Chromatography, Instrumentation, retention behavior, resolution, selection of gel type, applications, **Ion exclusion** – Principle and applications.

Supercritical fluid chromatography (SFC) – Instrumentation of SFC, stationary and mobile phases used in SFC, Detectors, Advantages of SFC. Technique and applications of SFC.

GC-FT-IR: Instrumentation, Principles and Applications

IC-28: Optical Methods

CD, ORD and Fluorescence: Optical rotator dispersion and Circular dichorism: Principles - Optical rotation, circular birefringence, circular dichroism and Cotton effect, Octet Rule, Experimental Techniques, Use of CD in the conformational studies of metal complexes, DNA and DNA-metal complexes.Theory and principles of fluorescence spectroscopy. Characteristic of fluorescence emission, Fluorescence life time, quantum yield, Static and dynamic/collisional quenching and comparison.
Fluorescence polarization and polarization spectra of a fluorophore. Application of Fluorescence quenching in general and ligand/drug/metal complex DNA binding studies

SUGGESTED BOOKS

1. Principles of Instrumental Analysis: Holler, Skoog and Ccrouch, 6th edition ,Cengage Learning 2007.
2. Instrumental methods of chemical analysis B.K. Sharma, Goel Publishing House.
3. Instrumental Methods of analysis, Willard Mersritt, Dean and Settle, 7th edition, CBS Publishers 1986.
4. Analytical Chemistry – Gary D. Christian, 6th ed., John Wiley and sons. Inc., New York 1994.
5. Instrumental methods of Analysis - Willard, Merit, Dean, 6th ed., CBS Publishers & distributors, 1986.
6. Hand Book for Instrumental Techniques for Analytical Chemistry, Ed. Frank Settle, Prentice Hall, New Jersey, USA, 1997.
7. Vogel's Text book of Quantitative Analysis – GJ Jeffery, J Bassett et al, 5th ed., Longmann, ELBS Publications, 2000.
8. Principles of fluorescence spectroscopes – Lakowicz.
9. Fluorescence Quenching theory and applications – Maurice R. Eftink.
10. Circular Dichroism Spectroscopes of DNA Methods in Enzymology Vol 211.
11. Tris (Phenanthroline) Metal complexes: probes for DNA Helicity Journal of Biomolecular structure and Dynamics Adenine Press 1983. G.L. Eichorn.8
12. Tris (Phenanthroline) Ru(II) Enantiomers interactions with DNA : Mode and specificity of binding J.B. Chaires. Biochemistry 1993 (32) 2573

PAPER IV

CH(IC) 304T (Elective IVb): Nuclear Chemistry, Zeolites, Solid State, and Surface Chemistry

IC-29: Nuclear Chemistry
IC-30: Zeolites and Molecular Sieves
IC-31: Solid State Chemistry
IC-32: Surface Chemistry & Superconductors

IC-29: Nuclear Chemistry

Introduction: The atomic nucleus-elementary particles, quarks, classification of nuclides based on Z and N values, nuclear stability, nuclear potential, binding energy.
Nuclear structure: Shell model-salient features, forms of the nuclear potential, magic numbers, filling of orbitals, nuclear configuration, Liquid drop model, Fermi gas model, Collective model and Optical model.
Nuclear reactors :- General aspects of reactor design, thermal, fast and intermediate reactors, reactor fuel materials, reactor moderators and reflects, coolants, control materials, shield, regeneration and breeding of fissile matter, types of research reactors.
Nuclear reactions, fission and fusion, radio-analytical

Radioactivity, radioactive decay kinetics, Parent-daughter decay-growth relationship-secular and transient equilibria, theories of α, β-, β+ and γ-decay, internal conversion, Auger effect. Radio isotopes & its applications.

IC-30: Zeolites and Molecular Sieves

Introduction to porous materials:

Classification into micro-, meso- and macro porous materials, the origin of pores and its significance, distinction from condensed materials.

Zeolites:

Definition, natural and synthetic zeolite or aluminosilicates, the primary and secondary building blocks, final framework structures, Lowensteins rule, sodalite and other structures, Nomenclature: Atlas of zeolite; structural distinctions, Novel zeolites, examplels of small, medium, large and extra large pore zeolites; general properties and application of molecular sieves.

Characterization of zeolite:

XRD, SEM and other techniques; spectral techniques: FT-IR and solid-state NMR; sorption capacity, surface area by BET method, pore volume and pore structure, the origin of Brönsted and lewis acidity in zeolites, the number and the strength, techniques for the estimation of acidity: adsorption of bases and IR spectra, temperature programmed desorption of bases.

IC-31: Solid State Chemistry

Electronic structure of solids and band theory, Fermi level, K Space and Brillouin Zones.

Structure of ionic Crystals & Compounds: Ionic Crystals with stoichiometry MX, Ionic Crystals with stoichiometry MX_2, spinel structure, perovskite structure. 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)].

Crystal Defects and non-stoichiometry:

Classification of Defects: subatomic, atomic and lattice defects in solids; Thermodynamics of vacancy in metals; Thermodynamics of Schottky defects in ionic solids ; Thermodynamics of Frenkel defects in silver halides; Calculation of number of defects and average energy required for defect, Other examples of defect structure; Non-stoichiometry and its classifications.

Preparative method of solids:

Introduction, Ceramic method, microwave synthesis, Precursor method, Hydrothermal method, Chemical vapour deposition (CVD) Method, Chemical vapour Transport, Choosing a method for solids.

Crystal Growth: law governing nucleation; Growth of nuclei; Reaction between two solids; Improving the reactivity of solids; Zone refining method; Crystal growth.

IC-32: Surface Chemistry & Superconductors

Surface Chemistry:

Mechanism of catalytic reactions on the surfaces – diffusion of reactants to the surfaces, adsorption of reactants, reaction within the adsorbed layer, desorption of the products, diffusion of the products away from the surface; The mechanism of chemisorption on metals – The formation of chemisorptions layer, the character and nature of the chemisorption bond, the mechanism of chemisorptions for some gases; Nature of adsorbates on surfaces.

Superconductors:

Discovery of super conductors, Meissner effect, Type I and II conductors, Leavitation, BCS theory and Cooper pairs, High Tc Super Conductors, applications of super conductors.

SUGGESTED BOOKS

1.Essentials of nuclear chemistry, 4th edition; H. J. Arniker, NAIL publishers (1995);
Chapters 1, 3 and 4.

2. Nuclear and Radioactive chemistry; Friedlander, Kennedy and Miller; Chapters 8and 9.
3.Introduction to zeolite science and practice, H. Van Bekkum, E. M. Flanigen, P. A. Jacobs and J. C. Jansen (Elseviver Pub. Amsterdam, 2001)
4.Breck.D.w. Zeolites molecular sieves- Structure, chemistry and use. John Wiley & Sons N.Y. (1974).
5.Solid-State Chemistry an Introduction (2nd Edition) – Lasley Smart and Elaine Moore (Chapman & Hall 1996)
6. Solid State Chemistry- D.K.Chakraborty(New Age International Pvt.Ltd.New Delhi, 2000)
7. Introduction to Soilds-L.V.Azaroff(tata McGraw Hill Publication Ltd. New York)
8. Principles of the Solid State-H.V.Keer(Wiley Eastern Ltd.New Delhi, 1994)
9. Solid state Chemistry –N.B.Hannay(Prentice Hall, New Jersey, 1967)
10.Superconductivity, Joi, Khachan& Stephen Bio Science, -----
11.Chemisorption, B. M. W. Trapnell, Butterworths Scientific Publications, London, 1955.
12.Adsorption on solids, VladimirPonec, ZlatkoKnor, SlavojCerny, Butterworth & Co – publishers, 1974.
13.Catalysis: Principle and Applications, B. Viswanathan, S. Sivasanker, A. V. Ramaswamy, Narosa Publishing House, 2002.

LABORATORY COURSES (III Semester)

Paper CH (IC) 351: Synthesis and Characterization of Metal Complexes

Laboratory preparation and characterization of *3d* transition metal complexes of *tetrahedral*, *square planar* and *octahedral* geometries.

1. $VO(acac)_2$
2. $CoCl_2(Py)_2$
3. $Na[Cr(NH_3)_2(SCN)_4]$
4. Prussian Blue, Turnbull's Blue Complexes
5. $K_3[Cr(C_2O_4)_3]$ $3H_2O$: UV, IR, TGA and estimation of oxalate.
6. Solid phase synthesis of trans-bis(glycinato)copper(II): IR, estimation of Cu by iodometry
7. $Fe(acac)_3$: FTIR
8. Cis and trans $[CoCl_2(en)_2]Cl$: conversion of cis to trans and trans to cis by IR.
9. Potassium bis(peroxo)oxo(1,10-phenanthroline)vanadium(V) trihydrate: IR,TGA, estimation of vanadium and peroxide
10. Tetra-butylammoniumhexamolybdate(VI): IR, estimation of Mo
11. MnO_2nano particles; SEM, SEM by adding CTAB

SUGGESTED BOOKS

1. *Practical Inorganic Chemistry*, G. Marr and B. W. Rockett.
2. Practical Inorganic Chemistry by G.Pass H.Sutchiffe,2ndedn John Wiley & Sons.
3. *Experimental Inorganic/Physical Chemistry,* M. A. Malati, HorwoodPublishing,Chichester, UK (1999)

Paper CH (IC) 352: Electro-analytical techniques

I Potentiometry

Potentiometric Titrations and Calculation of End Point Potentials for the following systems:
i) $Fe^{2+}$and VO^{2+} Mixture vs Ce^{4+}
ii) Assay of sulphanilamide
iii) Silver electrode for silver assay
iv) Mixture of halide anions using Silver electrode

II pH-metry

1. Determination of CO_3^{2-} and HCO_3^- in a mixture
2. Determination of the dissociation constants of

(i) Ethylenediamine (en)(H_2 L) (ii) Glycine (HL) (iii) Histidinemonohydrochloride (H_2L)

3. Determination of binary constants of i) Cu(II) -en and (ii) Ni(II) -His iii) Ni(II) – Gly Systems
4. Determination of stability constant of ternary (o-Phen-Ni(II)-His) system - Calculation of Log K.

III Conductometry:

1. Determination of the Composition of Cu(II)-oxine and Cu(II)-EDTA Complexes
2. Interaction of Pyrophosphate with Mg^{2+}, Ca^{2+}, Mn^{2+} and Cu^{2+}
3. Determination of Aspirin with KOH

IV Ion selective electrodes method (Ionimetry)

1. Estimation of fluoride ion in water
2. Estimation of nitrate ion in water
3. Estimation of ammonia in water

V Polarography

1. Determination of $E_{½}$ of Cd^{2+} and Pb^{2+}
2. Verification of Ilkovic equation by using Cd^{2+} solution
3. Determination of Stability Constants of Cd^{2+} and Pb^{2+} complexes

VI Electrogravimetry

1. Determination of Copper and Nickel individually and in a Mixture

SUGGESTED BOOKS

1. A Text Book of Quantitative Inorganic Analysis by A.I.Vogel 3rd Edition Elbs Publication 1969.
2. Vogel's Text Book Of Quantitative Inorganic Analysis Jeffery etal 4th edition Elbs Publications 1988.
3. Vogel's Text Book of Quantitative Chemical Analysis, 6th edition. Pearson Education Ltd 2002.
4. Determination and use of Stability Constants – Martell and Motekaitis VCH Publishers INC 1988.
5. Metal Complexes in Aqueous Solutions A.E.Martell and R.D. Handcock, Plenum Press, New York – 1996.
6. Analytical Chemistry by Gary D.Christian 6th EditionJohnWiley&SonsInc New York 1994.

M.Sc. INORGANIC CHEMISTRY SPECIALIZATION
SEMESTER-IV
PAPER I

CH(IC)401T: Molecular Spectroscopy of Inorganic Compounds

IC-33: Multinuclear NMR
IC-34: Advanced NMR techniques
IC-35:Applications of ESR to Metal Complexes
IC-36:Mossbauer Spectroscopy and Nuclear Quadrupole Resonance Spectroscopy

IC-33: Multinuclear NMR

^{13}C nmr spectroscopy: CW and PFT techniques. Types of ^{13}C nmr spectra: undecoupled, proton-decoupled, single frequency off-resonance decoupled (SFORD) and selectively decoupled spectra. ^{13}C chemical shifts, factors affecting the chemical shifts.

Chemical equivalence and magnetic equivalence. Virtual Coupling and its importance in study of Metal Complexes $[Pd\{P(CH_3)_3\}_2I_2]$. Spin Dilute Systems-Satellites in Pt(II) Complexes cis-$[Pt(PEt_3)_2Cl_2]$, $Sn(CH_3)_4$. NMR Time Scale and its use in studying Stereo chemical Non –rigidity (PF_5, $[Rh(PR_3)_5]^+$, $[Fe\{Cp\}_2(CO)_2]$) -ΔR, the Ring Contribution to ^{31}P Chemical Shifts –Metal and Chelate size on ΔR. Applications of ^1H, ^{13}C, ^{19}F, ^{31}P and ^{15}N to simple inorganic and Coordination Compounds - 1)^{1}H-NMR: $PtHCl(PEt_3)_2$,$Pt(NH_3)_3(CH_3)_3$, BH_4^-, NH_4^+, CH_3CN, [^{6}h- C_7H_8 $Mo(CO)_3$], [^{7}h-$C_7H_7Mo(CO)_3]^+$, B_2H_6; $^{29}SiH_3SiH_3$, 2)^{19}F: BF_4^-, H_2PF_3 3)^{31}P: $Mo(CO)_3(PPh_3)_3$, [Rh $(PPh_3)_3Cl$] ,trans-$[PtCl_4(PEt_3)_2]$, $^{31}PF_2H(^{15}NH_2)_2$ 4) 13C; [^{4}h $C_8H_8Ru(CO)_3$], $Fe(CO)_5$, $Fe_2(CO)_9$, $Fe_3(CO)_{12}$, $FeICp(CO)_{12}$, [$^{13}C^{15}N$ $Co(DH)_2$Pyridine]. $^{13}C\{^1H\}$ NMR spectrum of σ-bonded C_6H_5 ligand.

IC-34: Advanced NMR techniques

Spin-Lattice (T_1) and Spin-Spin Relaxation (T_2). Spin Echo Polarization Transfer – Spin Echo Measurements. ^{13}C-NMR spectral editing techniques: Attached proton test (APT spectra) by Gated Spin Echo, Cross polarization, INEPT spectra, DEPT spectra (Distortionless enhancement by polarization transfer). INADEQUATE spectra (Incredible Natural Abundance Double Quantum Transfer Experiment).

Two Dimensional NMR: Basic principles, Types of 2-D NMR ;i)J- resolved spectroscopy a)homo and b)Heteronuclear J- resolved spectroscopy ii) Correlation spectroscopy ; Homo nuclear shift correlation spectroscopy (COSY) and Hetero nuclear shift correlation spectroscopy (HETCOR) iii) NOESY(Nuclear Overhauser Enhancement Spectroscopy). HOESY (two dimensional heteronuclear NOE). Advantages of 2-D NMR

IC-35:Applications of ESR to Metal Complexes

Principle- Selection Rules – Instrumentation- Microwavesource (energy bands). Application of ESR to the study of simple free radicals: methyl ($CH_3^{\cdot}$), amine ($NH_2\cdot$), diphenylpicrylhydrazyl,cyclopentadienyl ($C_5H_5^{\cdot}$), hydroxy methyl ($CH_2OH\cdot$) radicals. Zero-Field Splitting (ZFS) - Effective Spin - Orbitally Non-degenerate and Degenerate States. ESR Spectra of d^1-d^9 Transition Metal Complexes with examples. Interpretation of g in cubic, axial and rhombohedral geometries. Factors affecting g values. Calculation of g values with simple examples. Intensities of '$g_\parallel$ and $g_\perp$peaks. Evidence for Metal-Ligand Bond Covalency- Cu(II)- Bis –Salicylaldimine. $[(NH_3)_5\ Co\ O_2\ Co\ (NH_3)_5]^{5+}$, Cu(II)- diethyldithiophosphinate, Vanadyldithiophsphinate, Copper(II) tetraphenylporphyrin, Co(II)- phthalocyanine, $K_2[IrCl_6]$. Interpretation of 'g' and 'A' values from esr spectral data in- i) MnF_6^{4-}, ii) CoF_6^{4-}, and CrF_6^{3-}. ESR spectra of dinuclear Cu (II) complexes.

IC-36 Mossbauer and Nuclear Quadrupole Resonance Spectroscopy

Mossbauer Spectroscopy: Principle, Experimental Considerations and Presentation of the Spectrum - Isomer Shifts – Quadrupole splitting and Magnetic hyperfine splitting - Selection Rules.

Applications

Iron Compounds: Low-spin and High-spin Fe(II) and Fe(III) Complexes - π-bonding Effects in Iron complexes - Study of High-spin Low-spin Cross-over c) Diamagnetic and Covalent Compounds - Structural aspects of Iron Carbonyls and Iron-Sulfur Proteins.

Tin Compounds: Tin Halides and Organotin Compounds.

Iodine Compounds: Isomer Shifts of ^{127}I and ^{129}I - Applications to Alkali metal iodides and Molecular Iodine. Mossbauer spectra of IF_6^- and IF_6^+

Nuclear Quadrupole Resonance Spectroscopy: Principle, nuclear quadrupole resonance experiment, Structural information from NQR spectra- $PFCl_4$, PCl_4Ph, $Ga_2Cl_7^-$ and $TeCl_4$ Interpretation of nuclear quadrupole coupling constants.

SUGGESTED BOOKS

1. Structural Methods in Inorganic Chemistry, E. A. V. Ebsworth, D. W. H. Rankin and
2. S. Craddock, ELBS.
3. Physical Methods in Chemistry, R. S. Drago, W.B. Saunders Co., 1977.
5. Physical Methods for Chemists, Russell S. Drago Second edition, Saunders College Publishing, 1992.
6. Principles of Mossbauer spectroscopy, T. C. Gibb, Chapman and Hall, London, 1976.
7. Mossbauer Spectroscopy, N. N. Greenwood and T. C. Gibb, Chapman and Hall, London, 1971.
8. Principles of Instrumental Analysis, Skoog, Holler and Nieman.
9. Instrumental Techniques for Analytical Chemistry, Frank Settle.
10. Principles of Analytical Chemistry, M. Valcarcel.
11. Physical Methods in Advanced Inorganic Chemistry, Hill and Day
12. Magneto Chemistry, Dutta &Shyamal Oxford Chemistry Primers, Vol 62

PAPER II

CH(IC) 402T: Bioinorganic Chemistry

IC-37: Metal ions Interactions with Nucleic acids and their constituents
IC-38: Transport of Electrons and Metal ions
IC-39: Metallo-Enzymes of Iron, Zinc and Nickel
IC-40: Metallo-Enzymes of Cobalt, Copper, Molybdenumand Manganese

IC-37: Metal ions Interactions with Nucleic acids and their constituents

Nucleic Bases, Nucleosides and Nucleotides. Proton Binding Sites of Nucleic Acid Constituents-Purine and Pyrimidine Bases, Nucleosides and Nucleotides. The covalent structure of polynucleotides, secondary structure of DNA: The double helix anti and syn conformations of nucleotides. B, A, & Z forms of DNA. General Factors that influence Metal Ion Binding Sites in Solution – Specific Metal Ion Binding to Nucleic Bases, Nucleotides and Nucleosides in Solution: Stability of Phosphate- Metal ion complexes, Metal binding Metal Ion Complexes, Metal Binding Sites in Nucleosides, Nucleotide - Metal Ion Interactions - Intramolecular Equilibrium Constant KI, Percentage of Closed Isomers - Outer Sphere and Inner Sphere Isomers of M-ATP Complexes and Metal Ion Nucleic Base Interactions.

Metal-DNA and RNA Interactions: Potential Binding Sites (Elementary Treatment) – Influence of Metal Ions on Stability of Nucleic Acids.

IC-38: Transport of Electrons and Metal ions

Transport of Electrons: Iron-Sulphur Proteins: Rubredoxins and Ferredoxins (2Fe,3Fe, 4Fe, 8Fe Proteins) -High Potential Iron-Sulphur Proteins – Structural andSpectral features of Iron-Sulphur Proteins - Electron-transport by Cytochromes,Azurin and Plastocyanin - Importance of Structures of Azurin and Plastocyanininfacilitating Rapid Electron Transport, acotinase- Fe-S enzyme.
Transport and Storage of Metal Ions: Iron-Transport by Transferrin and Siderophores – Ferritin in Iron Storage - Transport of Na+ and K+ across Cell Membranes by Na^+- K^+ ATPase - Transport of Calcium across Sarcoplasmic Reticulam by Ca^{2+}-ATPase.

IC-39: Metallo-Enzymes of Iron, Zinc and Nickel

Iron Enzymes: Structural and Mechanistic Aspects of Cytochrome P450, Cytochrome oxidase,Catalase and Peroxidase - Role of the Metal Ion.
Zinc Enzymes: Structural and Mechanistic Aspects of Carbonic Anhydrase, CarboxyPeptidase,Leucin – aminopeptidase, Thermolysin, Alcohol Dehydrogenase - Role of Zinc.
Nickel Enzymes: Urease, Hydrogenase and Factor F430: Reactions Catalyzed, MechanisticAspects.

IC-40: Metallo-Enzymes of Cobalt, Copper, Molybdenum and Manganese

Cobalt Enzymes: Cobalt in Vitamin B12 - Structural Features of Vitamin B12 with reference to coordination of Cobalt - Different Oxidation States of Cobalt - Various forms of Vitamin B12 and Active Enzyme forms - Types of Reactions Catalysed by i) Methyl Cobalamin ii)DeoxyadenosylCobalamin - Mechanism of the Methyl Malonyl CoA conversion to Succinyl CoA - Role of the Apoenzyme - Unique features of Cobalt to suit Vitamin B12.
Copper Enzymes: Types of Copper in Biological Systems - Structural and Mechanistic Aspects of Superoxide Dismutase, Laccase and Galactose oxidase.
Molybdenum Enzymes: Biological Roles and Mechanistic Aspects of Nitrogenase, Xanthineoxidase and Sulfite oxidase.
Manganese Enzymes*:*Arginase, Water – oxidase.

SUGGESTED BOOKS

1. Biochemistry - Geoffrey L. Zubay.
2. Biochemistry - Mary K. Campbell. (added these books)
3. Bioinorganic Chemistry, Bertini, Gray, Lippard and Valentine, University ScienceBooks, California USA 1994.
4. Principles of Bioinorganic Chemistry, S.J. Lippard and M.Berg University ScienceBooks, California 1994.
5. Biological Chemistry of Elements, J.J.R. Franstodasilva and R.J.P. Williams OxfordUniversity Press 1991.
6. Metal Ions in Biological Systems (Series), Ed. H. Sigel Marcel Dekkar, New York
7. Inorganic Biochemistry, J.A. Cowan, VCH publishers 1993.
8. Advances in Inorganic Biochemistry, edited by G.L.Eichorn&Marzilli
9. Bioinorganic Chemistry, Vol-I edited by G.L.Eichorn.
10. Interactions of metal ions with nucleotides and nucleic acids and their constituents Helmut Sigel Chem. Soc. Rev., 1993,22, 255-267.

PAPER III

CH(IC)403T(Elective IIIa):Medicinal Inorganic Chemistry, Spectroscopic Analysis of Drug/Metal Complexes and Applications of Nanomaterials

IC-41: Metal complexes in Clinical Chemistry
IC-42: Metal complexes as Drugs and Anticancer agents
IC-43: Spectroscopic analysis of drug/metal complexes binding to DNA
IC-44: Applications of Nanomaterials

IC-41: Metal complexes in Clinical Chemistry

Theory and mode of action of therapeutic chelating agents , Single ligand Chelation Therapy – Aminopolycarboxylic acids, Desferrioxamine, pencillamine, triethylenetetramine, Mixed ligand chelation therapy - Metallothionens in detoxification. Role of metal ions in the action of antibiotics: Bleomycin, adriamyacin and tetracyclines. Gold-Containing drugs used in therapy of Rheumatoid arthritis - A therapeutic agent for Menkes disease: Copper-histidine - Anti viral chemotherapy and metal peptide interaction.

IC-42: Metal complexes as Drugs and Anticancer agents

Introduction to Pt(II) chemistry– Thermodynamic and kinetic principles – *Cis*and*Trans* influences – Thermodynamic and kinetic aspects. Steric and electronic tuning of reactivity.

Platinum complexes in cancer therapy: Discovery applications and structure-effect Relationships. Cis-platin(cis$Pt(NH_3)_2Cl_2$) mode of action. Potential binding sites on nucleic acids and their bases and proteins. Drug resistance and DNA repair mechanism.

Physical effects of metal complex: DNA binding, unwinding, shortening and bending of the double helix. Biological consequences of platinum –DNA binding. Organic intercalatorsasdonor – acceptor pairs; Transition metal complexes as donor acceptor pairs. Non classical platinum antitumour agents.

IC-43: Spectroscopic analysis of drug/metal complexes binding to DNA

Introduction to DNA binding studies. Cooperativityanticooperativity, the excluded site model. UV-Vis Absorption Spectroscopy and ligand/drug/metal complex DNA binding studies. Application of Fluorescence quenching in general and ligand/drug/metal complex DNA binding studies. Fluorescence titrations and binding constants. Salt back titrations interpretation of the data, the binding analysis,obtaining equilibrium binding isotherms. Dependence of K_{obs}on salt concentration, cation effects on ligand nucleic acid equilibria, Competitive effects of monovalent and divalent cations for binding. Record's polyelectrolyte theory and its importance. Equilibrium dialysis. Partition analysis, competitive equilibrium dialysis to assess B & Z DNA binding. Competition dialysis to assess base and sequence specificity, viscosity studies. Tertiary structure of DNA, Supercoiled DNA(Form-I), Nicked DNA (Form-II) and Linear DNA(Form-III). DNA cleavage activity with ligand/metal complexes-Analysis by Gel electrophoresis.

IC-44: Applications of Nanomaterials

Nanotechnology in modern technology in relation to electronic, biological, consumer and domestic applications. Energy related application: photo-volatile cells. Energy storage nanomaterials.

Sensors: Agriculture, health and medical, food, security.

Applied nanobiotechnology and nanobiomedical science drug delivery, drug targeting, biosensors, bioimaging, neutron capture therapy.

SUGGESTED BOOKS

1. Bioinorganic Chemistry. Inorganic elements in the Chemistry of life, WolfgangKaim&BrigetteSchwederdki.
2. Bioinorganic Chemistry, Bertini, Gray, Lippard and Valentine, University ScienceBooks, California USA 1994.
3. Handbook of Metal-Ligand interactions in Biological fluid Bioinorganic medicine, Vol – Edt. Guy Berthon.
4. Bioinorganic Chemistry, Rosette M. RoatMalone.
5. Photoreactions of Metal complexes with DNA, A. Krisch – De Mesmacker et al.
6. Drug - Nucleic Acid Interactions, Volume 340 Jonathan B. Chaires, Michael J. WaringAcademicPress,2001.
7. Mechanistic Bioinorganic Chemistry Edited by byH.Holden Thorp and Vincent L. Pecoraro, Chemical Society, Washington DC 1995.
8. Metal Complex -DNA Interactions, Editor(s): Nick Hadjiliadis, EinarSletten, Copyright @ Blackwell Publishing Ltd.
9. Gel Electrophoresis - Principles and basics edited by SamehMagdeldin ISBN 978 - 958 -51-0458-2, 376 pages, Publisher: InTech, April 04, 2012
10. Encylopedia of nanomaterials and nanotechnologies, H. S. Nalva.
11. Nanostructures materials: Processing, Properties and applications, C. C. Kouch, WilliamAndrew publications, New york, 2002.
12. Introduction to nanotechnology, C. P. Poole Jr, F. J. Owens, 2nd edition, Wiley-India,Delhi, 2008.

PAPER III

CH(IC)403T(Elective IIIb):Analytical Techniques -III

IC-45: Electroanalytical Methods
IC-46: Radiochemical Methods
IC-47: Fluorimetry, Phosphorimetry, Nephelometry and Turbidimetry
IC-48: Industrial Analysis

IC-45: Electroanalytical Methods

pH-metry: Accuracy of direct potentiometer measurements. The Glass pH electrode – Theory, construction, standard buffers, accuracy of pH measurements, measurements with the pH – meter, pH titration of unknown soda ash.

Electrogravimetry: Basic principles of electrogravimetry, Instrumentation, electrogravimetry determination with constant applied voltage and at constant current. Applications of electrogravimetry. Problems based on effect of concentration on electrode potentials, calculation of theoretical cathode potential at the start of deposition, effect of pH in electrolytic separations.

Coulometry : Basic principles, Types of coulometers, constant current coulometric analysis, coulometric titrations – principle, circuit and cell for coulometry, Application to neutralization, Redox, precipitation, complexometric titrations, Advantages of coulometric titrations and errors. Controlled potential coulometry – Technique & applications of inorganic & organic compounds.
High Frequency Titrations: Introduction, Theory, Instrumentation, Applications, Advantages and disadvantages.

IC-46: Radiochemical Methods

Radioactive nucleotides, Instrumentation – measurement of alpha, Beta particles and Gamma radiation. Radio tracers and tracer techniques, applications of Tracer techniques,

Neutron activation analysis: Neutron sources, interaction of neutrons with matter. Theory of activation methods, Experimental considerations, Nondestructive and destructive methods, applications.

Isotopic dilution analysis: Principles, theory and Applications.

Radiometric titrations: Principle, Procedure, advantages & disadvantages, applications to various types of titrations, problems based on the techniques.

Applications of Radio Chemical Methods in Biology, Agriculture and Environment

IC-47: Fluorimetry,Phosphorimetry, Nephelometry and Turbidimetry

Fluorimetry and Phosphorimetry: Theory of Fluorescence and Phosphorescence- Excited states producing Fluorescence and Phosphorescence. Rates of absorption and emission. Deactivation processes, Variables affecting Fluorescence and Phosphorescence. Types of Photoluminescence spectra for Phenanthrene. Instrumentation – Components of Fluorimeter, Spectroflourimeters and Phosphorimeters. Applications of Fluorimetry - Determination of Inorganic Cations, Fluorimetric reagents. Fluorimetric determination of organic species – Thiamine, Aneurine Hydrochloride, Polycyclic aromatic hydrocarbons. Phosphorimetry- Determination of Aspirin in blood serum. Chemiluminescence-Origin, measurements. Analytical applications- Atmospheric pollutants (Oxides of Nitrogen and Sulphur compounds, Ozone).

Nephelometry and Turbidimetry: Light scattering, principle and theory ofNephelometry and Turbidimetry, Effect of concentration, particle size and wavelength on scattering, instrumentation for Nephelometry and Turbidimetry. Turbidimetric titrations. Applications of Nephelometry and Turbidimetry.

IC- 48: Industrial Analysis

Analysis of Ferroalloys: Analysis of steel - Molybdenum, Phosphorous.

Analysis of non- Ferrous alloys: Analysis of Tin, Zinc and Copper in Brass, Bronze. Analysis of Tin and lead in Solder.

Analysis of Cement: Composition of Portland cement, estimation of Aluminium oxide and Ferrous oxide. Determination of Alumina in Cement by Polarography.

Analysis of Oils & Fats: Theory, Melting point of fats, Chemical Characteristics: Saponification value, Iodine value, Thiocyanogen value, ketone or perfume rancidity.

Soaps & Detergents: Composition of Soaps. Determination of low level Surfactants, determination of Germicides in soaps and detergents by photometric method, analysis of phosphates by paper chromatography, determination of detergent alkylates by Mass Spectrometry.

Paints& Pigments: Constituents of Paints, Analysis of TiO_2 in Titanium dioxide pigments by XRD. Determination of Zn, Pb in Paint pigments by Polarographic method. Analysis of polyesters, acrylics by Gel permeation chromatography.

SUGGESTED BOOKS

1. Principles and practice of Analytical Chemistry, F.W.Fifield& D Kealey, 5th Ed.Blackwell Science, 2000
2. Principles of Instrumental Analysis: Holler, Skoog and Crouch, 6th education, Cengage Learning 2007.
3. Instrumental methods of chemical analysis B.K. Sharma, Goel Publishing House.
4. Analytical Chemistry: Gary D Christian.6th edition.
5. Principles of Instrumental Analysis - Skoog, Holler, Nieman, 5th ed., Harcourt College Publishers, 1998.
6. Principles and practice of Analytical Chemistry, F.W.Fifield& D Kealey, 5th Ed. Blackwell Science, 2000.
7. Quantitative Chemical Analysis, Daniel C. Harris, 6th Ed. WH Freeman & Co. NewYork, 2003.
8. Analytical Chemistry an Introduction, Crouch, 7th Ed. Saunders College Publishing,2000.

9. Standard methods of Chemical analysis, 6th ed., volumes I to IV. Edited by F.J. Welcher: D. Von NostrnadCo. Inc., Princeton N.J. 1966.
10. Biochemical Methods – S. Sadasivam, A. Manickam, 2nd ed., New Age International (P) Ltd., 1997.

PAPER IV

CH(ID) 404T(Elective IVa): Interdisciplinary Course (ID) (Environmental and Applied Analysis)

IC-49: Clinical and Pharmaceutical Analysis
IC-50: Food and Agricultural analysis
IC-51: Analysis of Air and Water Pollutants
IC-52: Drinking Water and Sewage Water Treatment

IC-49: Clinical and Pharmaceutical Analysis

Clinical analysis: Analysis of Carbohydrates and their significances – Fasting, random and post pandrial glucose tests, Estimation of Glucose in serum. Analysis of lipids and their significances –Test for cholesterol. Analysis of proteins and their significance – Estimation of total protein in serum.
Analysis of Major metabolites and their significance – Determination of Blood urea and Creatinine in urine. Analysis of ions and their significance: Estimation of Na, K, Ca, bicarbonates and phosphate in serum. Analysis of Hormones and their significance-ELISA and RIA.

Pharmaceutical analysis: Determination of Diclofenac (non-aqueous titration), Calcium inVitamin D and Calcium formulations (Complexometry), Sulphanilamide (potentiometry),Pethidine hydrochloride (UV-Vis), Frusemide (UV-Vis), Aspirin,paracetamol and codein in APC tablets (NMR), Phenobarbitone in tablets (IR), pivolic acid indipivefrin eye drops (GC), Assay of hydrocortisone cream. (HPLC).Impurity profiling of Propranolol (GC-MS), famotidine (LC-MS).

IC-50: Food and Agricultural analysis

Analysis of Chemical additives: Division of colour additives (Coal-tar dyes, vegetable colours and mineral colours). **Chemical preservatives** and synthetic sweetening agents (organic-ether extractable and non-ether extractable) SO_2, Sodium Benzoate, Sorbic acid, Benzoic acid.
Antioxidants: Types of Antioxidants used in foods, Analysis of Butylatedhydroxy toluene (BHT), propyl – gallates (PG), Octylgallates (GO), dodecyl gallates (DG) by TLC & GC.
Food adulteration: Common adulterants in food, contamination of food stuffs. Microscopic examinations for food adulterants.
Analysis of Soil – Determination of pH, conductivity, cation exchange capacity, total organic matter, nitrogen, phosphorous, potassium, S, Ca, Mg, Ca+Mg, Zn, Cu, Fe, Mn, B, Mo, Cd, Cr, Ni, Pb.
Analysis of Fertilizers – Moisture determination by Karl Fischer titration methods. Determination of Ammonical nitrogen and Ammonical nitrate nitrogen. Determination of total phosphates as P_2O_5. Estimation of potassium, Estimation of micronutrients by AAS.
Analysis of Pesticides: Analysis of Organo-chlorine pesticides (Cypermethrin) by Gas Chromatography. Determination of Malathion, Methyl parathion and DDT residues in vegetables and food grains.

IC-51: Analysis of Air and Water Pollutants

Air quality standards, sampling, analysis of air pollutants-SO_2 (UV-Vis, IR), H_2S (Spectrophotometry and Non-dispersive IR Spectrophotometry), NO-NOx (Chemiluminescence technique, Colorimetric technique- Saltzman method), CO & CO_2 (IR, AAS & GC), Hydrocarbons (GC, GC-MS), Aromatic hydrocarbons in automobile exhaust, petrol, air, O_3 (Chemiluminiscence& Spectrophotometry), particulate matter analysis. Objectives of analysis, sampling, preservation and pre-concentration methods, physical analysis - colour, odour, temperature, pH, EC, redox potential, total desolved solids (turbidimetry), Chemical analysis of anions – CN^-, Cl^-, F^-, NO_2^-, NO_3^- (spectrophotometry), SO_4, PO_4.

Determination of BOD, COD, TOC & DO. Analysis of Toxic Metals: Hg, As, Pb, Cd, Be, Al, Cr (Atomic Absorption Spectroscopy and Spectrophotometry)

IC-52: Drinking Water and Sewage Water Treatment

Hardness: causes, measurement of hardness, units- types of hardness, estimation of temporary and permanent hardness, Alkalinity of water and its estimation.

Treatment of Water for Municipal Supply: Characteristics of potable water/Domestic water, WHO standards, and Indian Standards. Aeration, Sedimentation with coagulation, Filtration, Sterilization and Disinfection: Physical Methods-Boiling, Exposure to Sunlight, Disinfection with UV light, Chemical Methods – Ozonization, Chlorination, Breakpoint chlorination and Dechlorination

Desalination of Brackish Water: Treating saline water: distillation, electrodialysis, reverse osmosis (RO).

Mineral Water and Purified Water: Typical Manufacturing Process, Flow Sheet Diagram of Mineral Water Manufacturing Process, Purified Water-Purification methods-Distillation, Double distillation, Deionization - Co-current deionization, Counter-current deionization, Mixed bed deionization, Demineralization, Uses of purified water- Laboratory use, Industrial uses and other uses; Health effects of drinking purified water

Sewage Water Treatment: Domestic sewage - Physical, Chemical, and Biological Characteristics of Domestic Sewage, Municipal sewage, Sewage Composition and Contaminants, Sewage Treatment - On-Site Sewage Treatment Systems and Off-Site Sewage Treatment Systems

SUGGESTED BOOKS

1. Medical Laboratory Technology – Mukherjee,McGraw Hills,1988.
2. Medical Laboratory Technology – RamnikSood, Medical Publishers Pvt. Ltd., 1999.
3. Biochemical Methods – S. Sadasivam, A. Manickam, 2nd ed., New Age International (P) Ltd., 1997.
4. Practical Pharmaceutical Chemistry, A.H. Beckett et al, 3rd ed. – Vol. 1 & Vol. 2 CBS Publishers & Distributors, 1986.
5. Pharmaceutical Analysis - P. Primoo. CBS Publishers, New Delhi, 1999.
6. Text book of Pharmaceutical Analysis – Kenneth. A. Connors, John Wiley & Sons, 1999.
7. Pharmaceutical Chemistry, Instrumental techniques vol-2, Ed. Lesile. G.Chatten.
8. Pharmaceutical Drug Analysis – Asuthoshkar, Minerva Press, 2001.
9. Handbook of analysis and quality control for fruit and vegetables products – S. Ranganna, 2nd edition, Tata McGraw-Hill Publishing Ltd., 1986
10. Introduction to the Chemical Analysis of Foods, S. Suzanne Neilsen, CBSPublishers, New Delhi, 2002.
11. A Text book of Soil Chemical Analysis – P.R. Hesse, CBS Publications, 1998.
12. Methods of Analysis of Soils, Plants, Water and Fertilizers – Ed, HLS Tandon, FDCO publications, New Delhi, 1999.
13. Vogel's Text Book of Quantitative Chemical Analysis, 6th Ed, Pearson Education Ltd.
14. Environmental Pollution Analysis, S M Khopkar, Wiley Eastern Ltd 1995.
15. Environmental Analytical Chemistry, F W Fifield, P J Haines, Blackie AcademiProfessional.
16. Environmental Chemistry, B K Sharma, Goel Publishing House, Meerut.
17. "A Textbook of Engineering Chemistry", Dr. Y. BharathiKumari and Dr. JyotsnaCherukuri, VGS Publications, First Edison, India, 2009.
18. "Engineering Chemistry", Jain P C and Monica Jain, 15th Edition, DhanpatRai Publishing Company Ltd, New Delhi, India, 2005.
19. Textbook of Engineering Chemistry, C Parameswara Murthy, C V Agarwal, Andra Naidu, BS Publications, Hyderabad, India
20. Water Encyclopedia - Domestic, Municipal, andIndustrialWaterSupply and Waste Disposal, Jay H. Lehr and Jack Keeley, Wiley-Interscience, Published by John Wiley & Sons, Inc., Hoboken, New Jersey.
21. Handbook of Water and Wastewater Treatment Technologies, Nicholas P. Cheremisinoff, PublishedbyButterworth-Heinemann, 225Wildwood Avenue, Woburn, MA 01801-2041
22. Purified water: https://en.wikipedia.org/wiki/Purified_water#Purification_methods

PAPERIV

CH(ID) 404T(Elective IVb): Interdisciplinary Course (ID) (Inorganic Material Chemistry)

IC-49: Composite Materials
IC-50: Liquid Crystals
IC-51: Explosives and Propellants
IC-52: Fuels and Combustion

IC-49: Composite Materials

Introduction, Advantageous Properties of the Composites, Constituents of Composites, Types of Composites – Fibre-reinforced composites (Glass, carbon, Armid, Alumina reinforced composites), Particulate composites, Layered composites, Processing of Fibre-reinforced Composites, Micromechanics of Fibre and Particle Reinforced Composites, Fabrication of the Composites.

Refractories: Characteristics and Classification of Refractories, Properties of Refractories, Manufacture of Refractories, Common Refractories Bricks – Silica Bricks, Alumina Bricks, Magnesite Bricks, Dolomite Bricks, Carbon Bricks and Chromite Bricks.

Ceramics: Plasticity of Clays, Whitewares or White-Pottery, Manufacture of White-Pottery, Glazing, Methods of glazing, Earthenwares and Stonewares.

IC-50: Liquid Crystals

Introduction, Types of Mesophases, Characterization of Liquid Crystals, Physical Properties of Liquid Crystals, Structure of Liquid Crystal forming compounds, Classification of Liquid Crystals-Thermotropic Liquid Crystals and Lyotropic Liquid Crystals, Chemical Properties of Liquid Crystals, Applications with special reference to Display systems, Applications and Importance of Lyotropic Liquid Crystals, Future of Liquid Crystals.

IC-51: Explosives and Propellants

Explosives: Introduction, Classification of Explosives, Primary Explosives, Low Explosives, High Explosives, Precautions During Storage of Explosives, Blasting Fuses, Manufacture of Important Explosives-Lead azide, Diazonitrophenol (DDNP), Trinitrotoluene (TNT), Nitroglycerine (NG) or Glycerol trinitrate (GTN), Pentaerythritaltetranitrate (PETN) and RDX; Recent uses of Explosives

Propellants: Rocket Propellants - Introduction, Principle of Rocket Propulsion, Classifications of Propellants-Solid propellants, Composite propellants, Liquid Propellants, Mono-propellants, Bi-propellants; Differences between Solid propellants and Liquid Propellants

IC-52: Fuels and Combustion

Introduction, Classification of Fuels, Calorific Value, Characteristics of a Good Fuel, Theoretical Calculation of Calorific value of a Fuel, Coal, Classification of Coal by Rank, Analysis of Coal – Proximate analysis and Ultimate analysis, Metallurgical Coke, Types of Carbonization of Coal – Low-temperature and high temperature carbonization, Manufacture of Metallurgical Coke by Beehive oven process, Petroleum, classification of petroleum, Refining of crude oil, Cracking – Thermal cracking, Catalytic cracking- Moving-bed catalytic cracking, LPG as a Fuel, Natural Gas, Producer Gas, Water Gas (or Blue Gas), Non-Conventional Sources of Energy-Solar energy, Solar cells and Uses of solar cells.
Combustion: Combustion, Mass Analysis from Volume Analysis and Vice Versa, Analysis of Flue Gas

SUGGESTED BOOKS

1. "Liquid Crystals, Nature's delicate phase of matter", Peter J Collings, Princeton University Press, 2002
2. "Liquid Crystals: Fundamentals", Shri Singh, World Scientific Publishing Company; 1st edition (November 7, 2002)
3. "Science of Engineering Materials", C.M. Srivastava and C. Srinivasan, Wiley-Eastern Ltd. (1991).
4. "Engineering Chemistry", Jain P C and Monica Jain, 15th Edition, DhanpatRai Publishing Company Ltd, New Delhi, India, 2005.
5. A Text book of Engineering Chemistry", Shashi Chawla" DhanpatRai Publishing Company (P) Ltd., New Delhi, India, 2007.
6. Textbook of Engineering Chemistry, C Parameswara Murthy, C V Agarwal, Andra Naidu, BS Publications, Hyderabad, India.
7. "A Textbook of Engineering Chemistry", Dr. Y. BharathiKumari and Dr. JyotsnaCherukuri, VGS Publications, First Edison, India, 2009

Paper CH (IC) 451: Conventional Methods of Analysis

I. Titrimetry:

1. Determination of Ca^{2+}, Mg^{2+}, CO_3^{2-}, HCO_3^- in soil sample
2. Determination of saponification value, Iodine number, acid value and ester value of an oil sample (5-6 samples and comparative study)
3. Determination of Ascorbic acid in Vit.C tablet by iodometry (2-3 samples)

II Water analysis:

1. Determination of Dissolved Oxygen
2. Determination of COD
3. Determination of residual Chlorine in water by Iodometry
4. Determination of Fluoride by Zirconium Alizarin Method
5. Determination of Sulphate by spectrophotometry, turbidimetry or nephelometry

III Separation Methods

1. Separation of Fe^{3+} and Ni^{2+} using tri-n-butyl phophite (TBP) from HCl medium (Solvent extraction)
2. Determination of cations by paper chromatography; Co(II), Ni(II) and Cu(II)
3. Separation of Fe(III) and Al(III) by column chromatography
4. Separation of Fe^{3+} and Ni^{2+} using strongly basic anion resin.

SUGGESTED BOOKS

1.Chemistry Experiments for Instrumental Methods, Donald T Sawyer WilliamR.Hememan et.al John Wiley & Sons 1984.
2.Analytical Chemistry by Gary D.Christian 6thEditionJohnWiley&Sons Inc New York 1994.
3.A Text Book of Quantitative Inorganic Analysis by A.I. Vogel 3rdEditionElbs Publication 1969.
4.Vogel's Text Book of Quantitative Inorganic Analysis Jeffery etal 4th edition ElbsPublications 1988.
5.Vogel's Text Book of Quantitative Chemical Analysis, 6th edition. Pearson Education Ltd 2002.
6.Analytical Chemistry Theory and Practice by R.M. Verma 3rd Edn.CBS Publishers &Distrbutors1994.
7.Comprehensive Experimental Chemistry by V.K. Ahluwalia et.al New Age Publications 1997.
8. Laboratory hand Book of Instrumental Drug Analysis.by B.G. Nagavi 2ndedn. 1996.

LABORATORY COURSES (IV Semester)
Paper CH (IC) 452: Spectroscopic techniques

I Spectrophotometry

1. Estimation of manganese.
2. Estimation of chromium.
3. Simultaneous determination of Manganese and Chromium in a mixture.
4. Determination of pKa of indicator (methyl orange/ methyl red)
5. Estimation of Nickel.
6. Determination of composition of Complex by Job's Method and Mole ratio Method in the following:
   (i) Cu(II)-EDTA (ii)Fe(II) - o-Phen

II Colorimetry

1. Determination of blood sugar
2. Determination of blood cholesterol
3. Determination of creatinine
4. Determination of Paracetamol

III Fluorimetry

1. Determination of Riboflavin
2. Determination of Quinine Sulphate.

IV Flame photometry

1. Determination of Na
2. Determination of K
3. Determination of Ca
4. Determination of Li

V Atomic Absorption Spectroscopy

1. Determination of i) Fe, ii) Mg, iii) Cu, iv) Pb.

SUGGESTED BOOKS

Text Book of Quantitative Inorganic Analysis Jafferyetal 4th edn. EdnElbs Publication

1. A Text Book of Quantitative Inorganic Analysis by A.I. Vogel 3rd EdnElbs Publication 1969.
2. Quantitative Analysis by Day and Underwood Prentice Hall (India) VI Edn.
3. Analytical Chemistry Thoery and Practice by R.M. Verma 3rd Edn.CBS Publishers & Distrbutors1994.
4. Practical Pharmaceutical Chemistry, A.H. Beckett and J.B. Stenlake 4thedn. CBS publishers, 2001
5. Medical Laboratory Technology – Mukherjee,McGraw Hills,1988

M.Sc. CHEMISTRY

ORGANIC CHEMISTRY SPECIALISATION
SYLLABUS OF III & IV SEMESTERS
REVISED AS PER NEW (CB) SYLLABUS

FOR STUDENTS ADMITTED FROM THE YEAR 2016 ONWARDS

M.Sc. CHEMISTRY (ORGANIC CHEMISTRY SPECIALISATION)

Syllabus for III and IV Semesters

(for the batches admitted in academic year 2016 & later under CBCS pattern)

[Under Restructured CBCS Scheme]

Grand total marks and credits (all 4 semesters) 2400 marks – 96 credits

(Approved in the P.G.BOS meeting held on 01-07-2017)

SEMESTER-III

Paper	Instruction Hrs/Week	Internal assessment marks*	Semester marks	Total marks	Total credits
CH(OC)301T	4	20	80	100	4
CH(OC)302T	4	20	80	100	4
CH(OC)303T	4	20	80	100	4
CH(OC)304T	4	20	80	100	4
CH(OC)351P	9	-	100	100	4
CH(OC)352P	9	-	100	100	4
Total				**600**	**24**

SEMESTER - IV

Paper	Instruction Hrs/Week	Internal assessment marks*	Semester marks	Total marks	Total credits
CH(OC)401T	4	20	80	100	4
CH(OC)402T	4	20	80	100	4
CH(OC)403T	4	20	80	100	4
CH(OC)404T	4	20	80	100	4
CH(OC)451P	9	-	100	100	4
CH(OC)452P	9	-	100	100	4
Total				**600**	**24**

**** 15 marks for the written test and 5 marks for the assignment***

Grand total all 4 semesters: 2400 marks and 96 credits

PAPER TITLES , M.Sc. ORGANIC CHEMISTRY SPECIALISATION
(For the batch admitted during the academic year 2016 onwards under the CBCS pattern)

[Under Restructured CBCS Scheme]

III SEMESTER SYLLABUS	IV SEMESTER SYLLABUS
Paper-1CH (OC) 301T: Synthetic Reagents, Advanced NMR, Conformational Analysis and ORD OC-09: Synthetic Reagents-I OC-10: Synthetic Reagents-II OC-11: ^{13}C NMR and 2D NMR spectroscopy OC-12: Conformational analysis (Cyclic systems) and ORD	**Paper-1 CH (OC) 401T: Drug Design and Drug Discovery** OC-17: Principles of Drug design and drug discovery OC-18: Lead modification and SAR Studies OC 19: QSAR studies and computer aided drug design OC 20: Combinatorial Synthesis
Paper II– CH (OC) 302T: Modern Organic Synthesis OC-13: Asymmetric synthesis OC-14: Synthetic strategies OC-15: New Synthetic reactions OC-16:New techniques and concepts in organic synthesis	**Paper-II CH (OC) 402T:Drug synthesis and mechanism of action** OC-21: Drugs acting on metabolic process, cell wall and specific enzymes OC-22: Drugs acting on genetic material and immune system OC-23: Drugs acting on receptors and ion channels OC-24: Chiral drugs
Elective-3A **Paper-IIICH (OC)303T (CB1): Bioorganic Chemistry** OC(CB1)-1: Carbohydrates OC(CB1)-2: Nucleic acids and Lipids OC(CB1)-3: Proteins and Enzymes OC(CB1)-4: Coenzymes and Vitamins	**Elective-3A** **Paper-III CH (OC)-403T (CB1): Advanced Heterocyclic Chemistry** OC (CB1) 17: Non aromatic heterocyclics& aromaticity OC (CB1)18: Five and six membered heterocyclics with two hetero atoms OC (CB1) 19: Heterocyclics with more than two hetero atoms OC (CB1) 20: Larger ring and other heterocycles
Elective-3B: **Paper-III CH (OC) 303T (CB2): Forensic Chemistry and Toxicology** OC(CB2)-5: Forensic chemistry- I OC(CB2)-6: Forensic chemistry- II OC(CB2)-7: Forensic Toxicology-I OC(CB2)-8: Forensic Toxicology-II	**Elective-3B** **Paper-III CH (OC)-403T (CB2): Polymers , dyes and Pigments** OC (CB2) 21: Polymers- I OC (CB2) 22: Polymers- II OC (CB2) 23: Dyes-I OC (CB2) 24: Dyes-II and pigments
Elective-4A **Paper-IV CH (OC) 304T (CB3): Green chemistry and Organic materials** OC (CB3) - 9: Principles of Green chemistry OC (CB3) -10: Green Synthesis OC (CB3) -11: Organic nanomaterials OC (CB3) -12: Supramolecular chemistry	**Elective-4A (ID Paper)** **Paper-IV CH (OC) 404(CB3)T: Advanced Natural Products** OC(CB3)-25: Biosynthesis of natural products OC(CB3)-26: Structure determination of natural products -I OC(CB3)--27: Structure determination ofnatural products-II OC(CB3)--28: Total stereo selective synthesis of natural products.
Elective-4B **Paper-IV CH (OC) 304T (CB4): Pesticides** OC (CB4) - 13: Introduction to pesticides OC (CB4) - 14: Synthetic insecticides OC (CB4) - 15: Natural insecticides & herbicides OC (CB4) - 16: Fungicides, and Rodenticides	**Elective-4B (ID Paper)** **Paper-IVCH (OC) 404 (CB4) T: Biopharmaceutics and Pharmacodynamics** OC(CB4)-29 : Pharmacokinetics OC(CB4)-30 : Pharmacodynamics OC(CB4)-31 : Principles of Therapeutics OC(CB4)-32: Drug Interactions
LABORATORY COURSES **Paper-V CH (OC) 351P**: Synthesis of organic molecules, isolation of natural products & TLC. **Paper-VI CH (OC) 352P**: Separation and identification of organic compounds & Column chromatography	**LABORATORY COURSES** **Paper-V CH (OC) 451P**: Spectroscopic identification of organic compounds & practice of chemistry software prgrammes **Paper- VI CH (OC) 452P**: Synthesis and analysis of drugs

M.Sc. ORGANIC CHEMISTRY SPECIALISATION
III SEMESTER SYLLABUS

(For the batch admitted during the academic year 2016-2017)

Paper-1CH (OC) 301T: Synthetic Reagents, Advanced NMR,Conformational Analysis and ORD

OC-09: Synthetic Reagents-I
OC-10: Synthetic Reagents-II
OC-11: ^{13}C NMR and 2D NMR spectroscopy
OC-12: Conformational analysis (Cyclic systems) & ORD

Paper II– CH (OC) 302T: Modern Organic Synthesis

OC-13: Asymmetric synthesis
OC-14: Synthetic strategies
OC-15- New Synthetic reactions
OC-16: New techniques and concepts in organic synthesis

Elective-3A Paper-III CH (OC)303T (CB1): Bioorganic Chemistry

OC(CB1)-1: Carbohydrates
OC(CB1)-2: Nucleic acids and Lipids
OC(CB1)-3: Proteins and Enzymes
OC(CB1)-4: Coenzymes and Vitamins

Elective-3B: Paper-III CH (OC) 303T (CB2): Forensic Chemistry andToxicology

OC(CB2)-5: Forensic chemistry- I
OC(CB2)-6: Forensic chemistry- II
OC(CB2)-7: Forensic Toxicology-I
OC(CB2)-8: Forensic Toxicology-II

Elective-4A Paper-IV CH (OC) 304T (CB3): Green chemistry and Organic materials

OC (CB3) - 9: Principles of Green chemistry
OC (CB3) -10: Green Synthesis
OC (CB3) -11: Organic nanomaterials
OC (CB3) -12: Supramolecular chemistry

Elective-4B Paper-IV CH (OC) 304T (CB4): Pesticides

OC (CB4) - 13: Introduction to pesticides
OC (CB4) - 14: Synthetic insecticides
OC (CB4) - 15: Natural insecticides & herbicides
OC (CB4) - 16: Fungicides, and Rodenticides

Laboratory courses:

Paper-V CH (OC) 351P: Synthesis of organic molecules, isolation of natural products and TLC.

Paper-VI CH (OC) 352P: Separation and identification of organic compounds & Column chromatography.

M.Sc. CHEMISTRY (ORGANIC CHEMISTRY)
III SEMESTER SYLLABUS

(For the batch admitted during the academic year 2016 -2017 under the CBCS pattern)

Paper-1CH (OC) 301T: Synthetic Reagents, Advanced NMR, Conformational Analysis and ORD

OC-09: Synthetic Reagents-I
OC-10: Synthetic Reagents-II
OC-11: ^{13}C NMR and 2D NMR spectroscopy
OC-12: Conformational analysis (Cyclic systems) & ORD

OC-09: Synthetic Reagents I 15 Hrs

i)Protecting groups: a) Protection of alcoholsby ether, silyl ether and esterformation b) Protection of 1,2-diols by acetal, ketal and carbonate formation c) Protection of amines by benzyloxycarbonyl, t-butyloxycarbonyl,fmoc and triphenyl methyl groups. d) Protection of carbonyls by acetal, ketal and thiol acetal (Umpolung)groups. e) Protection of carboxylic acids by ester and ortho ester (OBO) formation.
ii) Organometallic Reagents: Preparation and application of the following in organic synthesis: 1) Organolithium 2) Organo copper reagents3) Organoboranes in C-C bond formation 4) Organo silicon reagents: reactions involving β-carbocations and α-carbanions, utility of trimethyl silyl halides, cyanides and triflates.
iii) Carbonyl methylenation:a) Phosphorousylide mediated olefination 1) Witting reaction, 2) Horner-Wordsworth-Emmons reaction.b) Titanium- Carbene mediated olefination 1) Tebbe reagent, 2) Petasis reagent 3) Nysted reagent.
iv) Carbene insertions: Rh based carbene complexes, cyclopropanations.
v) C-H Activation: Introduction, Rh catalysed C-H activation.

OC-10:Synthetic Reagents II 15 Hrs

i)Oxidations: a) Oxidation of active C-H functions: DDQ and SeO_2.b) Alkenes to diols: Prevost and Woodward oxidation c) Alcohol to carbonyls:Cr^{VI} oxidants (Jones reagent, PCC, PDC) IBX, DMP, CAN, TEMPO, TPAP, Swern oxidation d) Oxidative cleavage of 1,2-diols: Periodic acid and Lead tetra acetate.
ii) Reductions: a) Catalytic hydrogenation: Homogenous (Wilkinsons's catalytic hydrogenation)and heterogeneous catalytic reduction. b) Non-metallic reductions: Diimide reduction c)Dissolving metal reductions: Birch reduction. d) Nucleophilic metal hydrides: $LiAlH_4$, $NaBH_4$, and their modifications.e) Electrophilic metal hydrides: BH_3, AlH_3 and DIBAL. f) Use of tri-n-butyl tin hydride: Radical reductions.

OC-11: ^{13}C NMR and 2D NMR spectroscopy 15 Hrs
i)^{13}C NMR spectroscopy: Introduction**,** Types of ^{13}Cnmr spectra: undecoupled, proton-

decoupled and off-resonance decoupled (ORD) spectra. ^{13}C chemical shifts, factors affecting the chemical shifts, chemical shifts of organic compounds. Calculation of chemical shifts of alkanes, alkenes and alkynes. Homonuclear (^{13}C, ^{13}C J) and heteronuclear (^{13}C,^{1}H J and ^{13}C, ^{2}H J) coupling. Applications of ^{13}C-NMR spectroscopy: Structure determination, stereochemistry, reaction mechanisms and dynamic processes in organic molecules. ^{13}C-NMR spectral editing techniques: principle and applications of APT, INEPT and DEPT methods.

ii) 2D-NMR spectroscopy: Principles of 2D NMR, Classification of 2D-experiments. Correlation spectroscopy (COSY) HOMOCOSY (^{1}H-^{1}H COSY) , TOCSY (Total Correlation Spectroscopy), HeteroCOSY (^{1}H,^{13}C COSY,HMQC), long range ^{1}H,^{13}C COSY (HMBC),Homonuclear and Heteronuclear 2D-J-resolved spectroscopy, NOESY and 2D-INADEQUATE experiments and their applications.

OC-12: Conformational analysis (Cyclic systems) & ORD15 Hrs

Conformational analysis (Cyclic systems)

Study of conformations of cyclohexane, mono, di and tri substituted cyclohexanes, (1,3,5-trimethyl cyclohexanes and Menthols), cyclohexanone (2-alkyl and 3 -alkyl ketone effect), 2-halocyclohexanones, cycloheptane . Stereo chemistry of bicyclo[3,3,0]octanes,hydrindanes, decalins and perhydroanthracenes. Conformational structures of piperidine, N-Methylpiperidine, tropane, tropine, pseudotropine, decahydroquinolineand quinolizidine. Factors governing the reactivity of axial and equatorial substituents in cyclohexanes.

(oxidation, S_N2 reaction, rearrangements, Ester hydrolysis) Stereochemistry of addition to the carbonyl group of a rigid cyclohexanone ring.

Optical Rotatory Dispersion (ORD) and CD Spectroscopy: Optical rotation, circular birefringence, circular dichroism and Cotton effect. Plain curves and anomalous curves. Empirical and semiempiricalrules-The axial haloketone rule, the octant rule, Helicity rule, Exciton chirality method. Application of the rules to the study of absolute configuration and conformations of organic molecules.

Recommended Books:

1. Some modern methods of organic synthesis by W. Carruthers
2. Guidebook to organic synthesis, by R K Meckie, D M Smith & R A Atken
3. Organic Synthesis by O House
4. Organic synthesis by Micheal B Smith
5. Reagents for organic synthesis, by Fieser&Fieser, Vol 1-11 (1984)
6. Organic synthesis by Robert E Ireland
7. Handbooks of reagents for organic synthesis by Reich and Rigby, Vol-I-IV
8. Organic chemistry by Jonathan Clayden, Nick Greeves and Stuart Warren
9. Organic Reactions and their mechanisms by P.S.Kalsi
10. Organic reaction mechanisms by V.K.Ahulwalia and Rakesh Kumar Parashar
11. Spectroscopic identification of organic compounds by RM Silverstein, G C Bassler and T B Morrill
12. Organic Spectroscopy by William Kemp
13. Spectroscopic methods in Organic chemistry by DH Williams and I Fleming
14. Modern NMR techniques for chemistry research by Andrew B Derome

15. NMR in chemistry - A multinuclear introduction by William Kemp
16. Spectroscopic identification of organic compounds by P S Kalsi
17. Introduction to organic spectroscopy by Pavia
18. Carbon-13 NMR for organic chemists by GC Levy and O L Nelson
19. Nuclear Magnetic Resonance Basic principles by Atta-ur-Rahman
20. Basic one and two-dimensional NMR spectroscopy by Horst Friebolin
21. NMR spectroscopy by H.Gunther
22. Stereochemistry of organic compounds — Principles & Applications by D Nasipuri
23. Stereochemistry of Carbon compounds by Ernest L Eliel & Samuel H. wilen
24. Stereochemistry: Conformation & Mechanism by P S Kalsi
25. The third dimension in organic chemistry, by Alan Bassendale
26. Stereo selectivity in organic synthesis by R S Ward.
27. Advanced organic chemistry. Part A Structure & Mechanism by Francis A. Corey and Richard J. Sundberg
28. Optical rotatory dispersion by C Djerassi
29. Optical rotatory dispersion and circular dichroism by P Crabbe
30. Mechanism and Structure in Organic chemistry by S Mukherjee

Paper II– CH (OC) 302T:Modern Organic Synthesis

OC-13: Asymmetric synthesis
OC-14: Synthetic strategies

OC-15: New Synthetic reactions
OC-16: New techniques and concepts in organic synthesis

OC- l3:- Asymmetric synthesis15 Hrs

Introduction: Brief revision of classification of stereo selective reactions

Prostereoisomerism: Topicity in molecules Homotopic, stereoheterotopic (enantiotopic and diastereotopic) groups and faces- symmetry criteria.

Prochiral nomenclature: Pro chiraility and Pro-R, Pro-S, Re and Si.

Conditions forstereoselectivity: Symmetry and transition state criteria, kinetic and thermodynamic control. Methods of inducing enantioselectivityy.

Analytical methods: % Enantiomeric excess and diastereomeric ratio. Determination of enantiomeric excess: specific rotation, Chiral NMR; Chiralderivatizing agents, Chiral solvent, Chiral shift reagents and Chiral HPLC.

Chiral Substrate controlled asymmetric synthesis: Nucleophilic additions to chiral carbonyl compounds. 1, 2- asymmetric induction, Cram's rule and Felkin-Anh model.

Chiral auxiliary controlled asymmetric synthesis: α-Alkylation of chiral enolates, Evan's oxazolidinone, 1, 4-Asymmetric induction and Prelog's rule..

Chiral reagent controlled asymmetric synthesis: Asymmetric reductions using BINAL-H. Asymmetric hydroboration using IPC_2 BH and $IPCBH_2$.

Chiral catalyst controlled asymmetric synthesis: Sharplessepoxidation. Asymmetric hydrogenations using chiral Wilkinson biphosphincatalyst.

Asymmetric aldol reaction: Diastereoselective aldol reaction (achiral enolate& achiral aldehydes) its explanation by Zimmerman-Traxelmodel.

OC-14: SyntheticStrategies15 Hrs

Introduction: Terminology, Target, synthon, synthetic equivalent, functional group interconversion (FGI), functional group addition. Criteria for selection of target. Linear and convergent synthesis. Retrosynthetic analysis and synthesis involvingchemoselectivity, regioselectivity, reversal of polarity and cyclizations. .

Order of events: S-Salbutamol, Propoxycaine..

One group C-C and C-X disconnections: Introduction .One group C-C disconnections in alcohols and carbonyl compounds. One group C-X disconnections in Carbonyl compounds, alcohols,ethers and sulphides.

Two group C-C and C-X disconnections : Introduction .Two group C-X disconnections in 1,1-difunctionalised, 1,2-difunctionalised and 1,3-difunctionalised compounds.

Two group C-C disconnections: Diels-Alder reaction, 1,3-difunctionalised compounds, 1,5-difunctionalised compounds, Michael addition and Robinson annulation.

Control in carbonyl condensations:oxanamide and mevalonic acid.

Strategic bond: definition, guidelines for disconnection; disconnection of C-X bonds, disconnect to greatest simplification, using symmetry in disconnection, disconnection corresponding to known reliable reaction, high yielding steps and recognizable starting materials. Retrosynthesis ofRetronecene, longifoline.

OC-15: New Synthetic reactions 15 Hrs

1. Metal mediated C-C and C-X coupling reactions: Suzuki, Heck, Stille,Sonogishira crosscoupling,Buchwald-Hartwigand Negishi-Kumadacoupling reactions.

2. C=C Formation Reactions: Shapiro, Bamford-Stevens, McMurreyreactions,Julia-Lythgoeolefinationand Peterson's stereoselective olefination.

3. Multicomponent Reactions: Ugi,Passerini, Biginelli, Bergman and Mannichreactions.

4. Ring Formation Reactions: Pausan-Khand reaction, Nazerov cyclisation.

5. Click Chemistry: Click reaction, 1,3-dipolar cycloadditions.

6.Metathesis: Grubb's 1st and 2nd generation catalyst, Olefin cross coupling metathesis(OCM), ring closing metathesis(RCM), ring opening metathesis(ROM), applications.

7. Other important synthetic reactions: Baylis-Hilman reaction,Eschenmoser-Tanabe fragmentation,Mitsunobu reaction,Stork-enamine reaction and Michael reactions.

OC-16: New techniques and concepts in organic synthesis 15 Hrs

1. Techniques in peptide synthesis: Solid phase peptide synthesis, commonly used resins (Rink resin, Wang resin and Ellman resin,synthesis of cross linked Merrifield resin and drawbacks of solid phase synthesis.

2. Solid phase oligodeoxynucleotide synthesis: Phosphotriester, phosphitetriester and phosphoramidite pathway

3. Oligosaccharide synthesis: Glycosidation**:**cylicoxocarbeniumion, glycosyl donors and glycosyl acceptors, Kahneglycosidation, convergent and linear oligosaccharide synthesis.

4. Phase Transfer catalysis: Onium and crwon ethers as PTC.

5. Tandem synthesis: Tandem reactions; conjugate addition-aldol reaction, polymerization-cyclisation, elctrocylic-Diels Alder reaction.

6. Baldwin Rules: Exo and Endo cyclisation, tetrahedral, trigonal and diagonal systems, favoured and disfavouredcyclisations.

7.Chiron approach in organic synthesis: Nature's chiral pool, carbohydrates, amino acids, hydroxy acids, terpenes as chiral precursors. Synthesis of shikimic acid from D-arabinose, furanonycin from D-glucose, S-(-)-ipsenol from S-leucine.

8) Determination of absolute configuration: Mosher's method.

Recommended Books:

1. Asymmetric synthesis by Nogradi
2. Asymmetric organic reactions by J D Morrison and H S Moschcr
3. Principles in Asymmetric synthesis by Robert E. Gawley&Jeffrey aube
4. Stereo differentiating reactions by Izumi
5. Some modern methods of organic synthesis by W Carruthers
6. Guidebook to organic synthesis, by R K Meckie, D M Smith & R A Atken
7. Organic synthesis by Michael B Smith
8. Organic Synthesis-The disconnection approach by S Warren
9. Organic Synthesis by C Willis and M Willis
10. Problems on organic synthesis by Stuart Warren
11.Organic chemistry Jonathan Clayden, Nick Greeves and Stuart Warren
12.The logic of chemical synthesis by Elias James Corey and Xue-Min Cheng
13. Name reactions by JieJacj Li

Elective-3A

Paper-III CH (OC)303T (CB1): Bioorganic Chemistry

OC(CB1)-1: Carbohydrates
OC(CB1)-2: Nucleic acids and Lipids
OC(CB1)-3: Proteins and Enzymes
OC(CB1)-4: Coenzymes and Vitamins

OC(CB1)-1: Carbohydrates 15 Hrs

Introduction to the importance of Carbohydrates. Types of naturally occuring sugars. Deoxy sugars, aminosugars, branched chain sugars mrthyl ethers and acid derivatives of sugars. Determination of configuration and determination of ring size of D-glucose and D-Fructose. Conformational analysis of monosaccharides. $^4C_1$ and $^1C_4$ conformations of D-glucose. Reactions of six carbon sugars: Ferrier, Hanesian reaction and Ferrier rearrangement. Synthesis of amino, halo and thio sugars. Structure, ring size determination of sucrose and maltose.Conformational structures of sucrose, lactose, maltose, cellobiose and gentobiose. Structure and biological functions of starch, cellulose, glycogenand chitin. Role of sugars in cell to cell recognition, blood groups.

OC(CB1)-2: Nucleic acids & lipids 15 Hrs

Nucleic acids: Retro synthetic analysis of nucleic acids - Nucleotides, Nucleosides, Nucleotide bases and Sugars. Structure and synthesis of nucleosides and nucleotides. Primary, secondary and tertiary structure of DNA. Types of mRNA,tRNA and rRNA. Replication, transcription and translation. Genetic code. Protein biosynthesis. DNA finger printing.

Lipids: Introduction and classification of lipids. Stereochemical notation in lipids.Chemical synthesis and biosynthesis of phospholipids and glycolipids. Properties of lipid aggregates, micelles, bilayers, liposomes and biological membranes.

OC(CB1)-3: Proteinsand Enzymes15 Hrs

Proteins: Introduction. Peptide bond, classification and nomenclatue of peptides. Amino acid sequence of polypeptides and proteins: terminal residue analysis and partial hydrolysis. Peptide synthesis by solution phase and solid phase synthesis methods. Proteins - Biological importance and classification - Primary, secondary and tertiary structure of proteins.

Enzymes: Definition. Classification based on mode of action.Mechanism of enzyme catalysis - Lock and Key, Induced- Fit and three point contact models. Enzyme selectivity –chemo, regio, diastereo and enantio selectivity – illustration with suitable examples. Factors affecting enzyme catalysis.Enzyme inhibition- reversible and irreversible inhibition. Enzymes in organic synthesis. Immobilised enzymes

OC(CB1)-4: Coenzymes and Vitamins 15 Hrs

Coenzymes: Introduction. Co-factors -cosubstrates -prosthetic groups.

Classification — Vitamin derived coenzymes and metabolite coenzymes.Structure and biological functionsof coenzyme A, thiamine pyrophosphate (TPP), pyridoxal phosphate (PLP), oxidized and reduced forms of I) nicotinamide adenosine dinucleotide / their phosphates (NAD), NADH, $NADP^+$ NADPH) ii) Flavin adenine nucleotide FAD, $FADH_2$ and iii) Flavin mononucleotide (FMN, $FMNH_2$) lipoic acid, biotin, tetrahydrofolate and ubiquinone. Adenosine triphosphate (ATP)and adenosine diphosphate (ADP), S-adenosyl

methionine (SAM) and uridine diphosphosugars (UDP-sugars) Mechanism of reactions catalyzed by the above coenzymes.

Vitamins: Introduction, classification and biological importance of vitamins. Structure determination and synthesis of vitamins A, B_1, and B_2. Synthesis of vitamins - B_6, C, E and K. Structure of vitamin B_{12}.

Reference Books:

1. Organic Chemistry Vol.I and Vol.II by I.L.Finar
2. Carbohydrate Chemistry by Barton Volumes
3. Carbohydrate chemistry by G.J.Boons
4. The chemistry of natural products:vol.V - carbohydrates by S.F.Dyke
5. Organic Chemistry by McMurry
6. Nucleic acids in Chemistry and Biology by G M Blackbum MI Gait
7. LehningerPrinciples of Biochemistry by D L Nelson and M MCoxon
8. Outlines of Biochemistry by Conn and Stumpf
9. Enzyme structure and mechanism by Fersht and Freeman
10. Enzymes for green organic synthesis by V.K.Ahluwalia
11. Biotransformations in Organic Chemistry by K Faber.
12. Principles of biochemistry by Horton &others.
13. Bioorganic chemistry - A chemical approach to enzyme action by Herman Dugasand Christopher Penney.
14. Concepts in Biotechnology by D.Balasubramanian& others
15. Chemistry and physiology of the vitamins by H.R.Rosenberg.

Elective-3B

Paper-III CH (OC)303T (CB2): Forensic Chemistry & Toxicology

OC(CB2)-5: Forensic chemistry- I
OC(CB2)-6: Forensic chemistry- II
OC(CB2)-7: Forensic Toxicology-I
OC(CB2)-8: Forensic Toxicology-II

OC(CB2)-5: Forensic chemistry-I 15 Hrs

Forensic Chemistry - Introduction - Types of cases / exhibits - Preliminary screening - presumptive tests (colour and spot tests) - Examinations procedures involving standard methodsand instrumental techniques

Qualitative and quantitative forensic analysis of inorganic and organic material - Chemical fertilizers (N,P,K) _ Insecticides (Endosulfan, Malathion, Carbaryl) - Metallurgical analysis (Fe, Cu, Zn, Au, Ag) – Natural products (tobacco, tea, sugars, rubber) – Industrial chemicals - Sulphuric, Nitric and Hydrochloric acids, Sodium, Potassium hydroxide, Ammonium nitrate, Potassium chlorate, Organic solvents like Methanol, Ethanol, Acetone, Chloroform and Ether Organic chemicals like Acetanilide, P- Aminophenol, and Nitrobenzene etc. with reference to forensic work.

OC(CB2)-6: Forensic chemistry-II 15 Hrs

Examination of petroleum products - Distillation and fractionation - various fractions and theircommercial uses - Standard method of analysis of petroleum products – Analysis of petroleumproducts for adulteration and arson residues. Chemistry of fire - Investigation and evaluation of fires – Causes of fire - Analysis of arsonresidues by conventional and instrumental methods. Analysis of trace evidence - Cosmetics, Dyes, Trap related evidence materials, Paints, Pigments,Fibres, Oils fats, Greases, Industrial dusts, Chemicals and Plant materials.

OC(CB2)-7: Forensic Toxicology-I15 Hrs

Toxicology- Introduction- History- Scope- Areas of Toxicology- Role of forensic toxicologist- Poisons- Classification of poisons- Types of poisoning- Sample collection and preservation oftoxicological exhibits in fatal and survival cases- Storage of samples- Signs and symptoms ofpoisoning- Toxicological investigation/examination of poisoned death- Interpretationoftoxicologicaldata- Courtroom testimony in toxicological cases.Case Histories.

OC(CB2)-8: Forensic Toxicology-II 15 Hrs

Principles of Toxicology- Introduction – Pharmacokinetics - Methods of transportation oftoxicant- Absorption- Distribution- Storage of toxicants- Redistribution - Metabolism- Oxidation

– Reduction – Hydrolysis – Conjugation - Excretion- Other routes of elimination-Toxicokinetics- one and two compartmental model – Toxicodynamics- Spectrum of undesired(toxic) effects- Interaction of chemicals- Tolerance- Dose response relationship- Developmentaland reproductive toxicity- Mutagenicity- Toxicity testing.

Recommended books:

1. James, S. H. and Nordby, J. J.: Forensic Science: An Introduction to Scientific and Investigative Techniques, 2003.
2. Saferstein, R: Criminalistics - An Introduction to Forensic Science, Prentice Hall, 1995.
3. Sarkar, S: Fuels and Combustion, Orient Longman, 1990
4. Verma, R. M: Analytical Chemistry – Theory and Practice, CBS Pub., 1994
5. Svehla, G. Ed.: Vogel's Qualitative Inorganic Analysis, Longman, 1998.
6. Bassett: Vogel's Text Book of Quantitative Inorganic Analysis, Longman, 1978
7. Vogel, A. I: Text Book of Practical Organic Chemistry including Qualitative OrganicAnalysis, ELBS, 1971.
8. Narayanan, T. V: Modern Techniques of Bomb Detection and Disposal, R. A. Security System, 1995.
9. Almirall, J. R. and Furton, K. G: Analysis and Interpretation of Fire Scene Evidence, CRC Press, 2004.
10. Bogusz, M. J: Handbook of Analytical Separations : Vol. 2 ,Forensic Science, Elsevier, 2000.
11. Bureau of Indian Standards: Specifications and Methods of Analysis for Petroleum Products.
12. Wilson and Wilson's Comprehensive Analytical Chemistry Volumes
13. Standard Methods of Chemical Analysiss
14. AOAC: Official Methods of Analysis
15. Daeid, N.N.: Fire Investigation: Theory and Practice, Taylor and Francis, 2003
16. Klaassen, C. D.,:Casarett and Doull's Toxicology: The Basic Science of Poisons, 5thed, McGraw-Hill, 1995.
17. Moffat, A.C. : Osselton, D. M. Widdop, B. : Clarke's Analysis of Drugs and Poisons in Pharmaceuticals, body fluids and postmortem material, 3rd ed., Pharmaceutical Press2004.
18. Bogusz, M. J.,: Hand Book of Analytical Separations, Vol. 2: Forensic Science, 1st ed., Elsevier Science ,2000.
19. Siegel, J.A., Saukko, P. J., Knupfer, G.,: Encyclopedia of Forensic Sciences (Vol3), Academic Press, 2000.
20. Paranjape, H.M., Bothara, G.K., Jain, M.M.: Fundamentals of Pharmacology, 1st ed.,Nirali Prakashan,1990.
21. Budhiraja, R.D.: Elementary Pharmacology and Toxicology, Popular Prakashan, 2nd ed., 1999.
22. Laboratory procedure Manual, Forensic Toxicology: DFS, 2005
23. Cravey, R.H; Baselt, R.C.: Introduction to Forensic Toxicology , Biochemical Publications, Davis, C.A. (1981)
24. Stolmen, A.; Progress in Chemical Toxicology: Academic Press, New York (1963)
25. Modi, Jaisingh, P.; Textbook of Medical Jurisprudence& Toxicology, M.M. TripathiPublication (2001)
26. Eckert; An Introduction to Forensic Science, CRC Press

Elective-4A

Paper-IV CH (OC) 304T (CB3): Green chemistry and Organic materials

OC (CB3) -9: Principles of Green chemistry
OC (CB3) -10: Green Synthesis
OC (CB3) -11: Organic nanomaterials
OC (CB3) -12: Supramolecular chemistry

OC (CB3)-9: Principles of Green Chemistry 15 Hrs

Green chemistry: Introduction

Principles of Green Chemistry: Designing a Green Synthesis using these principles; Prevention of Waste/by-products; maximum incorporation of the starting materials used in the synthesis into the final products (Atom Economy); prevention/minimization of hazardous/toxic products; designing safer chemicals ; selection of appropriate auxiliary substances - green solvents, ionic liquids and solvent-free synthesis: energy requirements for reactions - use of microwaves, ultrasonic energy in organic synthesis; prevention of unnecessary derivatization – careful use of protecting groups; use of catalytic reagents in preference to stoichiometric reagents; designing of biodegradable products; prevention of chemical accidents; strengthening/development of analytical techniques to prevent and minimize the generation of hazardous substances in chemical processes.

OC (CB3) -10: Green Synthesis 15Hrs

i)Microwave Assisted Organic Synthesis (MAOS): introduction, benefits and limitations

a) Microwave assisted reactions in organic solvents: Esterification, Fries rearrangement, Claisen rearrangement and Diels- Alder reaction.

b)Microwave assisted Solvent-free reactions: Deacetylation, saponification of esters, alkylation of reactive methylene compounds and synthesis of nitriles from aldehydes.

ii)Ultrasound Assisted Organic Synthesis: introduction, applications of ultrasound-Cannizaro reaction, Reformatsky reaction and Strecker synthesis.

iii)Organic Synthesis in Green Solvents: introduction

a) Aqueous Phase Reactions: Diels-Alder Reaction, Heck reaction, Hoffmann elimination, Claisen-Schmidt condensation hydrolysis and diydroxylationreactions.

b)Organic Synthesis using Ionic liquids: Introduction, applications-Beckmann rearrangement Suzuki Cross-Coupling Reaction and Diels- Alder reaction.

iv) Green Catalysts in organic synthesis: introduction

a) Phase Transfer Catalysts in Organic Synthesis: Introduction, Williamson ether synthesis and Wittig reaction

b) Biocatalysts in Organic Synthesis: Biochemical (microbial) oxidations and reductions.

OC (CB3) -11: Organic Nanomaterials 15Hrs

Introduction:The ‘top-down’ approach, the ‘bottom-up’ approach and Nanomanipulation.

Molecular Devices: Photochemical devices, Liquid crystals, Molecular wires, Rectifiers, Molecular switches and Molecular Muscles.

New Carbon family: Types of Fullerenes, Types of Carbon nanotubes (Zig-Zag, Armchair and Chiral), Graphenes. Growth, Chemical Synthesis and optoelectronic properties of Fullerenes, CNTs (Zig Zag, Armchair and Chiral), singlewalled CNTs (SWCNTs) and multi walled MWCNTs)and Graphenes.

Structures of aromatics belts, nano car and molecular machines.

Optoelectronic molecules: OLEDs, Organic Solar Cells (Basic OLED mechanism and structures)

Natural Benzheterazoles and their synthetic modifications as optoelectronic molecules.

OC (CB3) -12: Supramolecular Chemistry 15Hrs

I**ntroduction**: Supramolecular interactions (ion-ion, ion-dipole, H-bonding, cation-π, anion-π, π-π and Van der Walls interactions),Ionophore and molecular receptors.

Host-Guest Chemistry: Lock and key anology, Structures and applications of Cryptands,Spherands, Calixerenes, Cyclodextrins, Cyclophanes, Carcerands and hemicarcirands.

Self-assembly: Ladder, polygons, helices, rotaxanes, catanenes, Molecular necklace, dendrimers, self-assembly capsules their synthesis, properties and applications.

Enantioselective molecular recognition: Cyclodextrins, Crown ethers with chiral frame work, Chiral receptor from Kemp's triacid. Chiral receptors for tartaric acid.

Recommended books:

1.P.T. Anastes & J.K. Warmer: Oxford Green Chemistry- Theory and Practical, University Press (1998).

2. A.S. Matlack: Introduction to Green Chemistry, Marcel Deckkar, (2001).

3. M.C. Cann & M.E. Connely: Real-World cases in Green Chemistry, American Chemical Society, Washington (2000).

4. M.A. Ryan & M. Tinnesand, Introduction to Green Chemistry, American Chemical Society, Washington (2002).

5. V.K. Ahluwalia & M.R. Kidwai: New Trends in Green Chemistry, Anamalaya Publishers

6. Enantioselective organocatalysis, Peter I Dallco, Willey-VCH

7. Core Concepts in Supramolecular Chemistry and Nanochemistry by Jonathan W. Steed, David R. Turner and Karl J. Wallace; John-Wiley and Sons Publications

9. Supramolecular Chemistry by Jonathan W. Steed and Jerry L. Atwood, John-Wiley and Sons Publications

10. Supramolecular Chemistry-Concepts and Perspectives by J M. Lehn; Wiley-VCH (1995) Publications

11. Supramolecular Chemistry by P. D. Beer, P. A. Gale and D. K. Smith; Oxford University Press (1999)

12. Stereochemistry of organic compounds -Principles & Applications by D Nasipuri

13. Nanochemistry by G.B. Sergeev; Elsevier

14. Nanochemistry: A chemical approach to nano materials , G.A. Ozin& A.C. Arsenault; RSC publishers.

Elective-4B
Paper-IV CH (OC) 304T (CB4): Pesticides

OC(CB4)- 13:Introduction to pesticides
OC(CB4)- 14: Synthetic insecticides
OC(CB4)- 15:Natural insecticides& herbicides
OC(CB4)- 16:Fungicides, and Rodenticides

OC (CB4)-13: Introduction to pesticides 15 Hrs

i) Defination ,Classification and importance of pesticides

ii) Pest control: Different methods –chemical – insecticides, fungicides, herbicides, rodenticides, fumigants, chitin synthesis inhibitors and insect repellents.

a) Biological–pheremones: Definition and classification, synthesis of Disparlure, Exobrevicomin, Endobrevicomin, frontalin and grandiso pheromones, synthetic sex attractants.

b) Insect juvenile hormones: JH-A, JH-B,Synthesis of juvabione. Structural formula and importance of methopren.

c) Moultingharmones-structural formulae and mode of action of ecdysones

d) Antibiotics and secondary metabolites of microbial origin as insecticides and fungicides in agricultiure. Structural formula and importance of Blasticidin-S, Kasugamycin, Avermectin-B, Invermectin, piercidins and phytoalexins.

iii) Environmental pollution from pesticides.iv) Integrated pest management.

v) Pesticide formulations: Dusts, Granules, Wettable powders, Emmulsions and Aerosols.

OC (CB4)- 14: Synthetic insecticides 15 Hrs

i)**Organochlorine insecticides**- synthesis and mode of action of methoxychlor, perthan, Dicofol, Heptachlor, Dieldrin and Endosulfan.

ii) **Organophosphorous insecticides** –synthesis and mode action of Phosphoric acid derivatives, phosdrin, Dichlorophos, parathion, Zolone, Aninphomethyl, TEPP and Sachradan.

iii) **Carbamate insecticides**- synthesis and mode of action of carbamyl, Furadan, Baygon, Aldicarb and Zectron.

iv) Formulation and residue analysis of organochlorine, organophophorous and carbamate insecticides.

OC (CB4)- 15: Natural insecticidesand herbicides15 Hrs

i**) Insecticides of palnt origin** –synthesis and importance of pyrethrins (I and II), Rotenone and Nicotine. Main constituents Neem-structural formula of Azadirachtin. Synthesis of polygodial and warbunganol(Antifeedants).

ii)Synthesis of pyrethroids: synthesis of Allethrin, Bioallethrin, Cypermethrin, Fenvalerate, Decemethrin and pyrithrelone.

iii) Concept of Bioinsecticides – Bacillus thiuringiensis.

iv) Concept of pro-insecticides-structure and mode of action of pro-pheremones and pre-pro-insecticides.

v) Herbicides – synthesis,applications and mode of action of the following

a)Aryloxyalkyl carboxylic acid derivative:2,4-D, MCPA,2,4,5-T and 2,4,5-TP.b) Carbamates-propham and chloropham, c)Urea derivatives –Monouron and diuron, d) Aliphatic acids-Dalapon,TCA, e)Aromatic acids -2,3,6-TBA,Dicomba and Amiben, f)Nitrogen heterocyclic dericvatives –Simazine,Atrazine,Amitrole,Maleic hydrazide Diquat and paraquat, g) Phenols-PCP and Dinoseb, h) Benzonitrile compounds

OC (CB4)-16: Fungicides, and Rodenticides 15 Hrs

i) Fungicides –classification ,synthesis application and mode of action of the following classes: **a**)Carbamatesb)Quinones-chloranil,Dichloneand Benquinoxc)perchloromethylmercaptan derivative –captan,folpet,Difolatan and Mesulfan d) Benzimidazoles-carbendazim, Benomyl and Thiabandazole

ii) Rodenticides, a) Anticoagulents-synthesis and application of warfarin, Coumachlor, Vacor, Coumatetrallyl, Dicoumarol and Bromodiolen.b) Acute poisons- application of pindone,Ratindan,SodiumFluoroacetate ,Barium fluoroacetate,Antu,Tetramine,pindone and castrix.

Referencebooks:

1) Naturally occurring insecticides: M.Jacobson and D.G.Crosby.
2) Insecticides for future:Jacobson
3) Insect juvenile harmone chemistry and action : J.J Mann and M.Beroza
4) Polygodial and warburganal.Terpenoidantifeedants part-II rec,Tran,chin 106
5) Insect antifeedants :S.V.ley&P.L Toogood,chemistry in Britain ,Jan 1990 P.31
6) Synthesis of Insecticides :Metcalf
7) Fungicides-Frear
8) Fungicides-Nene
9) Residue reviews vol.36 : Melnikov
10) Safer insecticides :E.Hodgson
11) Crop protection agents from Nature: leonard G Copping
12) Biofertilizers and Bioinsecticides : A.M.Deshmukh
13) Insecticides and Fungicides :U Sriramulu.
14) Organo chlorine insecticides : persistent organic pollutants :F.Moriary
15) Herbicides :P.C.Kearney&D.D.Kaufnan
16) Analytical Method for pesticides :Z.Weig (Vol III)
17) Pesticide formulations :Van Valkenburg
18) Insecticides :A.S.Tahori
19) Herbicides,fungicides,formulation chemistry-A.S.Tahori
20) Environmental pollution by pesticides :C.A.Edwards
21) Pespticides managements and insecticide resistance :Watson and brown
22) Organo phosphorous pesticides M.eto

Laboratory courses:

Paper CH (O) 351P: Synthesis of organic molecules, isolation of natural products & TLC

(A) Laboratory synthesis of the following compounds:

2-Phenyl indole (Fischer indole synthesis), 7-hydroxy-3-methyl flavone (Baker-Venkatraman reaction), 2,5-Dihydroxy acetophenone (Fries reaction), 4- Chlorotoluene from p-toluidine (Sandmeyer reaction), Benzilic acid from benzoin (Benzillic acid rearrangement), Benzpinacol (photochemical reaction), 7-hydroxy coumarin (Pechman synthesis), Photo-dimerization of maleic anhydride, benzophenone (Friedel-Crafts reaction), Benzanilide (Beckmann rearrangement), Vanillyl alcohol from vanillin ($NaBH_4$ reduction), 2- and 4-nitrophenols (nitration and separation by steam distillation), Acridone from Phthalic anhydride.

(B) Isolation of the following natural products:

Caffeine from tea leaves (solvent extraction), Piperine from pepper (Soxhlet extraction), Eucalyptus oil from leaves (steam distillation),Lycopene from tomatoes.

(C)Thin layer chromatography : Thin layer chromatography: Determination of purity(All the above preparations) , monitoring the progress of chemical reactions (any of the four above preparations), identification of unknown organic compounds by comparing the R_f values of known standards.

Paper CH (O) 352P: Separation and identification of organic compounds & Column chromatography

Separation of two component mixtures by chemical methods and their identification by chemical reactions — separation by using solvent ether, 5 % aqueous sodium bicarbonate, 5% sodium hydroxide and dil hydrochloric acid, checking the purity of the two components by TLC, identification of the compounds by a systematic study of the physical characteristics (mp/bp), extra elements (nitrogen, halogens and sulfur), solubility, functional groups, preparation of crystalline derivatives and identification by referring to literature. A minimum of **09** mixtures should be separated and analyzed by these procedures.

Cannizzaro reaction: 4-Chloro benzaldehyde as substrate and separation of the resulting two component mixture

Separation of three component mixtures by chemical methods. A minimum of two mixtures should be separated and analyzed.

Column chromatography: Separation of a mixture of *ortho* and *para*-nitroanilinesand any one of the two component mixture using silica gel as adsorbent and chloroform as the eluent. The column chromatography should be monitored by TLC.

Recommended Books:

1. Practical organic chemistry by Mann & Saunders
2. Text book of practical organic chemistry by Vogel
3. The systematic identification of organic compounds by Ralph L. Shriner, Christine K. F. Hermann, Terence C. Morrill and David Y. Curtin

M.Sc. ORGANIC CHEMISTRY SPECIALISATION
IV SEMESTER SYLLABUS
(For the batch admitted during the academic year 2016-2017)

Paper-1 CH (OC) 401T: Drug Design and Drug Discovery

OC-17: Principles of Drug design and drug discovery
OC-18: Lead modification and SAR Studies
OC 19: QSAR studies and computer aided drug design
OC-20: Combinatorial Synthesis

Paper-II CH (OC) 402T: Drug synthesis and mechanism of action

OC-21: Drugs acting on metabolic process, cell wall and specific enzymes
OC-22: Drugs acting on genetic material and immune system
OC-23: Drugs acting on receptors and ion channels
OC-24: Chiral drugs

Elective-3A Paper-III CH (OC)-403T (CB1): Advanced Heterocyclic Chemistry

OC (CB1) 17: Non aromatic heterocyclics& aromaticity
OC (CB1) 18: Five and six membered heterocyclics with two hetero atoms
OC (CB1) 19: Heterocyclics with more than two hetero atoms
OC (CB1) 20: Larger ring and other heterocycles

Elective-3B Paper-III CH (OC)-403T (CB2): Polymers , dyes and Pigments

OC (CB2) 21: Polymers- I
OC (CB2) 22: Polymers- II
OC (CB2) 23: Dyes-I
OC (CB2) 24:Dyes-II and pigments

Elective-4A Paper-IV CH (OC) 404(CB3)T: Advanced Natural Products

OC(CB3)-25: Biosynthesis of natural products
OC(CB3)-26: Structure determination of natural products -I
OC(CB3)-27: Structure determination of natural products-II
OC(CB3)--28: Total stereo selective synthesis of natural products.

Elective-4B Paper-IV CH (OC) 404(CB4)T: Biopharmaceutics and Pharmacodynamics

OC(CB4)-29 : Pharmacokinetics
OC(CB4)-30 : Pharmacodynamics
OC(CB4)-31 : Principles of Therapeutics
OC(CB4)-32: Drug Interactions

Laboratory courses

Paper-VCH (OC) 451P: Spectroscopic identification of organic compounds & practice of chemistry software prgrammes
Paper-VI CH (OC) 452P: Synthesis and analysis of drugs

M.Sc. CHEMISTRY (ORGANIC CHEMISTRY)
IV SEMESTER SYLLABUS
(For the batch admitted during the academic year 2016 -2017 under the CBCS pattern)

Paper-1 CH(OC) 401T: Drug Design and Drug Discovery

OC-17: Principles of Drug design and drug discovery
OC-18: Lead modification and SAR Studies
OC 19: QSAR studies and computer aided drug design
OC 20: Combinatorial Synthesis

OC- 17: Principles of Drug design and drug discovery 15 Hrs

Introduction to drug discovery. Folklore drugs, stages involved in drug discovery- disease, drug targets, bioassay. Discovery of a lead- screening of natural products and synthetic compound libraries. Existing drugs as leads (me too drugs). Pharmacokinetics (ADME), pharmacodynamics. Nature of drug – receptor interactions and their theories – Occupancy theory, Induced – fit theory, Macromolecular purturbation theory and Two-state model of receptor activation. Natural products as lead structures in drug discovery – Pharmacophore - structure pruning technique e.g. morphine.Discovery of lead structure from natural hormones and neurotransmitters.Principles of design of agonists (e.g.Salbutamol), antagonists e.g. cimitidine) and enzyme inhibitors (e.g. captopril). Drug discovery without lead – serendipity- Penicillin and Librium as examples. Principles of prodrug design. Introduction to drug patents and Clinical trials.

OC-18: Lead modification and SAR Studies 15 Hrs

SAR*:* Lead modification strategies, Bioisosterism, variation of alkyl substituents,chain homologation and branching, variation of aromatic substituents,extension of structure, ring expansion and ring contraction, ring variation, variation and position of hetero atoms, ring fusion, simplification of the lead, rigidification of lead.Discovery of oxaminquine, salbutamol, cimitidine and captopril Structure-Activity Relationship studies in sulfa drugs,benzodiazepines, and taxol analogs.

OC-19: QSAR studies and computer aided drug design 15Hrs

QSAR: Introduction, physicochemical properties - pKa, electronic effects and Hammett constants(σ), lipophilicity constant(π), steric effects and Taft's constant, linear and nonlinear relationship between biological activityLipophilicity Substituent constants. Lipinski rule of five. Hansch analysis, Craig's plot,Topliss scheme, Free Wilson approach, cluster significant analysis. Two case studies (QSAR study on pyranenamine and design of Crizotinib).

Computer aided drug design: Introduction, active site, allosteric binding site,use of grids in docking , rigid docking , flexible docking and induced fit docking of ligands. Basic principles and difference between structure and ligand based drug design, denovo drug design and utility to optimize the lead structure.

OC-20: Combinatorial Synthesis 15Hrs

Introduction. Combinatorial approach. Combinatorial libraries, technologies. Solid phase synthesis, types of resins. Linkers. Reactants for solid phased synthesis. Methods of Parallel synthesis: Haughton's tea bag procedure. Automated parallel synthesis. Methods in Mixed combinatorial synthesis: general principles. Furkas mix and split combinatorial synthesis, Structure determination of active compounds-Deconvolution, Methods in deconvolution-recursive deconvolution, tagging and use of decoded sheets. Examples of Combinatorial Chemistry. Planning and designing of combinatorial synthesis, Spider like scaffolds, drug molecules. Automation in Combinatorial chemistry. High throughput screening.

Reference books

1. Burger's medicinal chemistry and drug discovery by Manfred E. Wolf.
2. Introduction to Medicinal chemistry by Patrick.
3. Introduction to drug design by R Silverman
4. Comprehensive medicinal chemistry. Vol 1-5 by Hanzsch.
5. Principles of medicinal chemistry. by William Foye
6. Biochemical approach to medicinal chemistry. by Thomas Nogrady.
7. Pharmaceutical Chemistry and Drug synthesis by Roth and Kleeman
8. Drug design by E.J.Arienes
9. Principles of Medicinal Chemistty Vol I & II by Kadam et al
10. Medicinal chemistry An introduction by Garreth Thomas
11.Organic and Pharmaceutical chemistry By Delgrado
12. Organic Pharmaceutical chemistry By Harikishansingh
13. Medicinal Chemistry By Ashtoshkar
14. Medicinal Chemistry By Chatwal
15. Organic Drug synthesis By Ledneicer Vol 1-6

1 6.Strategies for organic drug synthesis and design By Daniel Ledneicer.

1 7.Top Drugs: Top synthetic routes By John Saunders

I 8.Chirotechnoiogy By Roger A. Sheldon

19. Burger's Medicinal Chemistry and Drug Discovery: Principles and Practices. Vol. 1.
20. Medicinal Chemistry by G. Patricks.
21. Text book of Drug Design and Discovery, Edited by PovlKrogsgaard – Larsen Tommy Liljefors.
22. Structure Based Drug Design of Crizotinib (PF-02341066), a Potent and Selective Dual Inhibitor of Mesenchymal–Epithelial Transition Factor (c-MET) Kinase and Anaplastic Lymphoma Kinase (ALK) Martin P. Edwards, J. Med. Chem., 2011, 54 (18), pp 6342–6363.

http://www.pfizer.com/news/featured_stories/featured_stories_martin_edwards.jsp

Paper-II CH (OC) 402T: Drug synthesis and mechanism of action

OC-21: Drugs acting on metabolic process, cell wall and specific enzymes
OC-22: Drugs acting on genetic material and immune system
OC-23: Drugs acting on receptors and ion channels
OC-24: Chiral drugs

OC-21: Drugs acting on metabolic process, cell wall and specific enzymes

Basic concepts of mechanism of drug action: Introduction to macromolecular targets, carbohydrates, proteins, lipids and nucleic acids as possible drug targets. Classification of drugs. Enzyme inhibition and its types.

a**)** Drugs acting on metabolic process:

Antifolates –Discovery and mechanism of action of sulphonamides, Synthesis of sulfomethoxazole, sulfodoxine, sulfaguanidine and dapsone.

Diaminopyrimidines -trimethoprim, bacterial resistance to sulfonamides and drug synergism

b**)**Drugs acting on cell wall: Structure of bacterial cell wall, β-Lactam antibiotics – mechanism of action of penicillins and cephalosporins. Synthesis of pencillin-G and cephalosporin-C, cefalexin and cycloserine. Resistance to pencillins, broad spectrum penicillins – cloxacillin, methicillin, ampicillin, amoxicillin and carbenicillin. β-Lactamase inhibitors- Structural formulae and mode of action of clavulanic acid and sulbactum

c)Drugs acting on specific enzymes: H^+/K^+ -ATPase inhibitors- synthesis of Omeprazole and Carbonic anhydrase inhibitors-synthesis of Acetazolamide.

OC-22: Drugs acting on genetic material and immune system

Drugs acting on genetic material:Introduction, classification and mechanism of action.

a) DNA-intercalating agents-Anticancer and antimalarial agents. Structural formulae of Daunomycin, Adriamycin and Amsacrine. Synthesis of Amscarine, Nitracrine, Quinacrine and Chloroquine.

b) DNA- Binding and nicking agents: Antiprotozoal drugs. Synthesis of Metronidazole, Dimetridazole and Tinidazole.

c) DNA-Alkylators: Synthesis of Cyclophosphamide and Bisulphan.

d) DNA-Polymerase inhibitors: Antiviral agents- Synthesis of Acyclovir and AZT.

e) DNA-Topoisomerase inhibitors: Anti bacterial agents.Synthesis of Ciprofloxacin and Norfloxacin. Structural formulae ofloxacin and Lomefloxacin.

f) Inhibitors of transcribing enzymes: Anti-TB and antileprosy agents-structural formulae of Rifamycins and partial synthesis of Rifampicin.

g) Drugs interfering with translation process: Antibacterial drugs- Structural formulae of Erythromycin, 5-Oxytetracycline and Streptomycin. Synthesis of Chloromycetin

Drugs acting on immune system: Introduction to immune system. Immunosupressing agent-structural formula of Cyclosporin. Immunoenhancers-use of vaccines and strucrural formula of levamisol.

OC-23: Drugs acting on receptors and ion channels

Introduction to nervous system: structure of neuron, nerve transmission. Definition and examples of agonist, antagonist, neurotransmitters and receptors.

Drugs acting on receptors:

a)Adrenergic receptors - Introduction and classification. α-Adrenergic-receptor agonists and antagonists- Synthesis and biological activity of Nor-adrenaline, Methyl L dopa and Tetrazosin.

β-Adrenergic-receptor - agonists and antagonists – Synthesis and pharmacological activity of Salbutamol, Tetrabutalin, Propranolol and Atenolol.
b)Cholinergic-receptors: Introduction and classification.Cholinergic-receptor agonists and antagonists- Structural formulae of Nicotine, Atropine and Tubocurarine. Synthesis of Acetyl choline and Succinyl choline
c)Dopamine receptors: Introduction and classification.Dopamine- receptoragonists and antagonists- Biosynthesis of Dopamine. Synthesis of L-Dopa and Chlorpromazine.
d)Serotonin receptors: Introduction and classification.Serotonin receptoragonists and antagonists-synthesis and pharmacological activity of Serotonin and Metoclopramide.
e)Histamine receptors:Introduction and classification.Histamine receptor agonists and antagonists-synthesis and biological action of Histamine, Chloropheneramine, and Ranitidine.
f) Hormones and their receptors: Introduction to estrogen receptors, Structural formulae of Tamoxifen
Drugs acting on ion channels: Introduction to ion channels, drugs acting on Ca^{2+}, Na^{+} and Cl^{-} channels and their mode of action. Structural formulae of Tetracaine and synthesis and of Nifedipine, Diltiazem, Tetracine and 4-Aminopyridine.

OC-24: Chiral drugs
Introduction to chiral drugs. Three-point contact model, Eutomer, Distomer and eudesmic ratio. Pfeiffer's rule. Role of chirality on biological activity: Distomers – a) with no side effects b)with undesirable side effects c) both isomers having independent therapeutic value d)combination products having therapeutic advantages e) metabolic chirality inversion.
Synthesis and pharmacological activity of S-Ibuprofen, S- Metaprolol, Ininavir sulfate, Levocetrazine, 2S-Verapamil, S,S-Ethambutol , (+)Lomefloxacin, Fluvastatin, Dextropropoxyphen, (+)Ephedrine, (+)Griseofulvin, Dexormaplatin, R-Indacrinone, Nateglinide, Oxybutynin hydrochloride, S,S- Captopril and S,S,S- Enalaprilate.

Reference Books:

1. Burger's medicinal chemistry and drug discovery. By Manfred B. Wolf.
2. Introduction to Medicinal chemistry. By Graham Patrick.
3. Introduction to drug design. By R.B.Silverman
4. Comprehensive medicinal chemistry. Vol 1-5 by Hanzsch.
5. Principles of medicinal chemistry. By William O. Foyeetal.
6. Biochemical approach to medicinal chemistry. By Thomas Nogrady.
7. Pharmaceutical Chemistry and Drug synthesis By Roth and Kleeman
8. Drug design By E.J. Arienes
9. Principles of Medicinal Chemistry. Vols.1 & 2 By Kadam etal
10. Medicinal chemistry An introduction By Gareth Thomas
11. Wilson and Gisvold,s text book of Organic, Medicinal and Pharmaceutical chemistry By J.N.Delgado and W.A.Remers.
12. Organic Pharmaceutical chemistry By Harikishansingh.
13. Medicinal Chemistry By Ashutoshkar
14. Medicinal Chemistry By G.Chatwal
15. Organic Drug synthesis By Ledneiser Vol 1-6
16. Strategies for organic drug synthesis and design By Daniel Ledneiser
17. Top Drugs: Top synthetic routes By John Saunders
18. Chirotecchnology By Roger A. Sheldon

Elective-3A

Paper-III CH (OC)-403T (CB1): Advanced Heterocyclic Chemistry

OC (CB1) 17: Non aromatic heterocyclics& aromaticity
OC (CB1) 18: Five and six membered heterocyclics with two hetero atoms
OC (CB1) 19: Heterocyclics with more than two hetero atoms
OC (CB1) 20: Larger ring and other heterocycles

OC (CB1) 17: Nonaromatic heterocyclics& Aromaticity15 Hrs

Different types of strains, interactions and conformational aspects of nonaromatic heterocycles. Synthesis, reactivity and importance of the following ring systems. Azirines, Aziridines, Oxiranes, Thiiranes, Diazirenes, Diaziridines, Oxaziridines, Azetidines, Oxetanesandthietanes

Aromaticity: Introduction, Aromatic and anti aromatic compounds. Criteria for aromaticity. Huckel's 4n+2 electron rule for benzene and non benzenoid aromatic compounds. Eg. Cyclopropenium ion, cyclopentadienyl ion, cycloheptatrienium ion, azulene and annulenes.

OC (CB1) 18: Five and six membered heterocyclics with two hetero atoms 15 Hrs

Synthesis, reactivity, aromatic character and importance of the following heterocycles: Pyrazole, Imidazole, Oxazole, Thiazole, Isoxazole, Isothiazole, Pyridazine, Pyrimidine. Pyrazine, Oxazine, thiazine, benzimidazole, benzoxazole and benzthiazole.

OC (CB1) 19: Heterocyclics with more than two hetero atoms 15 Hrs

Synthesis, reactivity, aromatic character and importance of the following Heterocycles: 1,2,3-triazoies,1,2,4-triazoles, Tetrazoles, 1,2,4-oxadiazole, 1 ,3,4-oxadiazole, 1,2,5- oxadiazole, 1,2,3-thiadiazoles, 1,3,4- thiadiazoles, 1,2,5- thiadiazoles, 1,2,3-triazine, 1,2,4- triazine, 1,3,5-triazine, tetrazines. Synthesis and importance of purines and pteridines. Syntheis of Caffeine, theobromine and theophylline.

OC (CB1) 20: Larger ring and other Heterocycles 15 Hrs

Synthesis, structure, stability and reactivity ofAzepines, Oxepines and Thiepines. Synthesis of Diazepines rearrangements of 1,2 - diazepines. Synthesis of Benzoazepines, Benzodiazepines, Benzooxepines, Benzothiepines, Azocines and Azonines. Synthesis of selenophenes, Tellerophenes,Phospholesand Boroles.

Recommended Books:

1. Heterocyclic Chemistry, T.Gilchrist
2. An introduction to the Chemistry of heterocyclic compounds, R.M.Acheson
3. Heterocyclic Chemistry, J.A.Joule&K.Mills
4. Principles of Modern Heterocyclie Chemistry, A.Paquette
5. Heterocyclic Chemistry, J,A.Joule& Smith
6. Handbook of Heterocyclic Chemistry, A.R.Katritzky
7. The aromaticity III level, units 17-19 British open university volumes
8. Aromatic character and aromaticity by G.M.Badger
9. Non-benzenoid aromatic compounds by D.Ginsberg
10. Nonbenzenoid compounds by Lloy

Elective-3B
Paper-III CH (OC)-403T (CB2): Organic Polymers, Dyesand Pigments

OC (CB2) 21: Polymers- I
OC (CB2) 22: Polymers- II
OC (CB2) 23: Dyes-I
OC (CB2) 24:Dyes-II and pigments

OC (CB2) 21:Organic Polymers - I15 Hrs

Introduction, Classification of Polymers – according to origin, structure, intermolecular interactions. Types of polymerization – addition, condensation, radical, ionic and coplymerization with mechanism, Ziegler-Natta polymerization with mechanism. Stereochemistry of polymers, Plasticity – types of plastics. Molecular mass of polymers. Resins and plastics – Polystyrene and styrene copolymers, poly(vinyl chloride/vinyl acetate)and related polymers, acrylic polymers, polyesters, phenol-formaldehyde polymers, polyurethanes and epoxide polymers with examples. Natural and synthetic rubbers.

OC (CB2) 22: Organic Polymers - II 15 Hrs

a) Functional polymers :

i) Electrically conducting polymers: Introduction, basic principles. Brief description of polyanilines, polypyrroles, polyacetylenes, polythiophenes and their applications.

ii) Photoconductive polymers: Liquid crystal polymers, smectoc, nematicamd cholesteric structures, ion-exchange polymers – cationic, anionic exchange polymers and their uses.

iii) Smart materials: Uses in sensing device and communication networks.

iv)Biodegradable polymers: Definition, classification. Brief description polyhydroxyalkanoates, polycaprolactones, polyactic, polyvinyl alcohol and their applications.

b) Membranes: Filtration, micro, ultra, nano filtration. Separation of gases-Permeselectivity and gas permeability representative polymers. Liquid separation-dialysis, electroosmosis and reverse osmosis.

c) Fire retarding polymers and photonic polymers.

Polymers in biomedical application, artificial organs and controlled drug delivery.

OC (CB2) 23: Dyes – I 15 Hrs

Synthetic and Natural dyes

Introduction, nomenclature and classification of synthetic dyes. Color and constitution - chromospheres and auxochromes with suitable examples, Witt's theory, Armstrong's theory, Baeyer's theory, Nietzki's theory, Waston's theory, Modern theories, Valence Bond Theory and Molecular orbital theory. Chemistry and synthesis of triphenyl methane dyes[malachite green, rosaniline, para aniline blue, crystal violet methyl violet, hydroxytriphenyl methane dyes, Aurin, chrome violet], Azo dyes - types of azo dyes, synthesis of acidic and basic azo dyes, mono azo, di azo, tri azo and poly azo dyes. Chemistry and synthesis of cyanine dyes. Natural dyes – structure determination and synthesis of alizarine, Quinazarin and Indigo.

OC (CB2) 24:Dyes–II and Pigments 15 Hrs

a)**Introduction to Fluorescence dyes**

Interaction of organic molecules with electromagnetic radiation. Energy diagram. Activation and deactivation of organic molecules by light. Fluorescence and delayed fluorescence. Effect of molecular structure on fluorescence. General properties of fluorescent dyes and their requirements. Triplet-triplet absorption of organic molecules. Fluorescent quantum

yields and factors affecting them. Synthesis of Fluorescent aromatic hydrocarbons. and Fluorescent heteroaromatic compounds.

b)**Introduction to laser dyes**. Synthesis of Oligophenylenes. Oxazoles and benzoxzoles. Stilbenoid compoundsCoumarin laser dyes, Rhodamine laser dyes.

c) **Pigments:** Introduction, Structures of Porphyrins , Bile pigments. Synthesis of Haemin and Chlorophyll. Synthetic pigments – preparation of phthalocyanines.

ReferenceBooks

1.Organic polymer chemistry by K.J.Sanders
2. Polymer syntheses, Vol.I by S.R.Sandler and W.Karo
3. The elements of Polymer Science and Engineering by A.Rudin
4. Principles of Polymer Chemistry by A.Ravve
5. Polymer Science by V.R.Gowariker , N.V.Viswanathan and J.Sreedhar
6. Polymer Chemistry by C.E.Carraher , Jr.
7. A text book of polymers, Vol. I,II,III, M.S. Bhatnagar , S. Chand
8. Polymer Chemistry, B. Vollmert
9. Textbook of Polymer Science, F. W. Billmeyer Jr, John Wiley & sons
10. Organic Chemistry , Vol.1,2 by I.L.Finar
11. Color and constitution of organic molecules by J.Griffiths
12. Functional Dyes, Elsevier BV 2006,,,,,,S H.KIM
13. Colorants for non-textile Applications, Elsevier BV 2000 …H S Freeman and A T Peters
14. Industrial Dyes-Chemistry, Properties, Applications. WILEY-VCH Verlag, 2003 Klaus Hunger
15. Introduction to Fluorescence Sensing, Springer 2009, by A P Demchenko
16. Natural Dyes and their Applications in Textiles by M. L. Gulrajani, IIT Delhi
17. Handbook on Natural Dyes for Industrial Applications by P. S. Vankar, National Institute of Industrial Research
18. Steroelectronic Effects in Organic Chemistry by Pierre Deslongchams, Pergamon Press
19. Chemistry and Biochemistry of plant pigments, Vol. 2, by T.W.Goodwin
20. Contemporary Polymer Chemistry, H. R. Alcock& F. W. Lambe, Prentice Hall
21. Materials scince and engineering an introduction by William D Callister, Jr. Wiley Publishers

Elective-4A(ID Paper)
Paper-IVCH (OC) 404(CB3)T: Advanced Natural Products

OC(CB3)-25: Biosynthesis of natural products
OC(CB3)-26: Structure determination of natural products-I
OC(CB3)--27: Structure determination of natural products-II
OC(CB3)--28: Total stereo selective synthesis of natural products.

OC(CB3)-25: Biosynthesis of natural products 15 Hrs

Biosynthesis of secondary metabolites: Introduction,Difference between Laboratory synthesis and biosynthesis. Methods for determination of biosynthetic mechanism. Isolation and identification of Biosynthetic precursors, Feeding experiments – use of radioisotopes Measurement of incorporation – absolute incorporation, specific incorporation. Identification of the position of labels in labeled natural products by chemical degradation and spectral methods. Major biosynthetic pathways: 1) Acetate-Malonate pathway: Biosynthesis of aromatic compounds, 2) Shikimic acid pathway ; Biosynthesis of essential amino acids – phenylalanine, tyrosine and tryptophan, carboxylic acid derivatives, flavonoids and morphine alkaloids. 3) Mevalonic acid pathway : Biosynthesis of terpenes – mono,sesqui, di, tri (β-amyrin) and carotenoids, steroids – cholesterol.

OC(CB3)-26:Structure determination of natural products-I15Hrs

Determination of structure and stereochemistry of morphine, reserpine, abietic acid, cholesterol and rotenone.

OC(CB3)-27: Structure determination of natural products-II 15 Hrs

Spectroscopic techniques IR, UV, ^{1}Hnmr, ^{13}Cnmr, COSY, HETEROCOSY, NOESY, 2D-INADEQUATE and MS in the structure elucidations of natural products, Examples, flavones, biflavones, flavanones, isoflavones, coumarins, quinolines, isoquinolines.

Study of the following solved problems: Mass, IR, ^{1}H, ^{13}C NMR, HOMOCOSY, HECTOR, DEPT, 2D-INADEQUATE and NOE of Geraniol, INEPT of **menthol**, APT of **apparicine**,

Heteronuclear 2D-J resolved spectrum of **stricticine**,NOESY of **buxaquamarine**, HETEROCOSY of **strictanol**, 2D-INADEQUATE of **α-picoline** and **β-methyl tetrahydran furan**.

OC(CB3)-28: Total stereoselective synthesis of natural products. 15 Hrs

Nicalou's synthesis of Dynemicin A , Corey's synthesis of prostaglandins (E2, F2α) and paeoriflorin, Sharpless synthesis of L-hexoses, Nicolaous synthesis of taxol, Danishefsky synthesis of indolizomycin, Takasago synthesis of menthol, Hoffmann-LaRoche synthesis of Biotin.

Reference books:

1.Textbook of organic chemistry, Vol II by I L Finar
2. Chemistry of natural products, Vol 12, by Atta-Ur-Rahman
3. An introduction to the chemistry of terpenoids and steroids, by William templeton
4. Systematic identification of flavonoid compounds by Mabry &Markham
5. Steroids by Fieser arid Fieser
6. Alkaloids by Manske
7. Alkaloids by Bentley
8. The chemistry of terpenes by A Pinder
9. The terpenes by Simenson
10. Terpenoids by Mayo
11. Alkaloids by Pelletier
12. Total synthesis of Natural Products by Apsimon Vol 1-5
13. Biosynthesis by Geismann
14.Principles of organic synthesis 3rd Ed.R O C Norman and J M Coxen
15.One and two dimensional nmr spectroscopy by Atta Ur Rahman
16.Classics in total synthesis K C Nicolaou and E J Sorenson
17. Spectrometric identification of organic compounds by Silverstein and Webster

Elective-4B(ID Paper)
Paper-IV CH (OC) 404(CB4)T: Biopharmaceutics and Pharmacodynamics

OC(CB4)-29 : Pharmacokinetics
OC(CB4)-30 : Pharmacodynamics
OC(CB4)-31 : Principles of Therapeutics
OC(CB4)-32: Drug Interactions

OC(CB4)-29: Pharmacokinetics.
Introduction and importance of ADME studies of drugs. Routes of administration . i)Absorption: Definition, absorption of drugs across the membranes. Physico chemical factors affecting the drug absorption (emphasis on pH partition hypothesis and Drug Dissolution). Methods of determination of drug absorption. Bioavailability. ii)Distribution: Apparent volume of drug distribution. Factors affecting distribution, plasma protein binding. iii) Metabolism: Sites of drug metabolism, metabolic rate constant, bioactivation and biotransformation of drugs (phase I and phase II reactions) iv)Elimination: Types of elimination and overall apparent elimination rate constant and half-life, concept of clearance.

OC(CB4)-29: **Pharmacodynamics.**
Introduction, targets for drug action, receptor concept. Pharmacological binding terms. Two-statereceptor model, receptor families- structure and signal transduction mechanisms- channel linked proteins, gating mechanism, G-protein coupled receptors, G-protein and their role, Targets for G-proteins, Kinase linked receptors, receptors that regulate gene transcription. Theories of concentration -response relationship, dose-response curves.

OC(CB4)-30: **Principles of Therapeutics**
Plasma Drug concentration vs Time profile,Definition and explanation of various terms: MEC, MSC, MTC, AUC(graph). Peak plasma concentration, time of peak concentration. Therapeutic range. Steady state concentration, onset of action, onset of time, duration of action, intensity of action. LD50, ED50. Therapeutic objective. Dosage regimen, Design of dosage regimes: Dose size, dosing frequency, drug accumulation during multiple dosing, time to reach steady-state during multiple dosing, average concentration and body content on multiple dosing to steady state, loading dose, maintenance dose, maintenance of drug within the therapeutic range, design of dosage regimen from plama concentration. Kinetics of fixed dose, fixed time interval regimes. Modification to dosage regime: Dosing of drugs in obese patients, dosing of drugs in Neonates, infants & children, dosing of drugs in geriatrics (elderly), dosing of drugs in Hepatic disease, dosing of drugs in renal disease.

OC(CB4)-31: Drug Interactions.
Introduction, classification, Mechanisms of drug interactions.– pharmacokinetic interactions(alteration of gastrointestinal absorption, compexation and adsorption, alteration of distribution, alteration of metabolism and alteration of excretion) & pharmacodynamic interactions (antagonistic effects, synergistic effects, alteration of electrolyte levels, interactions involving adrenergic system, alteration of receptor site interaction and antibiotic combinations). Influence of alcohol(Anti biotics, Anti coagulants, Anti histamines, Anti psychotic drugs, sedatives and Hypnotics), smoking(Theophylline, Diazepam, a Tri cyclic antidepressants), food (Bronchodaliators, Diuretics, ACE Inhibitors, Anti coagulants,Tetracyclines) on drug action.

Reference books:

1. Pharacokinetics. By Shobha Rani
2. Elements of Pharmacology. By Gandhi,Desani& Goyal.
3. Goodmann&Gilmann's " The pharmacological basis of therapeutics. By Gilman &Rali.
4. Pharmacology. By Rang.
5. Biopharmaceutics and pharmacokinetics By Brahmanikar
6. Pharmacology By Lippincot
7. Modern Pharmacology with Clinical Applications. By R.Craig.
8. Compehensive pharmacy review by Leon Shargel
9. Hospital and clinical pharmacy
10. Burger's medicinal chemistry and drug discovery. By Manfred E. Wolf.
11. Introduction to Medicinal chemistry. By Patrick.
12. Comprehensive medicinal chemistry. Vol 1-5 By Hanzsch.
13. Principles of medicinal chemistry. By William Foye
14. Biochemical approach to medicinal chemistry. By Thomas Nogrady.

Laboratory courses

Paper CH (OC) 451P: Spectroscopic identification of organic compounds & practice of chemistry software prgrammes

1. Identification of unknown organic compounds by interpretation of IR, UV, ^{1}H -NMR, ^{13}C NMR, and mass spectral data(two examples with 2D-NMR). A minimum of 30 representative examples should be studied.

2. Chemistry software programmes: Chem Draw, analysis of IR and NMR using ACD/Id NMR processor. EXCEL: Drawing graphs, Molecular docking.

Paper CH (OC) 452P: Synthesis and analysis of drugs

(A) Laboratory Synthesis of the following drugs:

Paracetamol, Phenytoin, Benzocaine, 6-Methyluracil, Chloritone,FIuorescien, 4-Aminobenzene sulfonamide, antipyrineand phenothiazine

(B) Estimation of the following drugs*:*

Aspirin (titrimetry), Ibuprofen (titrimetry), Analgin (titrimetry), Chloride in Ringer's lactate (argentometry), ascorbic acid {titrimetry, Iodometry and Cerimetry), colorimetry}, Isoniazid(Iodometry), Riboflavin(colorimetry),Zn ions in Bactracin Zinc, Ca^{+2} ions in Calcium gluconate injection(complexometry), Riboflavin (UV-Visible Spectrophotometer).

Reference books:

1. Practical organic chemistry by Mann & Saunders
2. Text book of practical organic chemistry by Vogel
3. The systematic identification of organic compounds by Shriner et.al
4. Analytical chemistry by G N David Krupadanam et.al
5. Advanced practical medicinal chemistry by Ashutoshkar
6. Pharmaceutical drug analysis by Ashutoshkar
7. Quantitative analysis of drugs in pharmaceutical formulations by P D Sethi
8. Practical pharmaceutical chemistry part-1 and part-2 by A H Beekett and J B Stenlake
9. Spectroscopic identification of organic compounds by R M Silverstein and F X Webster

M.Sc. CHEMISTRY (PHARMACEUTICAL CHEMISTRY SPECIALISATION)

SYLLABUS OF III & IV SEMESTERS

REVISED AS PER NEW (CB) SYLLABUS

FOR STUDENTS ADMITTED FROM THE YEAR

2016 ONWARDS

M.Sc. CHEMISTRY (PHARMACEUTICAL CHEMISTRY)
Syllabus for III and IV SEMESTERS
(For the batch admitted in the academic year 2016 and later under the CBCS pattern)
[Under Restructured CBCS Scheme]
Grand total marks and credits (all 4 semesters) 2400 marks – 96 credits

(Approved in the P.G.BOS meeting held on 01-07-2017)

SEMESTER-III

Paper	Instruction Hrs/Week	Internal Assessment marks*	Semester marks	Total marks	Total credits
CH(PhC)301T	4	20	80	100	4
CH(PhC)302T	4	20	80	100	4
CH(PhC)303T	4	20	80	100	4
CH(PhC)304T	4	20	80	100	4
CH(PhC)351P	9	-	100	100	4
CH(PhC)352P	9	-	100	100	4
			Total	600	24

SEMESTER - IV

Paper	Instruction Hrs/Week	Internal Assessment marks*	Semester marks	Total marks	Total credits
CH(PhC)401T	4	20	80	100	4
CH(PhC)402T	4	20	80	100	4
CH(PhC)403T	4	20	80	100	4
CH(PhC)404T	4	20	80	100	4
CH(PhC)451P	9	-	100	100	4
CH(PhC)452P	9	-	100	100	4
			Total	600	24

*** 15 marks for the written test and 5 marks for the assignment**
Grand total all 4 semesters: 2400 marks and 96 credits

PAPER TITLES , M.Sc. Pharmaceutical Chemistry Specialization
(For the batch admitted during the academic year 2016 onwards under the CBCS pattern)
[Under Restructured CBCS Scheme]

III SEMESTER SYLLABUS	IV SEMESTER SYLLABUS
Paper-1 CH(PhC)301T: Basics of Pharmaceutal Chemistry PhC 9 : Introduction to I.P, B.P & USP monographs, Errors in Pharmaceutical analysis and statistical validation. PhC 10: Rheology and micromeritics PhC 11: Physical pharmacy PhC 12::Introduction to pharmaceutics Paper-II CH(PhC) 302T: Pharmacokinetics and Pharmacodynamics PhC 13 : Pharmacokinetics PhC 14 : Pharmacodynamics PhC 15 : Principles of Therapeutics PhC 16 : Drug Interactions **Elective-3A** Paper -IIICH(PhC) 303T(CB1): Synthetic Reagents, Advanced NMR, Conformational Analysis and ORD PhC(CB1)-1: Synthetic Reagents-I PhC(CB1)-2:Synthetic Reagents-II PhC(CB1)-3: ^{13}C NMR and 2D NMR spectroscopy PhC(CB1)-4: Conformational analysis (Cyclic systems) & ORD **Elective-3B:** Paper-III CH(PhC) 303T(CB2): Pharmaceutical Inorganic and Analytical Chemistry PhC(CB2)-5: Inorganic pharmaceuticals-I PhC(CB2)-6: Inorganic and Radio pharmaceuticals-II PhC(CB2)-7: Limit tests PhC(CB2)-8: Biochemical analysis **Elective-4A** Paper IV CH(PhC) 304T(CB3): Modern Organic Synthesis PhC(CB2)-9: Asymmetric synthesis PhC(CB2)-10: Synthetic stratagies PhC(CB2)-11: New Synthetic reactions PhC(CB2)-12: New techniques and concepts in organic synthesis **Elective-4B** Paper IV CH(PhC) 304T(CB4): Herbal drugs , synthetic pharmaceuticals and IPM PhC(CB4)-13 : Herbal Drugs PhC(CB4)-14: Synthetic pharmaceuticals -I PhC(CB4)-15 : Synthetic pharmaceuticals –II PhC(CB4)-16: Intellectual Property Management **LABORATORY COURSES** Paper-V CH(PhC) 351: Qualitative Analysis of Organic Mixtures Paper-VI CH (PhC) 352 P: Spectroscopic identification of organic compounds and Chromatography	Paper-1 CH (PhC) 401T: Drug Design and Drug Discovery PhC-17: Principles of Drug design and drug discovery PhC-18: Lead modification and SAR Studies PhC 19: QSAR studies and computer aided drug design OC 20: Combinatorial Synthesis Paper-II CH (PhC) 402T: Drug synthesis and mechanism of action PhC-21: Drugs acting on metabolic process, cell wall and specific enzymes PhC-22: Drugs acting on genetic material and immune system PhC-23: Drugs acting on receptors and ion channels PhC-24: Chiral drugs **Elective-3A** Paper-III CH(PhC)403T(CB1): Medicinal natural products and drug analysis PhC (CB1)-17 : Medicinal natural products PhC (CB1)-18 :Spectroscopic analysis of drugs PhC (CB1)-19 :Titrimetric analysis of drugs PhC (CB1)-20 :XRD and chromatographic analysis of drugs **Elective-3B** Paper-III CH(PhC) 403T(CB2): Industrial Pharmaceutical Chemistry PhC (CB2)-21:Unit Process PhC (CB2)-22:Industrial Synthesis PhC (CB2)-23:Quality Control and Quality Assurance PhC (CB2)-24:Effluents of Industrial Units and their purification **Elective-4A (ID Paper)** Paper IV CH(PhC) 404T(CB3): Biopharmaceutical Chemistry PhC(CB3)-25 : Enzymes – Enzyme Immobilisation PhC (CB3)-26 :Microbial Transformations PhC(CB3)-27:Pharmaceuticals From Fermentation Technology PhC(CB3)- 28:Pharmaceuticals From Recombinant DNA Technology **.Elective-4B (ID Paper)** Paper IV CH(PhC) 404T(CB4): Biomolecules and Molecular Modelling PhC (CB4)-29:Nucleic acids PhC (CB4)-30: Proteins: PhC (CB4)-31: Molecular Modelling PhC (CB4)-32: Modelling Biomolecules **LABORATORY COURSES** Paper-V CH (PhC) 451P: CH (PhC) 451P: Synthesis of drug molecules and QSAR studies Paper- VI CH (PhC) 452P: Titrimetric & Instrumental Drug analysis

M.Sc. CHEMISTRY (PHARMACEUTICAL CHEMISTRY)
III SEMESTER SYLLABUS
(For the batch admitted during the academic year 2016 -2017 under the CBCS pattern)

PAPER- I
CH (PhC) 301T BASICS OF PHARMACEUTICAL CHEMISTRY

PhC 9 : Introduction to I.P, B.P & USP monographs, Errors in Pharmaceutical analysis and statistical validation.
PhC 10 : Rheology and micromeritics
PhC 11: Physical pharmacy
PhC 12: Introduction to pharmaceutics

PhC 9: Introduction to I.P, B.P & USP monographs, Errors in pharmaceutical analysis and statistical validation. 15hrs

Introduction to I.P, B.P & USP monographs. Errors in pharmaceutical analysis: Introduction, classification, accuracy, precision, minimization of systemic errors. Statistical validation- Statistical treatment of finite examples (mean, median, average deviation, standard deviation, coefficient variation and variance calculations). Distribution of random numbers. Significant figures- computation rules. Comparison of results (students t-test, variance-ratio test or f-test), method of least squares.

PhC 10 : Rheology and Micromeritics 15hrs

Introduction, concept of viscosity, kinematic viscosity, mechanism of enhanced viscosity, factors influencing viscosity-intrinsic and extrinsic factors. Newtonian flow, non-Newtonian flow. Thixotropy, negative thixotropy, Rheopexy & measurement of thixotropy. Determination of rheological properties(flow properties).Selection of viscometers. Newtonian flow – Ostwald viscometer, falling sphere viscometer. Non Newtonian flow – cup & bob viscometer & cone & plate viscometer. Applications to pharmacy.

Micromeritics Introduction, particle size analysis- concepts of particle size, size distribution, mean size of particulate system, methods of particle size analysis (sieving, microscopic method, sedimentation methods, electrical sensing zone method, optical sensing zone and light diffraction method).

PhC 11: Physical Pharmacy 15hrs

Physical properties of drug molecules: Dielectric constant, Induced polarization, refractive index, molar refraction, optical rotation, Colligative properties.

Buffered and isotonic solutions: Buffer equation, common ion effect, buffer equation for weak acid and its salt and weak base and its salt. Factors influencing PH of buffer solutions. Drugs as buffers. PH of indicators,buffer capacity and its calculations, Van Slyke equation, influence of concentration on buffer capacity and maximum buffer capacity. Buffers in pharmaceutic and biological system- in vivo biologic buffer systems, pharmaceutical buffers and their preparation. Influence of buffer capacity and PH on tissue irritation, stability vs. optimum therapeutic response. PH and solubility. Buffered isotonic solution, measurement of tonicity. Calculating tonicity and methods of adjusting tonicity and PH.

PhC 12 : Introduction to pharmaceutics **15hrs**

Introduction to pharmaceutical dosage forms- Definition and requirement for formulation of pharmaceuticals. Classification of dosage forms. Routes of administration- Advantages and Disadvantages. Solid dosage forms: Tablets-Classification. Properties of tablets, evaluation of tablets. Capsules..Liquid dosage forms: monophasic-for internal and external use, Monophasic-Syrups, Elixirs. Biphasic: Emulsions(various types), stability and evaluation of emulsions. Suspensions: Flocculated and nonflocculated systems, evaluation of suspensions. Semisolid dosage forms: Suppositories Types, suppository bases, evaluation. Ointments: Special types and evaluation, Creams. Parenteral Products.

Recommended text books:

1. Practical pharmaceutical chemistry. By A.H.Backette, J.B.Stenlake, Part-A & B.
2. Pharmaceutical analysis by Ashtoshkar
3. Fundamentals of analytical chemistry by Skoog & West
4. Physical Pharmacy by AN.Martin,J, Swarlbick etal
5. Physical pharmaceutics by Shotton and Ridgeway
6. Text book of Physical Phamacy by Hadkar
7. Text book of physical pharmaceuticals by Subramaniyan
8. Essentials of Physical chemistry and pharmacy by Arnikar & Kadam
9. Introduction to pharmaceuticals by Mittal
10. Pharmaceutical dosage forms and drug delivery systems by Ansel
11. Introduction to Pharmaceuticals by Gupta, Volume I & II.
12. Modern pharmaceutics by Banker and Rhode

References:

1. British Pharmacopoeia vol I,II
2. Indian Pharmacopoeia vol I,II
3. Bently's Text book of pharmaceutics by Rowlins
4. The science and practice of pharmacy by Remington

PAPER-II CH (PhC) 302T PHARMACOKINETICS AND PHARMACODYNAMICS

PhC 13 : Pharmacokinetics
PhC 14 : Pharmacodynamics
PhC 15: Principles of Therapeutics
PhC 16 : Drug Interactions

PhC 13 : Pharmacokinetics **15hrs**

Introduction and importance of ADME studies of drugs. Routes of administration . i)Absorption: Definition, absorption of drugs across the membranes. Physico chemical factors affecting the drug absorption (emphasis on pH partition hypothesis and Drug Dissolution). Methods of determination of drug absorption. Bioavailability. ii)Distribution: Apparent volume of drug distribution. Factors affecting distribution, plasma protein binding. iii) Metabolism: Sites of drug metabolism, metabolic rate constant, bioactivation and biotransformation of drugs (phase I and phase II reactions) iv)Elimination: Types of elimination and overall apparent elimination rate constant and half-life, concept of clearance.

PhC14 :Pharmacodynamics 15hrs

Introduction, targets for drug action, receptor concept. Pharmacological binding terms. Two-statereceptor model, receptor families- structure and signal transduction mechanisms- channel linked proteins, gating mechanism, G-protein coupled receptors, G-protein and their role, Targets for G-proteins, Kinase linked receptors, receptors that regulate gene transcription. Theories of concentration -response relationship, dose-response curves.

PhC15 : Principles of Therapeutics 15hrs

Plasma Drug concentration vs Time profile,Definition and explanation of various terms: MEC, MSC, MTC, AUC(graph). Peak plasma concentration, time of peak concentration. Therapeutic range. Steady state concentration, onset of action, onset of time, duration of action, intensity of action. LD50, ED50. Therapeutic objective. Dosage regimen, Design of dosage regimes: Dose size, dosing frequency, drug accumulation during multiple dosing, time to reach steady-state during multiple dosing, average concentration and body content on multiple dosing to steady state, loading dose, maintenance dose, maintenance of drug within the therapeutic range, design of dosage regimen from plama concentration. Kinetics of fixed dose, fixed time interval regimes. Modification to dosage regime: Dosing of drugs in obese patients, dosing of drugs in Neonates, infants & children, dosing of drugs in geriatrics (elderly), dosing of drugs in Hepatic disease, dosing of drugs in renal disease.

PhC16: Drug Interactions. 15hrs

Introduction, classification, Mechanisms of drug interactions.– pharmacokinetic interactions(alteration of gastrointestinal absorption, compexation and adsorption, alteration of distribution, alteration of metabolism and alteration of excretion) & pharmacodynamic interactions (antagonistic effects, synergistic effects, alteration of electrolyte levels, interactions involving adrenergic system, alteration of receptor site interaction and antibiotic combinations). Influence of alcohol(Anti biotics, Anti coagulants, Anti histamines, Anti psychotic drugs, sedatives and Hypnotics), smoking(Theophylline, Diazepam, and
Tri cyclic antidepressants), food (Bronchodaliators, Diuretics, ACE Inhibitors, Anti coagulants,Tetracyclines) on drug action.

Recommended text books:

1. Pharacokinetics. By Shobha Rani
2. Elements of Pharmacology. By Gandhi,Desani & Goyal.
3. Goodmann & Gilmann's " The pharmacological basis of therapeutics. By Gilman & Rali.
4. Pharmacology. By Rang.
5. Biopharmaceutics and pharmacokinetics By Brahmanikar
6. Pharmacology By Lippincot
7. Modern Pharmacology with Clinical Applications. By R.Craig.
8. Compehensive pharmacy review by Leon Shargel
9. Hospital and clinical pharmacy
10. Burger's medicinal chemistry and drug discovery. By Manfred E. Wolf.
11. Introduction to Medicinal chemistry. By Patrick.
12. Comprehensive medicinal chemistry. Vol 1-5 By Hanzsch.
13. Principles of medicinal chemistry. By William Foye
14. Biochemical approach to medicinal chemistry. By Thomas Nogrady.

PAPER III -CH (PhC) 303T(CB1): Synthetic Reagents, Advanced NMR, Conformational Analysis and ORD

PhC-(CB1) -1: Synthetic Reagents-I
PhC-(CB1) -2: Synthetic Reagents-II
PhC-(CB1) -3: ^{13}C NMR and 2D NMR spectroscopy
PhC-(CB1) -4: Conformational analysis (Cyclic systems) & ORD

PhC-(CB1) -1: Synthetic Reagents I
15 Hrs

i) Protecting groups: a) Protection of alcohols by ether, silyl ether and ester formation b) Protection of 1,2-diols by acetal, ketal and carbonate formation c) Protection of amines by benzyloxycarbonyl, t-butyloxycarbonyl, fmoc and triphenyl methyl groups. d) Protection of carbonyls by acetal, ketal and thiol acetal (Umpolung) groups. e) Protection of carboxylic acids by ester and ortho ester (OBO) formation.

ii) Organometallic Reagents: Preparation and application of the following in organic synthesis: 1) Organo lithium 2) Organo copper reagents 3) Organo boranes in C-C bond formation 4) Organo silicon reagents: reactions involving β-carbocations and α-carbanions, utility of trimethyl silyl halides, cyanides and triflates.

iii) Carbonyl methylenation: a) Phosphorous ylide mediated olefination 1) Witting reaction, 2) Horner-Wordsworth-Emmons reaction. b) Titanium- Carbene mediated olefination 1) Tebbe reagent, 2) Petasis reagent 3) Nysted reagent.

iv) Carbene insertions: Rh based carbene complexes, cycloprpanations.

v) C-H Activation: Introduction, Rh catalysed C-H activation.

PhC-(CB1) -2: Synthetic Reagents II **15 Hrs**

i) Oxidations: a) Oxidation of active C-H functions: DDQ and SeO_2. b) Alkenes to diols: Prevost and Woodward oxidation c) Alcohol to carbonyls: Cr^{VI} oxidants (Jones reagent, PCC, PDC) IBX, DMP, CAN, TEMPO, TPAP, Swern oxidation d) Oxidative cleavage of 1,2-diols: Periodic acid and Lead tetra acetate.

ii) Reductions: a) Catalytic hydrogenation: Homogenous (Wilkinsons's catalytic hydrogenation) and heterogeneous catalytic reduction. b) Non-metallic reductions: Diimide reduction c) Dissolving metal reductions: Birch reduction. d) Nucleophilic metal hydrides: $LiAlH_4$, $NaBH_4$, and their modifications. e) Electrophilic metal hydrides: BH_3, AlH_3 and DIBAL. f) Use of tri-n-butyl tin hydride: Radical reductions.

PhC-(CB1) -3: ^{13}C NMR and 2D NMR spectroscopy **15 Hrs**

i) ^{13}C NMR spectroscopy: Introduction**,** Types of ^{13}C nmr spectra: undecoupled, proton-decoupled and off-resonance decoupled (ORD) spectra. ^{13}C chemical shifts, factors affecting the chemical shifts, chemical shifts of organic compounds. Calculation of chemical shifts of alkanes, alkenes and alkynes. Homonuclear (^{13}C, ^{13}C J) and heteronuclear (^{13}C,^{1}H J and ^{13}C, ^{2}H J) coupling. Applications of ^{13}C-NMR spectroscopy: Structure determination, stereochemistry, reaction mechanisms and dynamic processes in organic molecules. ^{13}C-NMR spectral editing techniques: principle and applications of APT, INEPT and DEPT methods.

ii) 2D-NMR spectroscopy: Principles of 2D NMR, Classification of 2D-experiments. Correlation spectroscopy (COSY) HOMO COSY (^{1}H-^{1}H COSY) , TOCSY (Total Correlation

Spectroscopy), Hetero COSY ($^{1}H,^{13}C$ COSY,HMQC), long range $^{1}H,^{13}C$ COSY (HMBC), Homonuclear and Heteronuclear 2D-J-resolved spectroscopy, NOESY and 2D-INADEQUATE experiments and their applications.

PhC-(CB1) -4: Conformational analysis (Cyclic systems) AND ORD 15 Hrs

Conformational analysis (Cyclic systems) Study of conformations of cyclohexane, mono, di and tri substituted cyclohexanes, (1,3,5-trimethyl cyclohexanes and Menthols), cyclohexanone (2-alkyl and 3 -alkyl ketone effect), 2-halocyclohexanones, cycloheptane . Stereo chemistry of bicyclo [3,3,0] octanes, hydrindanes, decalins and perhydroanthracenes. Conformational structures of piperidine, N-Methylpiperidine, tropane, tropine, pseudotropine, decahydroquinoline and quinolizidine. Factors governing the reactivity of axial and equatorial substituents in cyclohexanes.

(oxidation, S_N2 reaction, rearrangements, Ester hydrolysis) Stereochemistry of addition to the carbonyl group of a rigid cyclohexanone ring.

Optical Rotatory Dispersion (ORD) and CD Spectroscopy: Optical rotation, circular birefringence, circular dichroism and Cotton effect. Plain curves and anomalous curves. Empirical and semiempirical rules-The axial haloketone rule, the octant rule, Helicity rule, Exciton chirality method. Application of the rules to the study of absolute configuration and conformations of organic molecules.

Recommended Books:

1. Some modern methods of organic synthesis by W. Carruthers
2. Guidebook to organic synthesis, by R K Meckie, D M Smith & R A Atken
3. Organic Synthesis by O House
4. Organic synthesis by Micheal B Smith
5. Reagents for organic synthesis, by Fieser & Fieser, Vol 1-11 (1984)
6. Organic synthesis by Robert E Ireland
7. Handbooks of reagents for organic synthesis by Reich and Rigby, Vol-I-IV
8. Organic chemistry by Jonathan Clayden, Nick Greeves and Stuart Warren
9. Organic Reactions and their mechanisms by P.S.Kalsi
10. Organic reaction mechanisms by V.K.Ahulwalia and Rakesh Kumar Parashar
11. Spectroscopic identification of organic compounds by RM Silverstein, G C Bassler and T B Morrill
12. Organic Spectroscopy by William Kemp
13. Spectroscopic methods in Organic chemistry by DH Williams and I Fleming
14. Modern NMR techniques for chemistry research by Andrew B Derome
15. NMR in chemistry - A multinuclear introduction by William Kemp
16. Spectroscopic identification of organic compounds by P S Kalsi
17. Introduction to organic spectroscopy by Pavia
18. Carbon-13 NMR for organic chemists by GC Levy and O L Nelson
19. Nuclear Magnetic Resonance Basic principles by Atta-ur-Rahman
20. Basic one and two-dimensional NMR spectroscopy by Horst Friebolin
21. NMR spectroscopy by H.Gunther
22. Stereochemistry of organic compounds — Principles & Applications by D Nasipuri
23. Stereochemistry of Carbon compounds by Ernest L Eliel & Samuel H. wilen
24. Stereochemistry: Conformation & Mechanism by P S Kalsi

25. The third dimension in organic chemistry, by Alan Bassendale
26. Stereo selectivity in organic synthesis by R S Ward.
27. Advanced organic chemistry. Part A Structure & Mechanism by Francis A. Corey and Richard J. Sundberg
28. Optical rotatory dispersion by C Djerassi
29. Optical rotatory dispersion and circular dichroism by P Crabbe
30. Mechanism and Structure in Organic chemistry by S Mukherjee

Paper III CH (PhC) 303T (CB2) PHARMACEUTICAL INORGANIC AND ANALYTICAL CHEMISTRY

PhC (CB2) -5 : Inorganic pharmaceuticals
PhC (CB2) -6 : Inorganic and Radio pharmaceuticals
PhC (CB2) -7 : Limit tests
PhC (CB2) -8: Biochemical analysis

PhC (CB2) -5 : Inorganic pharmaceuticals 15hrs

:i)Antioxidants : Introduction, criteria for action as anti oxidants, mechanism of action. Preparation, properties and assay of hypophosphorus acid and sodium meta bisulphate ii) Gastrointestinal agents: Acidifiers, antacids. Acidifiers- dil. HCl; Antacids- evaluation of antacid activity, drug interactions. Aluminium compounds- aluminium hydroxide gel, dry tablets, dried aluminium phosphate gel; calcium compounds- calcium phosphate, calcium carbonate; magnesium compounds- milk of magnesia, magnesium oxide; sodium compounds - sodium bicarbonate; combination of antacids. iii) Antidiarrhoeals: Bismuth compounds - bismuth sub carbonate iv) Laxatives: Magnesium sulfate , milk of magnesia v) Topical agents: Introduction, categories. vi) Astringents: alum

PhC (CB2) -6: Inorganic and radio pharmaceuticals 15hrs

i) Dental products. Introduction, anticaries agents-sodium flouride, dentifriers-dibasic calcium phosphate. ii) Inhalants: Introduction, role of oxygen, carbon dioxide and ammonia, nitrous oxide as inhalant.iii) Expectorants-Ammonium chloride and Potassium iodide. iv) Respiratory stimulants: Dil. ammonia solution, aromatic spirit of ammonia.v) Emetics: Ammonium chloride, potassium iodide. vi) Intra cellular and extra cellular electrolytes- body fluid compartments, role of major physiological cations and anions, sodium chloride. Metal ions as pharmaceuticals; i) Anti neoplastic agents: Cis-Platin and Carboplatin and their mechanism of action at molecular level.ii) Anti arthritics- Auranofin iii)Antiinfectives- Silver(I) sulphadiazine. **Radio pharmaceuticals**: Introduction, types of radio nuclides, units of radioactivity, 131I, 125I and barium sulfate.

PhC (CB2) -7: Biochemical analysis 15hrs

Principles and practical aspects of i)Microbiological assay- Zone inhibition method, serial dilution method (eg: antibiotics); ii) Competitive protein binding assay (eg. testosterone); iii) Radioimmuno assay(eg. morphine, insulin); iv)Radioreceptor assay(eg. benzodiazepine); v) Enzyme linked immunosorbent assay (eg. cocaine, opiates,); vi) Flourescence immuno assay(eg. galactosyl umbelliferone drug, cortisol).vii) Test for pyrogens.

PhC (CB2) -8 : Limit tests **15hrs**

Limit tests for insoluble matter, limit tests of soluble matter, limits of moisture, volatile matter, residual matter, residual solvents, limits of nonvolatile matter, limits of residue on ignition, limits of loss on ignition, limits on ash value. Limit tests for metallic impurities: lead, arsenic, iron: Limit tests for acid radical impurities, chlorides, sulfates, arsenate, carbonate, cyanide, oxalate, phosphate.Limit tests for nonmetallic impurities: Boron, free Halogens, Selenium.

Recommended text books:

1. Vogel's text book of quantitative chemical analysis
2. Pharmaceutical analysis By Chapman
3. Pharmaceutical analysis By Ashtoshkar
4. Inorganic pharmaceutical chemistry By Chatwal
5. Inorganic pharmaceutical chemistry By Mohammadali
6. Inorganic pharmaceutical and medicinal chemistry By Quadri and Quadri

References

1. Practical pharmaceutical chemistry. By A.H.Backette, J.B.Stenlake.
2. British Pharmacopoeia vol I,II
3. Indian Pharmacopoeia vol I,II
4. Pharmaceutical analysis. By Takeru,Higuchi
5. Pharmaceutical analysis By. David G.Watson
6. Bently's Text book of pharmaceutics by Rowlins
7. The science and practice of pharmacy by Remington

Paper IV -CH (PhC) 304T (CB3): Modern Organic Synthesis

P**h**C (CB3)-9: Asymmetric synthesis
P**h**C (CB3)-10: Synthetic strategies
P**h**C (CB3)-11: New Synthetic reactions
P**h**C (CB3)-12: New techniques and concepts in organic synthesis

PhC (CB3)-9:- Asymmetric synthesis **15 Hrs**

Introduction: Brief revision of classification of stereo selective reactions

Prostereoisomerism: Topicity in molecules Homotopic, stereoheterotopic (enantiotopic and diastereotopic) groups and faces- symmetry criteria.

Prochiral nomenclature: Pro chiraility and Pro-R, Pro-S, Re and Si.

Conditions for stereoselectivity: Symmetry and transition state criteria, kinetic and thermodynamic control. Methods of inducing enantioselectivityy.

Analytical methods: % Enantiomeric excess and diastereomeric excess. Determination of enantiomeric excess: specific rotation, Chiral NMR; Chiralderivatizing agents, Chiral solvent, Chiral shift reagents and Chiral HPLC.

Chiral Substrate controlled asymmetric synthesis: Nucleophilic additions to chiral carbonyl compounds. 1, 2- asymmetric induction, Cram's rule and Felkin-Anh model.

Chiral auxiliary controlled asymmetric synthesis: α-Alkylation of chiral enolates, Evan's oxazolidinone, 1, 4-Asymmetric induction and Prelog's rule..

Chiral reagent controlled asymmetric synthesis: Asymmetric reductions using BINAL-H. Asymmetric hydroboration using IPC_2 BH and $IPCBH_2$.
Chiral catalyst controlled asymmetric synthesis: Sharpless epoxidation. Asymmetric hydrogenations using chiral Wilkinson biphosphin catalyst.
Asymmetric aldol reaction: Diastereoselective aldol reaction (achiral enolate & achiral aldehydes) its explanation by Zimmerman-Traxel model.

PhC (CB3)-10: Synthetic Strategies 15 Hrs
Introduction: Terminology, Target, synthon, synthetic equivalent, functional group interconversion (FGI), functional group addition. Criteria for selection of target. Linear and convergent synthesis. Retrosynthetic analysis and synthesis involving chemoselectivity, regioselectivity, reversal of polarity and cyclizations. .
Order of events : S-Salbutamol, Propoxycaine..
One group C-C and C-X disconnections: Introduction .One group C-C disconnections in alcohols and carbonyl compounds. One group C-X disconnections in Carbonyl compounds, alcohols, ethers and sulphides.
Two group C-C and C-X disconnections : Introduction .Two group C-X disconnections in 1,1-difunctionalised, 1,2-difunctionalised and 1,3-difunctionalised compounds.
Two group C-C disconnections: Diels-Alder reaction, 1,3-difunctionalised compounds, 1,5-difunctionalised compounds, Michael addition and Robinson annulation.
Control in carbonyl condensations: oxanamide and mevalonic acid.
Strategic bond: definition, guidelines for disconnection; disconnection of C-X bonds, disconnect to greatest simplification, using symmetry in disconnection, disconnection corresponding to known reliable reaction, high yielding steps and recognizable starting materials. Retrosynthesis of Retronecene, longifoline.

PhC (CB3)-11: New Synthetic reactions 15 Hrs
1. Metal mediated C-C and C-X coupling reactions: Suzuki, Heck, Stille, Sonogishira cross coupling, Buchwald-Hartwig and Negishi-Kumada coupling reactions.
2. C=C Formation Reactions: Shapiro, Bamford-Stevens, McMurrey reactions, Julia-Lythgoe olefination and Peterson's stereoselective olefination.
3. Multicomponent Reactions: Ugi, Passerini, Biginelli, Bergman and Mannich reactions.
4. Ring Formation Reactions: Pausan-Khand reaction, Nazerov cyclisation.
5. Click Chemistry: Click reaction, 1,3-dipolar cycloadditions.
6.Metathesis: Grubb's 1^{st} and 2^{nd} generation catalyst, Olefin cross coupling metathesis (OCM), ring closing metathesis(RCM), ring opening metathesis(ROM), applications.
7. Other important synthetic reactions: Baylis-Hilman reaction, Eschenmoser-Tanabe fragmentation, Mitsunobu reaction, Stork-enamine reaction and Michael reactions.

PhC (CB3)-12: New techniques and concepts in organic synthesis 15Hrs
1. Techniques in peptide synthesis: Solid phase peptide synthesis, commonly used resins (Rink resin, Wang resin and Ellman resin, synthesis of cross linked Merrifield resin and drawbacks of solid phase synthesis.
2. Solid phase oligodeoxynucleotide synthesis: Phospho triester, phosphite triester and phosphoramidite pathway

3. Oligosaccharide synthesis: Glycosidation**:** cylic oxocarbenium ion, glycosyl donors and glycosyl acceptors, Kahne glycosidation, convergent and linear oligosaccharide synthesis.
4. Phase Transfer catalysis: Onium and crwon ethers as PTC.
5. Tandem synthesis: Tandem reactions; conjugate addition-aldol reaction, polymerization-cyclisation, elctrocylic-Diels Alder reaction.
6. Baldwin Rules: Exo and Endo cyclisation, tetrahedral, trigonal and diagonal systems, favoured and disfavoured cyclisations.
7. Chiron approach in organic synthesis: Nature's chiral pool, carbohydrates, amino acids, hydroxy acids, terpenes as chiral precursors. Synthesis of shikimic acid from D-arabinose, furanonycin from D-glucose, S-(-)-ipsenol from S-leucine.
8) Determination of absolute configuration: Mosher's method.

Recommended Books:

1. Asymmetric synthesis by Nogradi
2. Asymmetric organic reactions by J D Morrison and H S Moschcr
3. Principles in Asymmetric synthesis by Robert E. Gawley & Jeffrey aube
4. Stereo differentiating reactions by Izumi
5. Some modern methods of organic synthesis by W Carruthers
6. Guidebook to organic synthesis, by R K Meckie, D M Smith & R A Atken
7. Organic synthesis by Michael B Smith
8. Organic Synthesis-The disconnection approach by S Warren
9. Organic Synthesis by C Willis and M Willis
10. Problems on organic synthesis by Stuart Warren
11. Organic chemistry Jonathan Clayden, Nick Greeves and Stuart Warren
12. The logic of chemical synthesis by Elias James Corey and Xue-Min Cheng

Paper IV -CH(PhC) 304T (CB4): Herbal drugs , synthetic pharmaceuticals and IPM

PhC (CB4)-13: Herbal Drugs
PhC (CB4)-14 : Synthetic pharmaceuticals -I
PhC (CB4)-15 : Synthetic pharmaceuticals –II
PhC (CB4)-16: Intellectual Property Management

PhC (CB4)-13:Herbal Drugs 15hrs

i)Classification of herbal drugs- Taxonomical, Morphological, Pharmacological and Chemical classification. ii) Adulteration and evaluation of drugs. iii) Different chemical groups of Herbal drugs-- Alkaloids, Terpenoids, Glycosides, Volatile oils, Isolation of volatile oils, Tannins and carbohydrates. iv) Herbal drugs and their therapeutic efficacy. Laxative- Barbarian, Aloe emodin from Aloes. Ricinolic acid from castor oil. Cardiotonics- Digitoxigenin, Digoxigenin from Digitalis purpurea. Carminatives and Gastro-intestinal regulators--Coriandrol from coriander. Thymol from Azowan. Zinguone from zinger. Vanillin, Eugenol from clove. Piperine from pepper. Astringents - Catechin, epicatechin from Black catechue. Nervous system drugs- Depressants - Reserpine from Rawolfia, Hallucinogens- LSD (ergot), Stimulants- Caffeine (coffee), Cocaine (coca), Analeptics- Strychnine (St.Nuxvomica), Camphor (Cinnamonam camphora), Analgesics- Morphine and Codeine (Phapaver somniferum), Depressants- Tropane alkaloids (belladonna), Cannabinol (cannabis) Anti-hypertensive- Reserpine (rawolfia), Anti-tussive- Eugenol, Cineole (tulasi). Vasicine (vasalca). Anti-rheumatics- Guggulosterol (Guggul), Colchicin (colchicum).Anti-tumor- Colchicin (colchicum), Vinblastin (vincarosea), Taxol (taxus bacetta), Anti-diabetics- Neem oil (Neem). Anti-malarial- Quinine (cinchona).

PhC (CB4)-14: Synthetic pharmaceuticals –I **15hrs**

Synthesis and pharmacological activity of the following drugs. Diclofenac(anti-inflammatory), Tinidazole(anti-amebic), Pheniramine(anti-histamine), Ciprofloxacin(anti-bacterial), Cloxacillin, Cephalexin (anti-biotics), Miconazole (anti-fungal), Cisplatin (anti-neoplastic), Ethambutal (anti-tubercular) and Enalapril (anti-hypertensive).

PhC (CB4)-15: Synthetic pharmaceuticals-II **15hrs**

Benzocaine (localanesthetic), Phenobarbitone, Nitrazepam (Hypnotic) Isoprenalin (sympathomimetic) Celecoxib(antiinflammotory), Procainamide(cardiovascular), Omeprazole (antiulcer), 5-Floro uracil(anticancer), Ciprofloxacin, norfloxacin(antibacterials), Lamivudine(anti AIDs) and Clofazimine(anti leprosy and anti T.B).

PhC (CB4)-16: Intellectual Property Management **15hrs**

Introduction, Intellectual property-meaning of patent, definition, object of patent law, salient features of IPA 1970, Patentable invention, procedure for patentship, application, examination, exclusive marketing rights, opposition, grant and seal, patent addition, amendment in application, restoration of lapsed patent, surrender, revocation, register of patents, powers of controller, non-patentable inventions, transfer of patent, use of inventions by Government, Infringement, Reliefs, Patents (amendment) Act- 1999 and 2002(briefly) and any further amendments on that date. Case Laws-relating to Pharmaceuticals and drugs.

Recommended text books:

1. Natural products. By P.S.Kalsi
2. Medicinal chemistry. By Chatwal.
3. Medicinal chemistry. By Ashtoshkar.
4. Chemistry of Drugs. By V.N.Ivers.
5. May's chemistry of synthetic drugs. Hand Book of Reagents for organic synthesis. By Reich,Rigby
6. The organic chemistry of Drug synthesis.vol 1-6 By Ledneicer etal.
7. Top Drugs: The synthetic routes. J.Saunders
8. Organic natural products By Barton and Ollis
9. Organic natural products by OP Agarwal
10. Natural products. By P.S.Kalsi
11. Organic natural products By Barton and Ollis
12. Organic chemistry. By Finar. Vol.I & II
13. Intellectual property rights by N.K.Acharya
14. Law relating to patents, trademarks, Copyright designs and geographical indications by B.L.Wadehra

B Laboratory work

PAPER V–(PhC-351 P): Qualitative Analysis of Organic Mixtures.
Separation and identification of organic compounds:

Separation of two component mixtures by chemical methods and their identification by chemical reactions — separation by using solvent ether, dil hydrochloric acid, 5 % aqueous sodium bicarbonate and sodium hydroxide solutions, checking the puroty of two components by TLC, identification of the compounds by a systematic study of the physical characteristics (mp/bp), extra elements (nitrogen, halogens and sulfur), solubility, functional groups, preparation of crystalline derivatives and identification by referring to literature. A minimum of 10 mixtures should be separated and analyzed by these procedures.

Paper VI (PhC-352 P): Spectroscopic identification of organic compounds and Chromatography
Identification of unknown organic compounds by interpretation of IR, UV, ^{1}H NMR, ^{13}C NMR and mass spectra. A minimum of 30 representatives

Thin layer chromatography: Determination of purity of a given sample, monitoring the progress of chemical reactions and column .chromatographic separations, identification of unknown organic compounds by comparing the Rf values of known standards, and preparative TLC for separation of mixtures.

Paper chromatography- Separation and identification of amino acids by ascending and radial paper chromatography.

Separation / Purification by column chromatography: Separation of a mixture of ortho and para-nitroanilines using silicagel as adsorbant and chloroform as the eluent. The column chromatography should be monitored by TLC.

M.Sc. CHEMISTRY (PHARMACEUTICAL CHEMISTRY)
IV SEMESTER SYLLABUS
(For the batch admitted during the academic year 2016 -2017 under the CBCS pattern)

Paper-1 CH (PhC) 401T: Drug Design and Drug Discovery
PhC-17: Principles of Drug design and drug discovery
PhC-18: Lead modification and SAR Studies
PhC 19: QSAR studies and computer aided drug design
PhC 20: Combinatorial Synthesis

PhC- 17: Principles of Drug design and drug discovery 15 Hrs
Introduction to drug discovery. Folklore drugs, stages involved in drug discovery- disease, drug targets, bioassay. Discovery of a lead- screening of natural products and synthetic compound libraries. Existing drugs as leads (me too drugs). Pharmacokinetics (ADME), pharmacodynamics. Nature of drug – receptor interactions and their theories – Occupancy theory, Induced – fit theory, Macromolecular purturbation theory and Two-state model of receptor activation. Natural products as lead structures in drug discovery – Pharmacophore - structure pruning technique e.g. morphine. Discovery of lead structure from natural hormones and neurotransmitters. Principles of design of agonists (e.g.Salbutamol), antagonists e.g. cimitidine) and enzyme inhibitors (e.g. captopril). Drug discovery without lead – serendipity- Penicillin and Librium as examples. Principles of prodrug design. Introduction to drug patents and Clinical trials.

PhC-18: Lead modification and SAR Studies 15 Hrs
SAR*:* Lead modification strategies, Bioisosterism, variation of alkyl substituents,chain homologation and branching, variation of aromatic substituents,extension of structure, ring expansion and ring contraction, ring variation, variation and position of hetero atoms, ring fusion, simplification of the lead, rigidification of lead.Discovery of oxaminquine, salbutamol, cimitidine and captopril Structure-Activity Relationship studies in sulfa drugs, benzodiazepines, and taxol analogs.

PhC-19: QSAR studies and computer aided drug design 15Hrs
QSAR: Introduction, physicochemical properties - pKa, electronic effects and Hammett constants(σ), lipophilicity constant(π), steric effects and Taft's constant, linear and nonlinear relationship between biological activity Lipophilicity Substituent constants. Lipinski rule of five. Hansch analysis, Craig's plot,Topliss scheme, Free Wilson approach, cluster significant analysis. Two case studies (QSAR study on pyranenamine and design of Crizotinib).
Computer aided drug design: Introduction, active site, allosteric binding site, use of grids in docking , rigid docking, flexible docking and induced fit docking of ligands. Basic principles and difference between structure and ligand based drug design, denovo drug design and utility to optimize the lead structure.

PhC-20: Combinatorial Synthesis 15Hrs

Introduction. Combinatorial approach. Combinatorial libraries, technologies. Solid phase synthesis, types of resins. Linkers. Reactants for solid phased synthesis. Methods of Parallel synthesis: Haughton's tea bag procedure. Automated parallel synthesis. Methods in Mixed combinatorial synthesis: general principles. Furkas mix and split combinatorial synthesis, Structure determination of active compounds-Deconvolution, Methods in deconvolution-recursive deconvolution, tagging and use of decoded sheets. Examples of Combinatorial Chemistry. Planning and designing of combinatorial synthesis, Spider like scaffolds, drug molecules. Automation in Combinatorial chemistry. High throughput screening.

Recommended books

1. Burger's medicinal chemistry and drug discovery by Manfred E. Wolf.
2. Introduction to Medicinal chemistry by Patrick.
3. Introduction to drug design by R Silverman
4. Comprehensive medicinal chemistry. Vol 1-5 by Hanzsch.
5. Principles of medicinal chemistry. by William Foye
6. Biochemical approach to medicinal chemistry. by Thomas Nogrady.
7. Pharmaceutical Chemistry and Drug synthesis by Roth and Kleeman
8. Drug design by E.J.Arienes
9. Principles of Medicinal Chemistty Vol I & II by Kadam et al
10. Medicinal chemistry An introduction by Garreth Thomas
11.Organic and Pharmaceutical chemistry By Delgrado
12. Organic Pharmaceutical chemistry By Harikishan singh
13. Medicinal Chemistry By Ashtoshkar
14. Medicinal Chemistry By Chatwal
15. Organic Drug synthesis By Ledneicer Vol 1-6
1 6.Strategies for organic drug synthesis and design By Daniel Ledneicer.
1 7.Top Drugs: Top synthetic routes By John Saunders
I 8.Chirotechnoiogy By Roger A. Sheldon
19. Burger's Medicinal Chemistry and Drug Discovery: Principles and Practices. Vol. 1.
20. Medicinal Chemistry by G. Patricks.
21. Text book of Drug Design and Discovery, Edited by Povl Krogsgaard – Larsen Tommy Liljefors.
22. Structure Based Drug Design of Crizotinib (PF-02341066), a Potent and Selective Dual Inhibitor of Mesenchymal–Epithelial Transition Factor (c-MET) Kinase and Anaplastic Lymphoma Kinase (ALK) Martin P. Edwards, J. Med. Chem., 2011, 54 (18), pp 6342–6363.
http://www.pfizer.com/news/featured_stories/featured_stories_martin_edwards.jsp

Paper-II CH (PhC) 402T: Drug synthesis and mechanism of action

PhC-21: Drugs acting on metabolic process, cell wall and specific enzymes
PhC-22: Drugs acting on genetic material and immune system
PhC-23: Drugs acting on receptors and ion channels
PhC-24: Chiral drugs

PhC-21: Drugs acting on metabolic process, cell wall and specific enzymes 15hrs

Basic concepts of mechanism of drug action: Introduction to macromolecular targets, carbohydrates, proteins, lipids and nucleic acids as possible drug targets. Classification of drugs. Enzyme inhibition and its types.

a**)** Drugs acting on metabolic process:

Antifolates –Discovery and mechanism of action of sulphonamides, Synthesis of sulfomethoxazole, sulfodoxine, sulfaguanidine and dapsone.

Diaminopyrimidines -trimethoprim, bacterial resistance to sulfonamides and drug synergism

b**)**Drugs acting on cell wall: Structure of bacterial cell wall, β-Lactam antibiotics – mechanism of action of penicillins and cephalosporins. Synthesis of pencillin-G and cephalosporin-C, cefalexin and cycloserine. Resistance to pencillins, broad spectrum penicillins – cloxacillin, methicillin, ampicillin, amoxicillin and carbenicillin. β-Lactamase inhibitors - Structural formulae and mode of action of clavulanic acid and sulbactum

c)Drugs acting on specific enzymes: H^+/K^+ -ATPase inhibitors- synthesis of Omeprazole and Carbonic anhydrase inhibitors-synthesis of Acetazolamide.

PhC-22: Drugs acting on genetic material and immune system 15hrs

Drugs acting on genetic material: Introduction, classification and mechanism of action.

a) DNA-intercalating agents-Anticancer and antimalarial agents. Structural formulae of Daunomycin, Adriamycin and Amsacrine. Synthesis of Amscarine, Nitracrine, Quinacrine and Chloroquine.

b) DNA- Binding and nicking agents: Antiprotozoal drugs. Synthesis of Metronidazole, Dimetridazole and Tinidazole.

c) DNA-Alkylators: Synthesis of Cyclophosphamide and Bisulphan.

d) DNA-Polymerase inhibitors: Antiviral agents- Synthesis of Acyclovir and AZT.

e) DNA-Topoisomerase inhibitors: Anti bacterial agents. Synthesis of Ciprofloxacin and Norfloxacin. Structural formulae ofloxacin and Lomefloxacin.

f) Inhibitors of transcribing enzymes: Anti-TB and antileprosy agents-structural formulae of Rifamycins and partial synthesis of Rifampicin.

g) Drugs interfering with translation process: Antibacterial drugs- Structural formulae of Erythromycin, 5-Oxytetracycline and Streptomycin. Synthesis of Chloromycetin

Drugs acting on immune system: Introduction to immune system. Immunosupressing agent-structural formula of Cyclosporin. Immunoenhancers-use of vaccines and strucrural formula of levamisol.

PhC-23: Drugs acting on receptors and ion channels 15hrs

Introduction to nervous system: structure of neuron, nerve transmission. Definition and examples of agonist, antagonist, neurotransmitters and receptors.

Drugs acting on receptors:

a)Adrenergic receptors - Introduction and classification. α-Adrenergic-receptor agonists and antagonists- Synthesis and biological activity of Nor-adrenaline, Methyl L dopa and Tetrazosin. β-Adrenergic-receptor - agonists and antagonists – Synthesis and pharmacological activity of Salbutamol, Tetrabutalin, Propranolol and Atenolol.

b)Cholinergic-receptors: Introduction and classification. Cholinergic-receptor agonists and antagonists- Structural formulae of Nicotine, Atropine and Tubocurarine. Synthesis of Acetyl choline and Succinyl choline

c)Dopamine receptors: Introduction and classification. Dopamine- receptor agonists and antagonists- Biosynthesis of Dopamine. Synthesis of L-Dopa and Chlorpromazine.
d)Serotonin receptors: Introduction and classification. Serotonin receptor agonists and antagonists-synthesis and pharmacological activity of Serotonin and Metoclopramide.
e)Histamine receptors: Introduction and classification. Histamine receptor agonists and antagonists-synthesis and biological action of Histamine, Chloropheneramine, and Ranitidine.
f) Hormones and their receptors: Introduction to estrogen receptors, Structural formulae of Tamoxifen

Drugs acting on ion channels: Introduction to ion channels, drugs acting on Ca^{2+}, Na^{+} and Cl^{-} channels and their mode of action. Structural formulae of Tetracaine and synthesis and of Nifedipine, Diltiazem, Tetracine and 4-Aminopyridine.

PhC-24: Chiral drugs 15hrs

Introduction to chiral drugs. Three-point contact model, Eutomer, Distomer and eudesmic ratio. Pfeiffer's rule. Role of chirality on biological activity: Distomers – a) with no side effects b)with undesirable side effects c) both isomers having independent therapeutic value d)combination products having therapeutic advantages e) metabolic chirality inversion.
Synthesis and pharmacological activity of S-Ibuprofen, S- Metaprolol, Ininavir sulfate, Levocetrazine, 2S-Verapamil, S,S-Ethambutol , (+)Lomefloxacin, Fluvastatin, Dextropropoxyphen, (+)Ephedrine, (+)Griseofulvin, Dexormaplatin, R-Indacrinone, Nateglinide, Oxybutynin hydrochloride, S,S- Captopril and S,S,S- Enalaprilate.

Recommended Books:

1. Burger's medicinal chemistry and drug discovery. By Manfred B. Wolf.
2. Introduction to Medicinal chemistry. By Graham Patrick.
3. Introduction to drug design. By R.B.Silverman
4. Comprehensive medicinal chemistry. Vol 1-5 by Hanzsch.
5. Principles of medicinal chemistry. By William O. Foye etal.
6. Biochemical approach to medicinal chemistry. By Thomas Nogrady.
7. Pharmaceutical Chemistry and Drug synthesis By Roth and Kleeman
8. Drug design By E.J. Arienes
9. Principles of Medicinal Chemistry. Vols.1 & 2 By Kadam etal
10. Medicinal chemistry An introduction By Gareth Thomas
11. Wilson and Gisvold,s text book of Organic, Medicinal and Pharmaceutical chemistry By J.N.Delgado and W.A.Remers.
12. Organic Pharmaceutical chemistry By Harikishan singh.
13. Medicinal Chemistry By Ashutoshkar
14. Medicinal Chemistry By G.Chatwal
15. Organic Drug synthesis By Ledneiser Vol 1-6
16. Strategies for organic drug synthesis and design By Daniel Ledneiser
17. Top Drugs: Top synthetic routes By John Saunders
18. Chirotecchnology By Roger A. Sheldon

SEMESTER-IV

Paper III -CH(PhC) 403T(CB1): Medicinal natural products and drug analysis
PhC(CB1) 17 : Medicinal natural products
PhC(CB1) 18 :Spectroscopic analysis of drugs
PhC(CB1) 19 :Titrimetric analysis of drugs
PhC(CB1) 20 :XRD and chromatographic analysis of drugs

PhC(CB1) 17 : Medicinal natural products 15hrs

Alkaloids:- Source, Isolation, structure determination, Synthesis of Atropine, and Reserpine stereochemical structures and pharmacological activity of (i) Morphine, (ii)Codine, (iii)Colichicine.

Glycosides: Source, Isolation, structure determination, Synthesis of Streptomycin. stereochemical structures and pharmacological activity of Digitoxin and Digoxin.

Prostaglandins:- Introduction,Classification, Source, Isolation, structure determination,and synthesis of PGE_2 . stereochemical structures and pharmacological activity of Prostacyclin and Thromboxane.

Steroids and Harmones: Source, Isolation, structure determination, Synthesis of Cholestrol , stereochemical structure and pharmacological activity of (i)Ergosterol (ii) testosterone (iii) Estrone (iv) Androsterone (v) Progesterone.

PhC(CB1) 18:Spectroscopic analysis of drugs 15hrs

Ultraviolet spectrospcopy : Quantitation methods- use of standard absorbivity value, calibration graph method, method of least squares, single point and double point standardization. Assay of substances in multi-component samples – assay as a single component sample, assay after solvent extraction, assay after correction for interference, simultaneous equation method. Specific applications – assay of frusemide in tablet form, assay of pethidine hydrochloride in injection; Difference spectrophotometry- analysis of aspirin in dextroproxyphene compound tablets.

Infrared spectroscopy: Measurement of infrared absorption bands: Quantitation methods-Direct application Beer-Lambert relationship, use of a calibration graph, standard addition method. Specific applications-determination of phenobarbitone in phenobarbitone tablets, determination of acetyl salicylic acid and phenacetin in tablets.

^{1}H-NMR spectrometry:- Quantitative analysis of (i) Aspirin – paracetamol - caffeine tablets.

Atomic absorption spectroscopy: Principle, instrumentation- Hollow Cathode Lamp, Applications: Assay of total zinc in insulin zinc suspension, determination of thiomersal as mercury in a solution for contact lenses.

Atomic emission spectroscopy (Flame photometry): Principle, instrumentation. Applications-Determination of calcium in magnesium chloride for dialysis, determination of the concentration of potassium in haemodialysis solution.

Spectrofluorimetry: Theory, instrumentation, applications- determination of proflavin hemisulphate in proflavin cream, determination of ethinyloestradiol in tablets.

PhC(CB1) 19 :Titrimetric analysis of drugs 15hrs

Introduction to titrimetry, primary standards. Acid -base titrations: Titration curves, systemic equilibrium,calculations.Non-aqueous titrartions- theory, saponification value of fixed oils, determination of ester value. eg. Assay of aspirin, ibuprofen, phenobarbitone, methyl dopa. Precipitation titrations: Solubility product, titration curves, determination of end points. Formation of a colored precipitate, formation of a soluble colored compound, use of adsorption indicators. eg. Determination of chloral hydrate in dichlorophenazine. Redox titrations: Electrode potentials, Nernst equation, calculations, formal potentials, titration curves. Feasibility of redox titrations, types and selection of redox indicators, structural chemistry of redox indicators. eg. Assay of ascorbic acid, analgin, isoniazid . Complexometric titrations: Stability of complexes, titration curves, metal ion indicators. Types of EDTA titrations. eg: Determination of calcium gluconate in calcium gluconate injection, Zinc in Bacitracin zinc.

PhC(CB1) 20: XRD and Chromatographic analysis of drugs 15hrs

X-ray Diffraction studies: Polymorphism, Miller indices, Bragg's equation. Experimental methods- the rotating crystal method, oscillating crystal method, powder method, indexing the reflections, systemic absences and applications.

Size-exclusion Chromatography: Principle, Instrumentation, stationary phases, retention behavior, applications: determination of relative component composition. Determination of molecular weight, eg. Corticotrophin and insulin.

Capillary electrophoresis: Types of Eletrophoresis, Electro osmotic flow, instrumentation, control of separation, applications: Separation of Atenolol and related impurities, analysis of non steroidal anti inflammatory drugs.

Super Critical fluid Chromatography: Principle, super critical fluids, instrumentation, stationary phases, mobile phases, and detectors.

Recommended books:

1. Natural products. By P.S.Kalsi
2. Organic natural products By Barton and Ollis
3. Organic natural products by OP Agarwal
4. Natural products. By P.S.Kalsi
5. Medicinal natural products by Dewick
6. Chemistry of steroids. By Fieser & Fieser.
7. Steroid chemistry. By Kalsi
8. Organic chemistry. By Finar. Vol.I & II
9. Prostaglandins. By Ramsay
10. Analytical chemistry by Christian
11. Fundamentals of analytical chemistry by Skoog, West, Holler
12. Vogel's text book of quantitative chemical analysis
13. Quantitative analysis by Day & Underwood
14. Pharmaceutical analysis By Ashtoshkar
15. Analytical chemistry by open learning by Clive Whatson
16. Physical chemistry by Atkins
17. Physical chemistry by Glasstone
18. Solid state chemistry by West
19. Instrumental methods of analysis by Willard

References

20. Practical pharmaceutical chemistry. By A.H.Backette, J.B.Stenlake.
21. Fundamentals of analytical chemistry. By Skoog and West.
22. Pharmaceutical analysis By. David G.Watson
23. Instrumental methods of chemical analysis By Sharma
24. Analytical chemistry By Harris

Paper III CH(PhC) 403T(CB2) INDUSTRIAL PHARMACEUTICAL CHEMISTRY

PhC(CB2)-21: Unit Process
PhC(CB2)-22 : Industrial Synthesis
PhC(CB2)-23::Quality Control and Quality Assurance
PhC(CB2)-24::Effluents of Industrial Units and their purification

PhC 21::Unit Processes 15hrs

Concept of unit processes in systematization of chemical reactions, explanation of one example each for unit processes:Thermodynamic and kinetic aspects of Alkylation, amination, (by ammonolysis, reduction), esterification, halogenation, hydroformylation, hydrogenation, nitration, oxidation and reduction.Mechanistic aspects of carbonylation, carboxylation, condensation, dehydration, diazotization, disproportionation, , hydration, hydrolysis, hydroxylation, sulphonation and acetylation.

PhC 22: Industrial Synthesis 15hrs

Introduction to pharmaceutical manufacturing - raw materials, detailed manufacturing procedure, therapeutic function, common name, chemical name, structural formulae of the following drugs. Acyclovir, alprazolam, Ibuprofen, cimetidine, sulphamethoxazole, ciprofloxacin, chloramphenicol maleate, licocaine, ethambutal hydrochloride, 5-fluorouracil, furazolidine.

PhC 23:: Quality Control and Quality Assurance 15hrs

Introduction, concepts and significance, Quality control charts, the X-quality control chart, the R-quality control chart and its interpretation, spiked sample control charts, blind samples in control .

Establishing Quality assurance programme-management commitment, writing standard operating procedures, topics for standard operating procedures, consolidating the programme, monitoring quality assurance data, reporting quality assurance problems, writing the quality assurance manuals. Good laboratory practices: Organization and personnel, quality programme, instrument and calibration, customer satisfaction. Laboratory Accreditation: need for laboratory accreditation, international aspects of laboratory accreditation and in India. Criteria for laboratory accreditation. Benefits of laboratory accreditation. Significance of ISO 9000-2000, 9001-2000, 9003-2000, 9004-2000 series of standards.

PhC 24: Effluents Of Industrial Units And Their Purification 15hrs

Introduction to industrial effluents. Classification of effluents. Classification of basic methods of purifying effluents.i) Purification of suspended and emulsified impurities by mechanical method. ii) Purification of dissolved impurities- a) from mineral matter by ion exchange, reverse osmosis, electrical and reagent methods. b) From organic matter by destructive methods, biological oxidation, ozonization, chlorination, extraction, adsorption and ion exchange) Purification of gases by desorption method. iii) Purification by elimination and destruction- by thermal destruction, burying and pumping into depth of oceans.

Recommended text books:

1. Industrial chemistry By B.K.Sharma
2. Bulk drug manufacture. Profile
3. Environmental chemistry By B.K.Sharma
4. Unit processes in chemical engineering By Groggins
5. Unit processes in chemical engineering By Drydens
6. Pharmaceutical manufacturing encyclopedia vol I&II

Paper IV CH(PhC) 404(CB3) T BIOPHARMACEUTICAL CHEMISTRY (ID Paper)

PhC(CB3) 25 :Enzymes – Enzyme Immobilisation
PhC(CB3) 26: Microbial Transformations
PhC(CB3) 27: Pharmaceuticals From Fermentation Technology
PhC(CB3) 28: Pharmaceuticals From Recombinant DNA Technology

PhC(CB3) 25 : Enzymes – Enzyme Immobilisation 15hrs

Introduction; Classification and nomenclature of enzymes; mechanism of enzyme action- lock and key model; induced fit model; enzyme kinetics-initial velocity, effect of enzyme concentration substrate concentration (Michaels- Menton equation Lineweaver-Berk representation), effect of pH, temp.; Enzyme inhibition- irreversible, reversible(competitive, non-competitive and uncompetitive). Immobilization of enzymes- adsorption method, chemical binding method, cross binding method, entrapping method, effect of immobilization on kinetics and properties of enzyme applications and production of penicillin's , steroids, L-DOPA

PhC(CB3) 26:Microbial Transformations 15hrs

Introduction; methods used in biotransformation process- fermentation, analysis and isolation of product and selection of organisms. biotransformations with special reference to steroids and sterols- hydroxylation, dehydrogenation, hydrogenation, epoxidation, ring A aromatization, synthetic routes. Biotransformations with reference to prostaglandins -synthhesis of PGE1 and sulprostone

PhC(CB3) 27 :Pharmaceuticals From Fermentation Technology 15hrs

Introduction; development of industrial microroganisms-mutatoins, selectiion of mutants, selection of secondary metabolite producing mutants, catalyst screening, industrial fermentation (brief discussion only), maintainance of aseptic conditions, oxygen transfer; applications; b-lactam antibiotics- penicillins, streptpmycin, tetracyclins, chloramphenicol, vitamins- vit.B2, vit C, ergot alkaloids.

PhC(CB3) 28: Pharmaceuticals From Recombinant DNA Technology 15hrs

Introduction; oligonucleotide synthesis , restriction enzymes, recombinant DNA technolgy using plasmids, phase and cosmids;Polimerase chain reaction- principle, components technique method, Sanger's methodautomated DNA sequencingApplications - Insulin, human growth hormone, vaccines, interferons, novel enzymes.

Recommended books:

1. Biochemistry. By Lehninger.
2. Biochemistry. By Rastogi.
3. Biochemistry. By Chatwal.
4. Biochemistry. By Well.
5. Pharmaceutical Biotechnology. By Kor and Hal Kari
6. An introduction to biotransformation in organic chemistry By JamesR.Hanson
7. Biotransformation by Faber
8. Goodmann & Gilmann's " The pharmacological basis of therapeutics.

Paper IV CH(PhC) 404(CB4)T: BIOMOLECULES AND MOLECULARMODELLING (ID Paper)

PhC (CB4)-29: Nucleic acids
PhC (CB4)-30: Proteins:
PhC (CB4)-31: Molecular Modelling
PhC (CB4)-32: Modelling Biomolecules

PhC (CB4)-29: Nucleic acids 15hrs

Structure of the bases- Adenine, Thiamine, Guanine ,Uracil and cytosine. Structure and synthesis of nucleosides and nucleotides. Structure of DNA and RNA. Conformational structures of nucleic acids. Synthesis of oligonucleotides, sequencing of DNA. Replication, transcription and translation. Genetic code as a means to protein synthesis. Biosynthesis of proteins and importance of heredity

PhC (CB4)-30: Proteins 15hrs

Introduction to proteins, color reactions, molecular weight determination. Classification into simple, conjugated and derived proteins. Peptide linkage, primary structureof proteins, C-terminal aminoacid determination, N-terminal amino acid determination. Partial hydrolysis. Determination of primary structure. Synthesis of peptides by various mehods. Spatial arrangement of protein molecule. Classification of proteins. Secondary and tertiary and quarternary structure of proteins.

PhC (CB4)-31: Molecular Modelling 15hrs

Introduction to molecular modeling; Coordinate systems – Cartisian coordinates, internal coordinates, Z-matrix. Potential energy surfaces (definition only). Empirical force field models-molecular mechanics, energy calculations. (bond stretch, bond angles, dihedral angle, Non bonded interactions). Energy minimizations. Molecular dimensions (ex: Noradrenalin), molecular properties (partial charges, electrostatic potentials). Molecular modeling studies on SB 206553 and analogues.

PhC (CB4)-32: Modelling Biomolecules **15hrs**

Introduction to modeling biomolecules, Protein structure prediction – Protein folding, secondary structure prediction, sequence alignment, the inverse folding problem. Modelling by homology – the alignment, construction of the frame work, selecting variable regions, side chain placement. Validation of protein models – Ramachandran plot. Molecular modeling in drug discovery, 3D pharmacophores and detection methods, molecular docking, Denovo ligand design.

Recommended Books

1. Biochemistry. By Lehninger.
2. Biochemistry. By Rastogi.
3. Biochemistry. By Chatwal.
4. Biochemistry. By Well.
5. Burger's medicinal chemistry and drug discovery. By Manfred E. Wolf.
6. Introduction to Medicinal chemistry. By Patrick.
7. Introduction to drug design. By Silverman
8. Comprehensive medicinal chemistry. Vol 1-5 By Hanzsch.
9. Principles of medicinal chemistry. By William Foye
10. Biochemical approach to medicinal chemistry. By Thomas Nogrady.
11. Organic chemistry. By Finar. Vol.I & II

References:

1. Drug design By E.J. Arienes
2. Jenkin's quantitative pharmaceutical chemistry By Knevel and Dryden
3. Recent advances in Bioinformatics By IA.Khan and A Khanum
4. Computational chemistry By GH. Grant and WG. Richards
5. Molecular modeling By Hans Dieter Holtje and Gerd Folkers
6. Molecular modeling By Leach
7. Computational Chemistry by Jenson

Laboratory work

PAPER-V: PhC-451P Synthesis of drug molecules and QSAR studies

(A) **Synthesis of drug molecules**

2-Phenyl indole, (Fischer Indole Synthesis), 7- Hydroxy-3-methylflavole (Baker-Venkatraman Reaction), 2, 5-Dihydroxy acetopheneone(Fries reaction). 4-ChloroToluene(Sandmeyer reaction), 7-Hydroxy Coumarin(Pechman synthesis), vanillyl alcohol form vanillin(NaBH4 Reduction) , Benzylic acid rearrangement, Beckmann rearrangement, Phenytoin, Fluorescein, 6-Methyl Uracil, Benzocaine, 4-Aminobenzene Sulphonamide, Phenacetin, phenothiazine, Tolbutamide

(B) Prepration of Pharmaceutical formulations

(i) Sulpha ointment (ii) salicylin ointment (iii) Benadryl Cough syrup

(C) QASR problems based on logP, π ans σ parameters.

PAPER-VI: PhC-452P Titrimetric & Instrumental Drug analysis

Assay of Aspirin, (Acid-base titrations).
Assay of Chloride in Ringers lactate (Precipitation titrations).
Assay of Codiene phosphate syrup
Assay of Ascorbic acid in raw material by iodometry
Assay of Calcium in Calcium tablets (single tablet method)
Assay Zinc in Bacitracin zinc
Assay of Ethambutol in Ethambutol tablets
Assay of Amlodipine in Amlodipine tablets
Assay of Ampicillin in Ampicillin Capsules.
Tests for hardness of tablets, Friability, Disintegration tests for uncoated, coated and enteric coated tablets, capsules.
Colorimetric estimation of dextrose in dextrose injection.
Conductometric assay of Aspirin
Assay of Riboflavin in tablets by UV-Visible Spectrophotometry
Dissolution profile of paracetamol
Determination of sodium and potassium ions in pharmaceuticals by flamephotometry
Determination of quinine sulphate by florimetry.
Potentiometric estimation of Sulphanilamide

M.Sc. CHEMISTRY

PHYSICAL CHEMISTRY SPECIALISATION
SYLLABUS OF III & IV SEMESTERS
REVISED AS PER NEW (CB) SYLLABUS

FOR STUDENTS ADMITTED FROM THE YEAR 2016 ONWARDS

M.Sc. CHEMISTRY (PHYSICAL CHEMISTRY SPECIALISATION)

Syllabus for III and IV Semesters
(for the batches admitted in academic year 2016 & later under CBCS pattern)
[Under Restructured CBCS Scheme]
Grand total marks and credits (all 4 semesters) 2400 marks – 96 credits

(Approved in the P.G. BOS meeting held on 01-07-2017)

Semester - III (Physical Chemistry)
[Under CBCS Scheme]
(for the batches admitted in academic year 2016 & later under CBCS pattern)

	Hrs/week	Internal assessment	Semester exam	Total	Credits
CH(PC)301T (core)	4	20 marks	80 marks	100 marks	4
CH(PC)302T (core)	4	20 marks	80 marks	100 marks	4
CH(PC)303T (Elective)	4	20 marks	80 marks	100 marks	4
CH(PC)304T (Elective)	4	20 marks	80 marks	100 marks	4
CH(PC)351P (LAB-I)	9			100 marks	4
CH(PC)352P (LAB-II)	9			100 marks	4
Total				**600 marks**	**24**

Semester - IV (Physical Chemistry)

	Hrs/week	Internal assessment	Semester exam	Total	Credits
CH(PC)401T (core)	4	20 marks	80 marks	100 marks	4
CH(PC)402T (core)	4	20 marks	80 marks	100 marks	4
CH(PC)403T (Elective)	4	20 marks	80 marks	100 marks	4
CH(PC)404T (Elective)	4	20 marks	80 marks	100 marks	4
CH(PC)451P (LAB-I)	9			100 marks	4
CH(PC)452P (LAB-II)	9			100 marks	4
Total				**600 marks**	**24**

Grand total marks and credits (all 4 semesters) 2400 marks - 96 credits

M.Sc. SEMESTER - III
PHYSICAL CHEMISTRY SPECIALIZATION
(for the batches admitted in academic year 2016 & later under CBCS pattern)

PAPER –CH(PC) 301T: QUANTUM CHEMISTRY AND GROUP THEORY
PC - 09: Applications of Schrödinger equation
PC - 10: Angular momentum & approximate methods
PC - 11: Bonding in molecules
PC - 12: Group theory

PAPER – II CH (PC) 302T : SPECTROSCOPY AND LASERS
PC- 13 : Physical principles of spectroscopy and Vibrational spectroscopy
PC- 14 : NMR , NQR and Mossbaur Spectroscopy
PC- 15 : X-ray Spectroscopy & Diffraction techniques
PC- 16 : Lasers in Chemistry

ELECTIVE 3A
PAPER III CH (PC) 303T(CB1) : APPLIED CHEMISTRY, MATERIAL SCIENCE AND RADIATION EFFECTS
PC(CB1)-1 : Applied kinetics
PC(CB1)-2 : Applied Electrochemistry
PC(CB1)-3 : Types of materials, conducting organics and NLO materials
PC(CB1)-4 : Radiation effects

ELECTIVE–3B
Paper-III CH (PC) 303T(CB2): Biopolymer Chemistry
PC-(CB2)- 5:Bioenergetics and physical properties of biopolymers
PC-(CB2)- 6:Biological membranes and binding of ligands by biopolymers
PC-(CB2) - 7: DNA, genes and cloning
PC-(CB2) - 8: Bioinformatics

ELECTIVE–4A
PAPER-IV CH(PC) 304T(CB3): Polymer Chemistry
PC-(CB3)-9: Polymerization and Kinetics of polymerization
PC-(CB3)-10: Structure and properties of polymers
PC-(CB3)-11: Processing of Polymers
PC-(CB3)-12: Functional polymers

ELECTIVE –4B
Paper IV CH(PC) 304T(CB4): Environmental Chemistry
PC(CB4)-13: Pollution in Atmosphere
PC(CB4)-14: Pollution in Hydrosphere
PC(CB4)-15: Heavy Metal and Radiochemical Pollution.
PC(CB4)-16: Analysis of Air, Water and Metal Pollutants

LABORATORY COURSES

Paper-V CH (PC) 351 P: **Chemical Kinetics**
Paper-VI CH(PC) 352P: Instrumentation

M.Sc. SEMESTER - IV
PHYSICAL CHEMISTRY SPECIALIZATION
(for the batches admitted in the academic year 2016 and later under CBCS pattern)

PAPER-1 CH(PC) 401T(CB1): Thermodynamics, Chemical Kinetics and Electrochemistry
PC- 17.Statistical Thermodynamics
PC- 18. Non-equilibrium Thermodynamics
PC- 19. Chemical Kinetics-II
PC- 20. Electrochemistry –II

PAPER-II CH(PC) 402T: Supramolecular chemistry, Photo Chemistry and Computational chemistry
PC-21 : Supramolecular Chemistry
PC-22 : Photochemistry-II
PC-23 : Computational Chemistry
PC-24: Theoretical treatment of bio polymers

ELECTIVE–3A
PAPER-III CH(PC) 403 T(CB1) : Catalysis
PC-(CB1)-17: Homogeneous catalysis
PC-(CB1)-18: Surface Chemistry and Micellar catalysis
PC-(CB1)-19: Heterogeneous catalysis
PC-(CB1)-20: Phase transfer , Anchored and Photo catalysis

ELECTIVE–3B
Paper IV CH(PC) 403 T(CB2) : Dynamics of chemical reactions and Sensors
PC-(CB2)-21: MO and VB theory of reactivity
PC-(CB2)-22: Kinetic, isotopic, structural, solvent, steric and conformatlonal effects
PC-(CB2)-23:Nucleophilic, electrophilic and free radical reactivity
PC-(CB2)-24: Sensors

ELECTIVE –4A (ID PAPER)
PAPER-IV CH(PC) – 404T(CB3) : Computational Chemistry and It's Applications
PC(CB3)-25: Computational Chemistry – I
PC(CB3)-26: Computational Chemistry – II
PC(CB3)-27: Drug Design Methods I - Ligand Based
PC(CB3)-28: Drug Design Methods II - Structure Based.

ELECTIVE–4B (ID PAPER)
PAPER-IV CH(PC) 404T(CB4): Engineering Chemistry
PC(CB4) -29: Water And Waste Water Treatment
PC(CB4) -30: Corrosion And Its Control
PC(CB4) -31: Energy Sources:
PC(CB4)- 32 Engineering Materials.

ELECTIVE–4C (ID PAPER)
PAPER-IV CH(PC) 405T(CB5): Sugar Chemistry and Sugar Technology
PC(CB5) -33: Advanced Sugar Chemistry
PC(CB5) -34: Sugar and Sugar byproducts
PC(CB5) -35: Methodology used in Sugar Analysis
PC(CB5)- 36: Sugar Technology and Management

LABORATORY COURSES
Paper-V CH (PC) 451P: Chemical Kinetics
Paper-VI CH (PC) 452P: Instrumentation

M.Sc. SEMESTER - III
PHYSICAL CHEMISTRY Specialization
(for the batches admitted in academic year 2016 and later under CBCS pattern)

PAPER –CH(PC) 301T: QUANTUM CHEMISTRY AND GROUP THEORY

PC -09: Applications of Schrödinger equation
PC -10: Angular momentum and approximate methods
PC -11: Bonding in molecules
PC -12: Group theory

PC–09: Applications of Schrödinger equation (15 hrs)

Systems with discontinuity in the potential field. A simple potential barrier. A potential barrier with a finite thickness. Quantum mechanical tunneling – examples - α-particle emission, inversion of NH_3, hydrogen transfer reactions.

The harmonic oscillator – detailed treatment. Wave functions and energies. Vibration of a diatomic molecule – harmonic oscillator model.

The rigid rotator – detailed treatment. Wave functions and energies. Spherical harmonics. Rigid rotator as model for a rotating diatomic molecule.

The hydrogen atom – detailed treatment. Angular and radial functions. Atomic orbitals. Measurability of the ground-state energy of hydrogen atom. Orthonormal nature of hydrogen-like wave functions. Probability calculations.

Atomic and molecular term symbols.
Atoms in external field, Zeeman and anomalous Zeeman effect.

PC–10: Angular momentum and approximate methods (15 hrs)

Angular momentum operators. Commutation relations of angular momentum operators and their consequence. Eigen functions of L^2 and L_z and the eigen values. Magnitude and orientation of angular momentum vectors.

Electron spin. Spin operators. Pauli principle and the Pauli exclusion principle.

Approximate methods- The variation method. Constuction of variation function by the method of linear combinations. H and He atom. Perturbation theory (first order and nondegenerate). Wave function and energy corrections. Application of perturbation theory to the helium atom.
Time- dependent perturbation theory. Interaction of radiation and matter. Allowed and forbidden transitions.

Multielectron atoms. The Hartree-Fock self-consistent field method. Basis functions. Slater-type orbitals (STOs).

PC–11: Bonding in molecules (15 hrs)

Born-Oppenheimer approximation. MO theory of H_2^+ ion. Calculation of MOs and their energies. Evaluation of the overlap integral. Probability curves and enegy diagram. MO theory of H_2 molecule. Calculation of energy. MO theory of polyatomic molecules (general ideas). MO treatment of H_2O. Symmetry-adapted linear combinations. MOs of H_2O.

Concept of hybridization – sp, sp^2, and sp^3 hybrid orbitals.

Semiempirical MO methods. The Huckel theory of conjugated systems. HMO calculations on ethylene, allyl system, butadiene, cyclopropenyl system and benzene. π–electron charges and bond orders. Simplification of secular determinants of cyclopropenyl system, cyclobutadiene and benzene using molecular symmetry. Introduction to extended Huckle Theory, extension of the Huckle's approach to molecules containing heteroatoms.

Orbital symmetry and reactivity: $H_2 + F_2 \rightarrow 2HF$ reaction. $2NO \rightarrow N_2 + O_2$ reaction.

PC–12: Group theory (15 hrs)

Matrices: Addition and multiplication of matrices. Diagonal matrix. Unit matrix. Transpose of a matrix. Adjoint of a matrix. Inverse of a matrix. The determinant of a square matrix. Expansion of a determinant. Properties of determinants.

Symmetry operations forming a group. Classes of symmetry operations. Matrix representation of symmetry operations and point groups. Generation of representations for point groups. Reducible and irreducible representations.

The Great Orthogonality theorem (proof not required) and its consequences. Relation between reducible and irreducible representations. Character tables. Construction of character tables for C_{2h}, C_{2v} and C_{3v} groups.

Quantum mechanics and group theory. Wave functions as bases for irreducible representations. The direct product – vanishing of integrals. Projection operators. Symmetries of vibrations. IR and Raman activity.

Books suggested:

1. Quantum Chemistry, Ira N. Levine, Prentice Hall
2. Introduction to Quantum Chemistry, A. K. Chandra, Tata McGraw Hill
3. Elementary Quantum Chemistry, F. L. Pilar, McGraw Hill
4. Molecular Quantum Mechanics, P. W. Atkins & R. S. Friedman, Oxford University Press
5. Coulson's Valence, R. McWeeny, ELBS
6. The Chemical Bond, J. N. Murrel, S. F. A. Kettle & J. M. Tedder, John Wiley
7. Valency Theory, J. N. Murrel, S. F. A. Kettle & J. M. Tedder, ELBS
8. Chemical Applications of Group Theory, F. A. Cotton, John Wiley & Sons
9. Symmetry and Group Theory In Chemistry, Mark Ladd, Harwood Publishers, London (2000).
10. Symmetry Through the Eyes of a Chemist, I. Hargittai and M. Hargittai, 2nd Edition, Plenum Press, NY (1995).
11. Molecular Symmetry and Group Theory, Robert L. Carter, John Wiley & Sons (1998).
12. Group Theory for Chemists, G. Davidson, Macmillan Physical Science Series (1991).

PAPER – II CH (PC) 302T : SPECTROSCOPY AND LASERS

PC- 13 : Physical principles of spectroscopy and Vibrational spectroscopy
PC- 14 : NMR , NQR and Mossbaur Spectroscopy
PC- 15 : X-ray Spectroscopy and Diffraction techniques
PC- 16 : lasers in Chemistry

PC-13: Physical principles of spectroscopy and Vibrational spectroscopy: (15 Hrs)

Interaction of electromagnetic radiation with matter. Absorption and emission of radiation. Induced absorption, spontaneous emission and stimulated emission. Oscillator strength, transition moment integral. Selection rules, Spectrum of formaldehyde. Factors affecting width and intensity of spectral lines -Line width and natural line broadening, doppler broadening. Intensity of spectral lines.

Infrared spectroscopy- Anharmonic oscillator. Morse potential energy diagram.
Vibration – rotation spectroscopy, P, Q, R branches. Vibration – rotation spectra of polyatomic molecules – linear, symmetric top and asymmetric top molecules. Principles of FTIR.

Raman spectroscopy- Classical and quantum theories of Raman effect. Pure rotational, vibrational and vibrational – rotational Raman spectra. Selection rules. Depolarization factors of Raman lines and their relevance. Instrumentation. Typical applications of Raman spectroscopy – Strucure determination of XY_4 molecules, Phase transitions.

PC-14: NMR, NQR and Mossbaur Specroscopy. (15hrs)

Prnciple of nmr. Derivation of $h\ v = g\ \beta\ H$. Larmor precessional frequency- spin-spin splitting (AX) - Qantitative treatment (proof for J= distance between two successive nmr spectral lines) – Instrumentation - CW instrument and FT instrument.

Two dimensional nmr spectroscopy:
Principles of 2D nmr-Graphical representation of 2D nmr specra – Homonuclear ^1H J, δ spectroscopy-its application for mixture analysis- (for instance mixture analysis of n-butyl bromide and n-butyl iodide) - The COSY experiment. Two dimensional ^1H, ^1H shift correlations. COSY spectra of an AX system, o-nitroaniline, alanine, glutamic acid and arginine.

The nuclear overhauser effect(NOE). wo dimensional nuclear overhauser spectroscopy(NOESY). Nuclear Quadrupole Resonance: Quadrupole nuclei and quadrupole moments-prolate and oblate nuclear charge distributions-energies of quadrupolar transitions-electric field gradient, coupling constants and splitting.

Mossbauer Spectroscopy - Mossbauer effect – Recoil energy, typical Mossbauer spectrum - isomer shift – quadrupole splitting – magnetic hyperfine interaction – ^{57}Fe – Mossbauer spectra of Fe^{2+} and Fe^{3+} (paramagnetic) and Fe^{3+} (magnetic) compounds.

PC-15: X-ray Spectroscopy and Diffraction techniques: (15 hrs)

X-ray fluorescence (XRF) : Experimental method, Processes in X-ray fluorescence, K-emission spectrum of tin, L-emission spectrum of gold.

X-ray absorption: Absorption techniques, Absorption edge fine structure (AEFS spectra) and extended X-ray absorption fine structure (EXAFS) spectra.

X-ray diffraction: Bragg condition. Miller indices, d-spacing formula, Lattice planes and number of d-spacings, experimental methods of X-ray diffraction. Laue method and Debye-Scherrer method. Primitive and nonprimitive unit cells. Indexing the reflections. Identification of unit cells from systematic absences in diffraction pattern. Structure factor and its relation to intensity and electron density. Description of the procedure for an X-ray structure analysis. Typical examples.

Electron diffraction. Scattering intensity versus scattering angle. Wierl equation. Measurement technique. Elucidation of structure of simple gas phase molecules.

PC-16:Lasers in Chemistry: (15 hrs)

General principles of laser action. Stimulated emission. Rates of absorption and emission. Population inversion. Three-level and four-level laser systems. Pumping. Laser cavity – resonant modes. Characteristics of laser light. Laser pulses and their characteristics. Pulse production, Q-switching. Pulse modification, mode-locking.

Practical lasers. Solid-state lasers, gas lasers, chemical and excimer lasers. Examples.

Applications of lasers in chemistry: Femtochemistry. The pump-probe technique. Time-resolved spectroscopy. Photodissociation of ICN. Formation and dissociation of CO-hemoglobin complex. Conversion of ethylene to cyclobutane. Bond selectivity in chemical reactions – the reaction between hydrogen atoms and vibrationally excited HDO molecules.

Lasers and multiphoton spectroscopy – underlying principles. Two-photon spectra of diphenyloctatetraene. Lasers in fluorescence spectroscopy and Raman spectroscopy.

Books suggested:

1. Modern Spectroscopy, J. M. Hollas, John Wiley & Sons
2. Fundamentals of Molecular Spectroscopy, Banwell & McCash
3. Introduction to Molecular Spectroscopy, G. M. Barrow, McGraw Hill
4. Molecular Spectroscopy, J. D. Graybeal, McGraw Hill
5. Basic principles of Spectroscopy, R. Chang, McGraw Hill
6. Physical Methods for Chemistry, R. S. Drago, Affiliated East West Press
7. Vibrational Spectroscopy: Theory and Applications, D. N. Sathyanarayana, New Age International
8. Introduction to Raman Spectroscopy, J. R. Ferraro & K. Nakamoto, Academic Press
9. NMR Spectroscopy: Basic principles, concepts and applications in chemistry, H. Gunther, John Wiley-VCH publishers
10. NMR, NQR, EPR and Mossbauer Spectroscopy in Inorganic Chemistry, R. V. Parish, Ellis Harwood
11. NMR basic principles - Atta-ur-Rahman, Springer.
12. Two dimensional NMR Spectroscopy-Applications for chemists and biochemists, edited by W. R. Croasmun & R. M. K. Carlson, Wiley-VCH
13. X-ray diffraction procedures for polycrysralline and amorphous materials, H. P. Klug & L. E. Alexander, John Wiley
14. Physical Chemistry, Ira N. Levine, McGraw Hill
15. Atkin's Physical Chemistry, P. Atkins & Julio de Paula, Oxford University Press
16. A Guide to Lasers in Chemistry, G. R. Van Hecke & K. K. Karukstis, Jones and Bartlett Publishers
17. Lasers in Chemical and Biological Sciences, S. Chopra & H. M. Chawla, Wiley Eastern Ltd.
18. Molecular structure and Spectroscopy, G.Aruldas, Eastern Economic Edn.

ELECTIVE 3A

PAPER III CH(PC) 303T(CB1) : APPLIED CHEMISTRY, MATERIAL SCIENCE AND RADIATION EFFECTS

PC(CB1)-1 : Applied kinetics
PC(CB1)-2 : Applied Electrochemistry
PC(CB1)-3 : Types of materials, conducting organics and NLO materials
PC(CB1)-4 : Radiation effects

PC(CB1)-1:Applied kinetics (15 hrs)

Kinetics and chemical reaction engineering. Reactor design: Basic objectives in design of a reactor. Parameters affecting the reactor performance. Balance equations for reactor design. Single ideal reactor models.

Batch reactors (BR): General features. Design equations for a BR. Material and energy balances. Isothermal operation, constant-density system.

Continuous stirred-tank reactors (CSTR): General features. Design equations for a CSTR. Material and energy balances. Constant-density system. Steady-state operation at specified temperature. Damkohler number – numerical problems.

Plug-flow reactors (PFR): General features. Design equations for a PFR. Material and energy balances. Constant-density system.

Comparisons of ideal reactors for a single reaction. Single-vessel comparisons. BR and CSTR. BR and PFR. Numerical examples.

PC(CB1)-2:Applied Electrochemistry (15 hrs)

Batteries: Battery parameters. Energy density power density and Ragone plot. Measures of battery performance. Primary and secondary batteries. Zn/MnO_2, lead-acid and Ni-Cd batteries and Lthium cells; Lithium-thionylchloride cell and lithium-ion battery.
Fuel cells: General Chemistry of Fuel cells. Types of fuel cells: H_2/O_2 and methanol/O_2 fuel cells. Use of porous electrodes in fuel cells. Advantages, limitations and efficiency of fuel cells.

Photovoltaic cells: Semiconductor based photoelctrochemical cells. Electrochemical energy from solar energy.

Anodic oxidation of metals. Characteristics of anodic oxide films. Industrial application of anodic oxide films.

Electroplating: Technical importance. Mechanism of electroplating. Alkaline and acid plating of copper, nickel.

Electro-organic synthesis: Reduction of carboxylic acids, the polymerization of acrylonitrile to adiponitriles in the synthesis of nylon. Reduction of nitro compounds.

PC(CB1)-3:**Types of materials, Conducting Organics and NLO materials** (15 hrs)

Classification of materials – metals, ceramics, polymers, composites, semiconductors and biomaterials.

Glassy state – glass formers and glass modifiers, applications
Ceramics – criteria for determining the crystal structure of ceramic materials – examples.
Composites – particle reinforced and fibre reinforced composites.

Preparative methods of solid materials - Ceramic method (Solid State method), co-precipitation as a precursor to solid state reaction, solutions and gels (Zeolite synthesis), crystallization from melts: Czochralski method, Kyropolous method; vapour phase transport method, modification of existing structure by ion-exchange and interaction reactions.

Techniques of single crystal growth – growth from solutions – growth from melts – growth from vapour. Non-linear optical (NLO) behavior– basic concepts, second and third harmonic generation, examples of organic, inorganic and polymer NLO materials.
Conducting organics – Fullerenes, alkali metal doped fullerides, fullerenes as superconductors

PC(CB1)-4: Radiation effects 15hrs

Radiation hazards and safety: Radiation effects. High-energy radiation and high-energy particles – types and sources. Radiation protecting materials.
Radiation chemistry of liquid water. Chemical yields. Dosimetry. Fricke dosimeter and thiocyanate dosimeter. Effect of radiation on DNA. Direct and indirect effects. Reaction of OH radicals with DNA constituents. General mechanism of strand break formation in DNA by OH radicals.

Radioactive wastemanagement: Introduction, Classification of radioactive waste, Treatment of Radioactive waste: Radioactive waste disposal.

Applications of radioisotopes in nuclear medicine and pharmaceuticals: general applications of radiopharmaceuticals, use of nuclear properties of indicator nuclides. In vivo diagnostic procedures, in vitro diagnostic testing therapeutic use of radiations, Use of radiation for food preservation and sterilization.

Books suggested:

1. Introduction to Chemical reaction Engineering and Kinetics, R. W. Missen, C. A. Mims & B. A. Saville, John Wiley
2. Chemical Reaction Engineering, O. Levenspiel, John Wiley
3. Chemical Engineering Kinetics, J. M. Smith, McGraw Hill
4. Elements of Chemical Reaction Engineering, H. Scott Fogler, Prentice Hall (page-114)
5. Modern Electrochemistry 2B, Bockris & Reddy, Plenum
6. Industrial Electrochemistry, D. Pletcher, Chapman & Hall
7. Introduction to Electrochemistry, S. Glasstone, EAST-WEST Press Pvt. Ltd, New Delhi
8. Electrochemistry – B K Sharma
9. Fundamental principles of Modern Electroplating, Lowenheim, John Wiley
10. The physics and chemistry of solids. Stephen Elliot, John Wiley & Sons
11. Solid state chemistry and applications. A.R.West, John Wiley & Sons

12. New directions in solid state chemistry. CNR Rao and Gopalakrishnan, Cambridge University Press
13. Principles of the Solid State, H. V. Keer, New Age International
14. Material Science and Engineering – An Introduction, William D. Callister, Jr., Wiley & Sons
15. Materials Science & Engineering – A First Course, V. Raghavan, Prentice Hall
16. Radiation Chemistry: Principles and Applications, Farhataziz and M. A. J. Rodgers (Eds.), VCH Publishers, New York (1987).
17. Radiation Chemistry: Present Status and Future Trends, C. D. Jonah and B. S. M. Rao (Eds.) Elsevier, Amsterdam (2001).
18. Essentials of Nuclear Chemistry: H. J. Arnikar. New Age Publication Ltd. (1995).
19. Radiation chemistry and Nuclear Methods of Analysis W. D. Ehmann, D. E. Vance. John Wiley (1991).
20. Nuclear and Radiochemistry G. Friedelarder, J. W. Kennedy, E.. S. Macias, J. M. Miller John Wiley (1981).
21. Source Book of Atomic Energy, S. Glasstone, D. Van Nostrand (1967)
22. Nuclear analytical chemistry- J. Tolgyessy and S. Verga Vol. 2 , University park press (1972)
23. Fundamental of Radiochemistry, D.D.Sood, A.V.R.Reddy, N.Ramamoorthy, IANCAs , Mumbai, 4th Edition

ELECTIVE –3B

Paper III CH(PC) 303T(CB2) : BIOPOLYMER CHEMISTRY

PC(CB2)-5: Bioenergetics & physical properties of biopolymers
PC(CB2)-6: Biological membranes & binding of ligands by biopolymers
PC(CB2)-7: DNA, genes and cloning
PC(CB2)-8: Bioinformatics

PC(CB2)-5: Bioenergetics and physical properties of biopolymers (15 hrs)

Bioenergetics: The standard state in biological processes. ATP – the currency of energy. Gibbs energy change in ATP hydrolysis, comparison with other phosphates. Principles of coupled reactions. Glycolysis and coupled reactions involving ATP. Biological oxidation-reduction reactions – transfer of H^+ ions and electrons. Synthesis of ATP in the mitochondria. The chemiosmotic theory. Gibbs energy change accompanying the proton movement.

Viscometry: Molecular weights. Use of viscometry in the study of ligand binding to DNA. Separation/molecular weight studies of biopolymers.Light scattering method.

Sedimentation: Sedimentation velocity. Sedimentation coefficient. The Sverdberg equation. Sedimentation equilibrium analysis. Ultra centrifugation Molecular weights. Light scattering method.

Electrophoresis : principle involved. Gel electrophoresis. Electrophoretic mobility. Applications.

PC(CB2)-6: Biological membranes and binding of ligands by biopolymers (15 hrs)

Structure and function of cell membrane. Membrane equilibria and thermodynamics of membrane equilibria. Dialysis equilibrium. Osmotic pressure. Membrane potentials. Transport across membranes. Passive transport, facilitated transport and active transport.

Sodium-potassium pump. Selective ion transport and membrane potential. The Goldman equation (derivation not required). Nerve cells. The transfer of information in the body. The action potential and the mechanism of action potential propagation. Signal transducing mechanism involving gated ion channels in the plasma membrane.
Binding of ligands and metal ions to macromolecules – one and n-euqivalent binding sites per molecule. Allosteric interactions – Oxygen binding to myoglobin and hemoglobin – Cooperative and non-cooperative binding. Hill equation and Hill plots. Transport of H^+ and CO_2 . Bohr effect.

PC(CB2)-7: DNA, genes and cloning (15 hrs)

Watson –Crick model of DNA. Types of DNA chains – linear, circular and supercoiled DNA. Types of RNA. Secondary structure of t-RNA

Genes and genome. Gene expression. Transcription and translation (general principles only). Codons and the genetic code. Sequence analysis of DNA by the Sanger chain-termination method.
Introduction to biotechnology and recombinant DNA technology. Molecular cloning. Restriction endonucleases and cloning vectors. Steps involved in the construction of recombinant DNA. DNA hybridization and hybridization probes.

Satellite DNAs – micro and mini satellites. Sequence polymorphisms – RFLPs. Principles of DNA finger printing technology.

PC(CB2)-8: Bioinformatics (15 hrs)

Introduction: Use of informatics and computers in biology. Homology as descendants of common ancestors, statistical analysis of sequence alignment.

General purpose Databases for Comparative Genomics: COGs, KEGG, MDGB -
Organism Specific Databases examples - E. Coli, Yeast, Oryza.

Introduction to Proteins - primary, secondary, tertiary and quaternary structures.

Structure databases – PDB, MMDB, CSD. Homology modeling – Flow chart, structure refinement - Ramachandra Plot.

Books suggested:

1. Biophysical Chemistry, Cantor & Schimmel, W. H. Freeman and Company
2. Principles of Physical Biochemistry, Kensal E van Holde, W. Curtis Johnson & P. Shing Ho, Prentice Hall
3. Physical Biochemistry : Principles and Applications, David Sheehan, John Wiley
4. Physical Chemistry for the Chemical and Biological Sciences, Raymond Chang, University Science Books
5. Lehninger Principles of Biochemistry, D. L. Nelson & M. M. Cox, MacMillan
6. Biochemistry, L. Stryer, W. H. Freeman and Company
7. Concepts in Biochemistry, Rodney Boyer, Books/Cole Publishing Company
8. Modern Electrochemistry 2B, Bockris & Reddy, Kluwer Academic/ Plenum
9. Introduction to Bioinformatics by Arthur Lesk, Oxford University Press, Inc, New York
10. Bioinformatics, A practical guide to the Genes and Proteins. Edited by Andreas. D. Baxevanis and B. F. Francis Wiley Publishers

ELECTIVE 4A

Paper IV CH(PC) 304T(CB3) :POLYMER CHEMISTRY

PC(CB3)-9: Polymerization and Kinetics of polymerization
PC(CB3)-10: Structure and properties of polymers
PC(CB3)-11: Processing of Polymers
PC(CB3)-12: Functional polymers

PC(CB3)-9: Polymerization and Kinetics of polymerization (15 hrs)

Classification of polymers. Types of polymerization.

Kinetics and mechanism of free radical polymerization. Degree of polymerization, kinetic chain length and chain transfer coefficient – Trommsdorff effect. Effect of pressure and temperature on chain polymerization.

Kinetics and mechanism of cationic, anionic polymerization, coordination polymerization, linear stepwise polymerization.

copolymerization reactions and copolymer composition. Reactivity ratios and their determination. Alfrey and Price Q-e scheme for monomer and radical reactivity. Block and graft copolymers.

Polymerization in homogeneous and heterogeneous systems. Techniques of polymerization-Bulk, solution, suspension and emulsion polymerizations.

PC(CB3)-10: Structure and properties of polymers (15 hrs)

Polymer solutions:

The process of polymer dissolution. Thermodynamics of polymer dissolution. Entropy, heat and free energy of mixing of polymer solutions. Conformations of dissolved polymer chains. The freely jointed chain. Short-range and long-range interactions. The Flory-Huggins theory of polymer solutions. Dilute polymer solutions. Flory-Krigbaum theory.

Mechanical properties of polymers:

The elastic state. Rubber-like elasticity and viscoelasticity. Newtonian and non-Newtonian behaviour. Maxwell and Voigt-Kelvin models of viscoelastic behaviour.

The crystal structure of polymers. Morphology of crystalline polymers. Crystallization and melting. Determination of Tm. Thermodynamics of crystalline melting. Heats and entropies of fusion. Degree of crystallinity. Factors affecting the crystallization.

The glassy state – glass transition temperature Tg of polymers. Factors influencing Tg. Glass transition temperature and melting point.

Molecular weight distribution – measurement of molecular weights by end group analysis, osmometry and GPC.

PC(CB3)-11: Processing of Polymers (15hrs)

General applications of Polymers. Polymer Additives - Fillers, plasticizers, lubricants, catalysts, stabilizers, colorants, antioxidants, flame retardents.

Processing techniques of polymers - one dimensional coating -Adhesives, Lamination; extrusion- calendering and thermoforming ; Molding of Polymers- Process, advantages and limitations of Compression molding, Injection Molding, Extrusion Molding, Blow Molding.

Casting - Types, Vacuum Casting, Potting, Encapsulation, Film Casting,.

Fibre Reinforced Plastics- preparation and properties. Synthetic Fibres- Rayons, (Nitro cellular, Cupammonium, Diacetate, Viscose), Nylons, Dacron.

Processing of fiber reinforced Composites- Pultrusion technique, prepreg production processes, filament winding.

PC(CB3)-12: Functional polymers (15hrs)

Smart materials – Their uses in sensing devices and in communication networks.

Electrically conducting polymers- Introduction, basic principles and their applications. Brief description of polyanilines, polypyrrole, polyacetylene and polythiophene.

Photoconductive polymers, Liquid crystal polymers – smectic, nematic and cholesteric structures, Ionic exchange polymers- Cationic and anionic exchange polymers and their uses.

Biodegradable polymers- Definition, classification, applications. Brief description of polyhydroxyalkanoates, polycaprolactone, polyacetic acid and polyvinylalcohol.

Polymers in Membrane separation. Filtration – micro, ultra and nanofiltration. Separation of gases – permeselectivity and gas permeability of representative polymers. Liquid separation – dialysis, electro osmosis and reverse osmosis.

Fire retarding polymers, photonic polymers.
Polymers in biomedical applications – artificial organs and controlled drug delivery.

Books suggested:

1. Textbook of Polymer Science, F. W. Billmeyer Jr, John Wiley & sons
2. Polymer Science, V. R. Gowarikar, N. V. Viswanathan & J. Sreedhar, Wiley Eastern
3. Contemporary Polymer Chemistry, H. R. Alcock & F. W. Lambe, Prentice Hall
4. Physics and Chemistry of Polymers, J. M. G. Cowie, Blackie
   Academic and professional
5. Materials scince and engineering an introduction by William D Callister, Jr. Wiley Publishers
6. Polymer Chemistry, B. Vollmert, Springer publishers
7. Physical Chemistry of Polymers, A. Tagers, Mir Publishers
8. A text book of polymers, Vol. I,II,III, M.S. Bhatnagar, S. Chand publishers

ELECTIVE 4B

Paper IV CH(PC) 304T(CB4) : ENVIRONMENTAL CHEMISTRY

PC(CB4)-13: Pollution in Atmosphere
PC(CB4)-14: Pollution in Hydrosphere
PC(CB4)-15: Heavy Metal and Radiochemical Pollution.
PC(CB4)-16: Analysis of Air, Water and Metal Pollutants

PC(CB4)-13: Pollution in Atmosphere

Typical Composition of Unpolluted Dry Air - Major Air Pollutants: Carbon Monoxide, Nitrogen Oxides, Sulphur Oxides, Particulate Matter, Hydrocarbons, Chloroflurocarbons.

Carbon Monoxide: Sources and Sinks, Concentration Profile, Effects on Human Health, Control of CO Emissions.

Nitrogen Oxides (NO_x): Reactions Leading to Formation of NO_x, Sources and Sinks, Concentration Profile, Harmful Effects of NO_x on Human Beings, Plants, Materials and Control of NO_x Emissions.

Sulphur Oxides (SO_x): Reactions Leading to Formation of SO_x, Sources of SO_x. Harmful Effects on Human Beings, Plants and Materials - Control of SO_x Emissions - Acid Rain: Formation and Toxic Environmental Effects.

Particulate Matter: Sources, Inorganic and Organic Particulate Matter - Effects on Human Beings, Materials and Climate - Control of Particulate Emissions.

Hydrocarbons: Sources - Types of Polluting Hydrocarbons - Hydrocarbons and Photochemical Smog Formation - Harmful Effects of Photochemical Smog - Control of Hydrocarbon Emissions .

Green House Effect: Causes, Consequences and Abatement of Green House Effect - Ozone Depletion - Mechanism, Causes, Consequences and Abatement of Ozone Depletion - Bhopal Gas Tragedy and Sevozo Disaster.

PC(CB4)-14: Pollution in Hydrosphere

Types of Water Pollutants and their Effects - Sources of Water Pollution: Domestic, Industrial, Agricultural, Soil, Thermal and Radioactive Wastes - Types of Persistent Pollutants - Biomagnification of Persistant Pollutants, Effects of Biomagnified Pollutants on Human Beings (DDT) – Tripolyphosphates: Their Role in Eutrophication of Water Bodies - Ecological Consequences of Eutrophication, Bacteriological Contamination of Water - Dissolved Oxygen in Natural Waters - Depletion of Dissolved Oxygen - Biological Oxygen Demand and Chemical Oxygen Demand as Indicators of Extent of Water Pollution - Nitrates, Nitrites, Nitrosoamines in Water: Their Toxic Effects On Human Beings - Treatment of Drinking Water Supplies.

PC(CB4)-15: Heavy Metal and Radiochemical Pollution.

Essential and Toxic Elements in Nature - Mechanism of Metal Ion Toxicity - Effects on Non-Metalloenzymes, Metalloenzymes, Cell Membranes, Nucleic Acids - Concepts of Speciation, Biomethylation and Biomagnification.

Mercury: Sources of Pollution. Speciation and Environmental Forms of Mercury - Biochemical Effects of Different Species of Mercury - Minamata Bay Episode as a Case Study of Mercury Poisoning.

Arsenic: Sources of Pollution - Speciation and Environmental Chemistry of Arsenic - Biochemical Effects of Different Species of Arsenic.

Lead: Sources of Lead Pollution - Speciation and Pathways of Lead in Environment - Biochemical Effects of Lead.

Cadmium: Sources of Pollution – Speciation - Biochemical Effects of Cadmium Poisoning.
Radiochemical Pollution: Sources, Chemical Changes due to Radiation on Water.

Organic Compounds - Harmful Effects of Radioactive Pollutants on Living Organisms - Permissible Limits of Radiation - Control and Disposal of Radioactive Wastes - Chernobyl Disaster.

PC(CB4)-16: Analysis of Air, Water and Metal Pollutants

Air Quality Standards - Sampling (Particulates and Gaseous Pollutants) - Analysis of Pollutants: SO_2 (Modified West-Gaeke Spectrophotometric Method, Pulsed Fluorescence Spectrometry), H_2S (Spectrophotometry – Ethelyne Blue Method), NO-NOx (Chemiluminescence Technique, Colorimetric Technique- Saltzman Method) – CO (NDIR Spectrometry, GC), Hydrocarbons (Ionization Analysis), Aromatic Hydrocarbons in Automobile Exhausts, Petrol, Air, O_3 (Chemiluminiscene and Spectrophotometry) - Particulate Matter Analysis (High Volume Method).

Water Sampling, Preservation and Preconcentration Methods and Physical Analysis - Colour, Odour, Temperature, pH, EC, Redox Potential and Total Dissolved Solids (Turbidimetry). Chemical Analysis of Anions: CN^-, Cl^-, F^- (Spectrophotometry, Ion Selective Potentiometry and Titrimetry), NO_2^- and NO_3^- (Spectrophotometry), SO_4^{2-}, PO_4^{3-}, HCO_3^-, CO_3^{2-}, Hardness of Water (Titrimetry), Ammonical Nitrogen (Spectrophotometry) - Determination of DO, BOD, COD, TOC in Water.

Books Suggested:

1. Environmental Chemistry, John. W. Moore and Elizabeth Moore Academic press New York
2. Principles of Environmental Chemistry, Stanley E. Manahan 2nd Ed.
3. Environmental Chemistry, 4th ed. A.K. De. New Age International Publishers, 2000
4. Environmental Pollution Analysis, S.M. Khopkar Wiley Eastern Ltd. 1995
5. Environmental Chemistry, Colin Baird W.H. Freeman and Company New York 1995.
6. Text Book of Environmental Chemistry, Ayodhya Singh, Campus Books International publishers
7. Chemistry of the Environment, II Edn Thomas G.Spiro William M.Stigliani
8. Fundamental Concepts of Environmental Chemistry, G.S.Sodhi Narosa Publishing House.
9. Environmental Analytical Chemistry, F.W.Fifield,P.J.Haines,Blackie Academic & Professional

III SEMESTER PRACTICALS

CH (PC) 351 P: Paper-V (Chemical Kinetics) **9** hrs/week

Note: The data obtained in all the experiments are to be analyzed by the students both *by the usual graphical methods and by regression (linear/nonlinear) techniques using a PC.*

- Study of peroxydisulphate – iodide reaction:
  1. Individual orders of the reactants by initial rate and isolation methods
  2. Effect of temperature on reaction rate
  3. Effect of ionic strength on reaction rate
- Study of peroxydisulphate – iodide clock reaction:
  1. Individual orders of the reactants ,
  2. effect of ionic strength on uncatalyzed and Cu(II)-catalyzed reactions
- Study of acetone – iodine reaction by titrimetry
  1. Order w.r.t.[iodine]
  2. Order w.r.t. [acetone]
  3. Order w.r.t. [H+]

CH (PC) 352 : Paper-VI (Instrumentation) 9 hrs/ week

Conductometry:

- Conductometric titrations:
  1. Mixture of strong and weak bases vs strong acid
  2. Mixture of strong and weak acids vs weak base
  3. Mixture of strong acid, weak acid and CuSO4 vs strong base
  4. Mixture of halides (chloride + iodide) vs AgNO3
  5. Formic acid, acetic acid, chloroacetic acid, dichloroacetic acid and Trichloroacetic acid
  6. and their mixtures vs strong base
  7. Precipitation titration: K2SO4 vs BaCl2
- Dissociation constants of weak acids
- Effect of solvent on dissociation constant of a weak acid
- Verification of Onsager equation
- Composition of Cu(II) – tartaric acid complex by Job's method

pH metry:

- pH – metric titrations:
  1. Monobasic acids vs strong base
  2. Dibasic acid vs strong base
  3. Tribasic acid vs strong base
  4. Mixture of strong and weak acids vs strong base
- Determination of dissociation constants of monobasic/dibasic acids by Albert- Serjeant method
- Determination of dissociation constant of acetic acid in DMSO, acetone anddioxane
- Determination of pKa and pKb of glycine (calculation using a computerprogram)
- Determination of stability constant of a metal complex

Suggested books:

1. A textbook of practical organic chemistry by A I Vogel, Vol 1&2.
2. Senior practical physical chemistry. B. D. Khosla, V.C. Garg, Adarsh Gulati
3. Experimental Physical Chemistry: V. Athawale and P. Mathur.
4. Practical Physical Chemistry: B. Vishwanathan and P.S. Raghavan.
5. Practical in Physical Chemistry: P.S. Sindhu
6. Advanced Practical Physical chemistry: J.B.Yadav

M.Sc. SEMESTER - IV
PHYSICAL CHEMISTRY SPECIALIZATION
(For the batches admitted in academic year 2016 and later under CBCS pattern)

PAPER I CH(PC)401: Thermodynamics, Chemical kinetics and Electrochemistry

PC-17 : Statistical Thermodynamics
PC-18 : Non-equilibrium Thermodynamics
PC-19 : Chemical Kinetics-II
PC-20 : Electrochemistry -II

PC -17: Statistical Thermodynamics (15 hrs)

Concepts of distribution and probability. Estimation of probability and the most probable distribution. Systems composed of noninteracting particles. Derivation of Boltzmann distribution law. The molecular partition function. Systems composed of interacting particles.

The concept of ensemble and canonical ensemble. Canonical partition function and its relation to molecular partition function. The factorization of molecular partition function – translational, rotational, vibrational and electronic partition functions. Derivation of expressions for translational, rotational (diatomic) and vibrational partition functions. Relationship between partition functions and thermodynamic functions. The relationship between partition functions and thermodynamic functions. Law of equipartition energy.

Specific heats of solids – Einstein equation of heat capacity of solids – derivation. Explanation of heat capacity at very low and very high temperatures – Dulong and Petits Law. Debye theory.
The entropy of a monoatomic ideal gas. The Sackur-Tetrode equation- derivation. Mean translational and vibrational energies.

The relation between equilibrium constant and partition function- derivation.

Basic ideas of Bose-Einstein statistics and Fermi-Dirac statistics and comparison of these with Maxwell-Boltzmann statistics.

PC-18: Non-equilibrium Thermodynamics (15hrs)

Thermodynamic criteria for non-equilibrium states. Entropy production in irreversible processes. Entropy production in heat flow and entropy production in material flow.

Fluxes and forces. Linear flux-force relations**.** Phenomenonological equations and coefficients. Microscopic reversibility. Onsager reciprocal relations.

Application of Onsager relations to electrokinetic phenomena – electroosmotic pressure and streaming current. The Onsager relations and the principle of detailed balance. Liquid junction potentials – derivation of equation for liquid junction potential in terms of transport numbers using Onsager relations. Steady states. Principle of minimum entropy production.

Irreversible thermodynamics as applied to biological systems - examples.

Application to thermoelectric circuits. Seebeck and Peltier effect.

PC-19: Chemical kinetics – II: (15hrs)

Reactions in solution: Factors affecting reaction rates in solution. Effect of pressure on rate of reaction. Diffusion controlled reactions. Influence of dielectric constant and ionic strength on ion-ion, ion-dipole and dipole-dipole reactions. Primary and secondary salt effects. Kinetic isotope effects: Primary and secondary isotope effects. Solvent isotope effects.

Fast reactions: Flow methods and the stopped-flow technique. The fluorescence technique. Shock tube method. Relaxation methods (T-jump and P- jump). Kinetic equations for chemical relaxation.

Enzyme kinetics: Michaelis - Menten mechanisms of enzyme catalyzed reactions involving one and two intermediates. Steady-state approximation. Derivation of kinetic equations. Evaluation of kinetic parameters. Enzyme- substrate complex: Fischer's lock and key and Koshland's induced fit hypotheses. Specificity of enzyme-catalyzed reactions. Discussion of the various types of forces involved in the formation of E-S complex. pH dependence of enzyme-catalyzed reactions – the kinetics and the equations involved.

PC –20 : Electrochemistry – II (15 hrs)

The electrode-electrolyte interface: The electrical double layer. The Helmholtz-Perrin parallel-plate model, the Gouy-Chapman diffuse-charge model and the Stern model. Quantum aspects of charge transfer at the interfaces. Tunneling.

Electrodics: Charge transfer reactions at the electrode-electrolyte interface. Exchange current density and overpotential. Derivation of Butler-Volmer equation. High field approximation. Tafel equation - low field - equilibrium, Nernst equation. The symmetry factor and its significance.

Corrosion: Electrochemical corrosion.Short-circuited energy producing cell. The definition and final expression of corrosion current and corrosion potential. Homogeneous theory of corrosion.Evans diagrams. Potential-pH (Pourbaix) diagrams of iron. Methods of corrosion rate measurement. Mechanism of anodic dissolution of iron. Protection against corrosion. Corrosion inhibition by organic molecules.

Books suggested:

1. Elements of Statistical Thermodynamics, L. K. Nash, Addison – Wesley
2. Introduction to Statistical Thermodynamics, T. L. Hill, Addison Wiley
3. Statistical Thermodynamics, M. C. Gupta, New Age International
4. Atkin's Physical Chemistry, P. Atkins & Julio de Paula, Oxford University Press
5. Molecular Thermodynamics, D. A. McQuarrie & J. D. Simon, University Science Books
6. Text book of Biochemistry by Stryer, W.H.Freeman & Co Ltd
7. Advanced physical chemistry by Gurtu and Gurtu, Pragati Edition
8. Physical chemistry by Puri and Sharma, Vishal Publishing Co.
9. Chemical Kinetics, K. J. Laidler, McGraw Hill
10. Kinetics and Mechanism, A. A. Frost & R. G. Pearson, John Wiley & sons
11. Kinetics and Mechanism of Chemical Transformations, J. Rajaraman & J. Kuriacose, McMillan
12. Chemical Kinetics and Reaction Mechanisms, J. H. Espenson, McGraw Hill
13. Physical Organic Chemistry, N. S. Isaacs, ELBS

14. The Physical basis of Organic Chemistry, Howard Maskill, Oxford University Press
15. Modern Electrochemistry, J. O. M. Bockris & A. K. N. Reddy, Plenum.
16. Modern Electrochemistry 2B, Bockris & Reddy, Plenum.
17. Introduction to Electrochemistry, S. Glasstone, EAST-WEST Press Pvt. Ltd, New Delhi

PAPER- CH(PC) 402T: SUPRAMOLECULAR CHEMISTRY, PHOTO CHEMISTRY AND COMPUTATIONAL CHEMISTRY

PC-21 : Supramolecular Chemistry
PC-22 : Photochemistry
PC-23 : Computational Chemistry
PC-24 : Theoretical treatment of bio polymers

PC-21: Supramolecular Chemistry

Concepts: Molecules, super molecules and supramolecules. Nature of Supramolecular interactions.

Molecular recognition – factors involved. Ionophores. Molecular receptors – design principles.

Molecular receptors for alkali metal ions, ammonium ions, anions and neutral molecules. Crown ethers, cryptands, spherands, calixaranes, and cyclodextrins - their selectivity, macrocyclic, and template effects. Fullerenes as supramolecules.

Threading of a linear molecule through a cyclic molecule –creation of Rotaxanes and Catenanes.

Thermodynamics of host-guest complexation. Enthalpy and entropy contributions. Complexation free energies.

Supramolecular catalysis- Crownether supported alkaline earth metal ions as catalysts, cyclodextrins and calixaranes as catalysts in chemical reactions. Transport of ions across membranes by biological molecules.

Molecular electronic devices: Molecular wires, molecular switches and machines.

PC-22: Photochemistry – Ii

Formation of excimers and exciplexes – PE diagram and quantum yields. Energy transfer mechanism for bimolecular quenching. Long-range coulombic energy transfer – critical transfer distance. Short-range electron exchange energy transfer. Triplet-triplet energy transfer and sensitization.

P-type delayed fluorescence. The experimental study of photochemical reactions: Product analysis, chemical methods in the study of intermediates, spectroscopic methods, ESR and CIDNP, rate coefficients for photochemical processes and identification of excited states.

Electronic transitions in transition metal complexes. Ligand field (LF) and charge transfer (CT) electronic states. $Ru(bpy)_3^{2+}$ as sensitizer for photoredox reactions, examples. Photochemical cleavage of water.

PC-23: Computational treatment of many electron systems (15hrs)

Multi-electron atoms. The antisymmetry principle and the Slater determinant. The Hartree-Fock method. The Hartree-Fock equations.(no derivation). The Fock operator. Core hamiltonian. Coulomb operator and exchange operator. Slater-type orbitals (STOs) as basis functions. Orbital energies and total energy. Helium atom example. Koopman's theorem. Hund's rules and theoretical basis of the Aufbau principle. Electron correlation energy.

The Hartree-Fock method for molecules. Restricted and unrestricted HF calculations. The Roothan equations. The Fock matrix. The Roothan matrix elements. GTOs and different types of basis sets. Minimal basis set. Model HF calculations on H_2. Discussion of results of HF calculations on simple molecules – H_2O and NH_3. Introduction to configuration interaction.

Density functional theory (DFT). Hohenberg-Kohn theorem. Kohn-Sham (KS) formulation of DFT. KS equations and KS orbitals. Brief explanation of exchange-correlation energy and exchange- correlation potential.

PC-24: Theoretical treatment of biopolymers (15 hrs)

Types of biopolymers. Methods of determining Size and shape of biopolymers - mean molecular masses, colligative properties, sedimentation, viscosity, light scattering methods.

Chain conformation and configuration of poly peptides. Random coils and measures of size – contour length, rms separation, radius of gyration, constrained chains.

Secondary structures of proteins- helices and sheets: The Corey-Pauling rules. Conformational energy of a polypeptide- bonding, nonbonding potentials, electrostatic interactions, dipole-dipole interactions and van der Waals interactions. Hydrogen bonds. Principles of molecular mechanics to calculate potential energy of a polypeptide. Ramachandran plots of α-helix and β-sheet.

Conformational entropy. Introductory treatment of the protein folding problem.

Books suggested:

1) J.W Steed and J.L Atwood, Supramolecular chemistry, John Wiley & Sons, Ltd. New York.
2) Piet W. N. M. van Leeuwen, Supramolecular Catalysis, Wiley-VCH Verlag GmbH & Co.
3) Principles and methods in supramolecular chemistry, Hans-Jorg Schneider and A.Yatsimirsky, John Wiley and Sons.
4) Analytical Chemistry of Macrocyclic and Supramolecular Compounds, S.M.Khopkar, Narosa Publishing House
5) Essentials of Molecular Photochemistry, A. Gilbert & J. Baggott, Blackwell Science
6) Quantum Chemistry, I. N. Levine, Prentice Hall
7) Molecular Quantum Mechanics, P. W. Atkins and R. S. Friedman, Oxford University Press
8) Introduction to Computational Chemistry, F. Jensen, John Wiley & Sons
9) Elementary Quantum Chemistry, F. L. Pilar, McGraw Hill
10) Modern Quantum Chemistry, A. Szabo and N. S. Ostlund, Dover publishers
11) Computational Chemistry: Introduction to the theory and Applications of Molecular and Quantum Mechanics, Errol Lewars, Springer Publications
12) Physical Chemistry, D. A. McQuarrie and J. D. Simon, Viva Books Ltd.
13) Physical Chemistry, P. W. Atkins, Oxford Unibersity Press.

14) Approximate Molecular Orbital Theory, J. A. Pople and D. L. Beveridge, McGraw Hill
15) Biophysical Chemistry, Cantor & Schimmel, W. H. Freeman and Company
16) Principles of Physical Biochemistry, Kensal E van Holde, W. Curtis Johnson & P. Shing Ho, Prentice Hall
17) Physical Biochemistry : Principles and Applications, David Sheehan, John Wiley
18) Physical Chemistry for the Chemical and Biological Sciences, Raymond Chang, University Science Books

ELECTIVE –3A:

PAPER III CH(PC)- 403T(CB1): CATALYSIS

PC(CB1)-17: Homogeneous catalysis
PC(CB1)-18: Surface Chemistry & Micellar catalysis
PC(CB1)-19: Heterogeneous catalysis
PC(CB1)-20: Phase transfer , Anchored & Photo catalysis

PC(CB1)-17: Homogeneous catalysis (15 hrs)

Introduction to catalysis. Types of catalysis, characteristics of catalyst, catalyst supports, promoters, general mechanism of catalysis, equilibrium treatment and steady state treatment. Activation energies of catalyzed reactions.

Acid-base catalysis, specific acid-base catalysis, general acid base catalysis, mechanism of acid – base catalysis, catalytic activity and acid-base strength- Bronsted relationships.
Acidity functions: Types of acidity functions. Hammett acidity function. Measurement of Hammett acidity function(Ho), usefulness of Hammett acidity function in understanding the mechanism of an acid catalyzed reactions. Zucker-Hammett hypothesis and its applications. Bunnett – Olson's criteria of acid-base catalyzed reactions with examples.

Catalysis by transition metal ions and their complexes. Use of Ziegler –Natta and metallocene catalysts as homogeneous catalysts for polymerization of olefins. Application of metal ion catalysis to the hydrogenation of alkenes, hydroformylation, oxidation and isomerization reactions. Asymmetric Catalysis–Introduction, Catalysts, Commercial Applications, Asymmetric Hydrogenation, Enantioselective Isomerization: L-Menthol, Asymmetric Epoxidation.

PC(CB1)-18: Surface Chemistry and Micellar catalysis (15hrs)

Surface tension. Curved interfaces. The Laplace equation. Capillary action. Thermodynamics of surface layers – Gibbs isotherm.

Adsorption. Types of adsorption, factors effecting adsorption, Chemistry and thermodynamics of adsorption. Determination of heats and entropies of adsorption.

Surface versus bulk structures. Adsorbate -induced restructuring of surfaces. Thermal activation of bond breaking on a surface. Co-adsorption. Chemisorption isotherms. Kinetics of chemisorption.

Surface films. Monometallic surfaces and bimetallic surfaces. Experimental techniques for the study of monolayer films. States and reaction in monomolecular films. Reaction between $H_2(g)$ and $N_2(g)$ catalyzed by surfaces to give $NH_3(g)$.

Micelles: Classification of surface active agents. Micellization and micellar interactions. Structure of micelles – spherical and laminar. Critical micellar concentration (CMC). Factors affecting the CMC of surfactants.

Counter ion binding to micelles. Thermodynamics of micellization. Phase separation and mass action models, solubilization, micro emulsion, reverse micelles. Reactions assisted by micelle formation. Examples of micelle-catalyzed reactions and their mechanisms.

PC(CB1)-19: Heterogeneous catalysis (15 hrs)

Heterogeneous catalysis. Broad categories of catalysts – metals, bimetals, semiconductors, insulators, zeolites, oxides, nano materials.

Preparation of metal catalysts, supported metal catalysts and non- metallic catalysts. Co-precipitation, Impregnation, sol-gel method, deposition-precipitation, hydrothermal synthesis, pulsed laser methods, plasma chemical methods, chemical vapor deposition methods

Steps in heterogeneous catalyzed reactions. Diffusion and adsorption. Mechanism of surface-catalyzed reactions. Adsorption isotherms - Langmiur Hinshelwood model, Rideal - Eley mechanism, Kinetics and thermodynamics of catalysed reactions. Catalytic activity – the determining factors. Structure sensitive and structure insensitive catalysts.

Characterization of catalysts: Surface area by BET method. Determination of pore volume and pore size distribution by BJH method. Pore size and specificity of catalysts. Surface acidity of catalysts- Determination of surface acidity by indicator method, IR spectroscopic method and TPD methods. Surface characterization by XRD, LEED, TEM & AFM, XPS, AES, techniques.

Auto exhaust emissions- catalytic converters. Catalytic hydrogenation and oxidation reactions.

Cracking and reforming. Fischer-Tropsch synthesis of methanol.

PC(CB1)-20: Phase transfer, Anchored and Photo catalysis **(**15 hrs)

Phase-transfer catalysis (PTC): Principles of phase-transfer catalysis. PTC classification.
Role of water in phase-transfer catalyzed reactions. Factors influencing the rate of PTC reactions.

Inverse phase transfer catalysis. Mechanism of nucleophilic displacement reactions.

Crown ethers: Crown ethers as phase transfer catalysts(PTC) in the reaction of alkyl halides with super oxide. Permanganate oxidation of alkenes and phenols in presence of PTC's viz., quarternary ammonium salts and crown ethers.

Anchored catalysis: Definition and examples of anchored catalysis- organic polymers, inorganic oxides and clays as supports. Structure of montmorillonite anchored catalysts- HEW structure and EF structure. Montmorillonite anchored catalysts- application of intercalated clay catalysts in hydrogenation reactions.

Photo catalysis: Photocatalytic effect, metal semiconductor systems as photo catalysts, nature of the metal loaded, extent of metal loading, nature of semiconductor, doped semiconductors, coupled Semiconductors. Application of photocatalysis for splitting of water by semiconductor particles, removal of organic and inorganic pollutants, for oxidation and reduction of organic compounds.

Books suggested:

1. Principles of Heterogeneous Catalysis in practice, G. C. Bond, Oxford Publishing
2. Heterogeneous Catalysis, C. Satterfield, McGraw Hill
3. Catalysis, Principles and applications, edited by B. Vishwanathan, S. Sivasanker & A. V. Rama Swamy, Narosa Publishing House
4. Catalysis, J. C. Kuriacose, Macmillan
5. Colloidal and surface chemistry , M. Satake, Y. Hayashi, Y.Mido, S.A.Iqbal and M.S.sethi
6. " Physical Organic Chemistry" by L.P.Hammett, chapter 9 , McGraw Hill .
7. Chemical Review, **57,** 1935(1957), M.A. Paul and F.A. Long
8. Phase Transfer Catalysis, Fundamentals, Applications and Industrial perspective, C. M. Stark, C. Liotta & M. Halpern, Academic Press
9. Phase Transfer Catalysis, E. V. Dehmlow & S. S. Dehmlow, Verlag Chemie, Weinheim
10. Phase Transfer Catalysis in Organic synthesis, W. P. Weber & G. W. Gokel, Springer
11. Hand book of phase transfer catalysisEdited by Y. Sasson and R. Neumann
12. Catalysis in Micellar and Macromolecular systems, J. H. Feudler & E. J. Feudler, Acad. Press
13. Reaction Kinetics in Micelles, E. H. Codes (ed), Plenum
14. Micelles – Theoretical and Applied aspets, V.Moroi, plenum
15. Physical Chemistry of surfaces, A.W.Adamson and A.P.gast, Wiley
16. Polymer supported Catalysts, C. U. Pittman Jr, vol 8, Comprensive Organometallic Chemistry
17. Principles and Practice of Heterogeneous Catalysis, J. M.Thomas andW.J.Thomas, VCH1997.
18. Spectroscopy in catalysis – An introduction by J. W. Niemantsverdriet.
19. Modern methods of Organic Synthesis: Ahluwalia.

ELECTIVE–3B

PAPER IV CH(PC) 403 T(CB2) : Dynamics of Chemical Reactions And Sensors

PC-(CB2)-21: MO and VB theory of reactivity
PC-(CB2)-22: Kinetic, isotopic, structural, solvent, steric and conformatlonal effects
PC-(CB2)-23:Nucleophilic, electrophilic and free radical reactivity
PC-(CB2)-24: Sensors

PC-(CB2)-21: Molecular Orbital (MO) and Valence Bond (VB) theory of reactivity 15 Hrs

Introduction to Huckel molecular orbital (MO) method as a means to explain modern theoretical methods. Advanced techniques in PMO and FMO theory. Molecular mechanics, semiemperical methods and ab inito and density functional methods. Scope and limitations of several computational programmes. Quantitative MO theory-Huckel molecular orbital (HMO) method as applied to ethane energy levels .Orbital symmetry, orbital interaction diagrams. MO of simple organic systems such as ethane, allyl, butadiene, methane and methyl group. Conjugation and hyperconjugation. Aromaticity. Valence bond (VB) configuration mixing diagrams. Relationship between VB configuration mixing and resonance theory. Reaction profiles. Potential energy diagrams. Curve crossing model nature of activation barrier in chemical reactions. Principle of reactivity Mechanistic significance of entropy, enthalpy and Gibbs free energy. Arrhenius equation, transition state theory. Uses of activation parameters.

PC-(CB2)-22: Kinetic, isotopic, structural, solvent, steric and conformational effects 15 Hrs

Theory of isotope effects, Primary and secondary kinetic isotope effects. Heavy isotope effects. Tunneling effect Solvent effects. Structural effects on reactivity: Linear free energy relationship (LFER.). The Hammett equation, substituent constants, theories of substituent effects. interpretation of σ-values. Reaction constant ρ. Deviations from Hammett equation. Dual—parameter correlations, inductive substituent constant The Taft model, σ1, σR scales. Solvation and solvent effects: Qualitative understanding of solvent- solute effects on reactivity Thermodynamic measure of solvation. Effects of solvation on reaction and equilibrium. Various empirical indexes of solvation based on physical properties, solvent- sensitive reaction rates, spectroscopic properties and scales for specific solvation. Use of solvation scales in mechanistic studies. Solvent effects from the curve-crossing model. Various type of steric strain and their influence on reactivity. Steric acceleration. Molecular measurements of steric effects upon rates. Steric LFER. Conformational barrier to bond rotation-spectroscopic detection of individual conformers. Acyclic and monocyclic systems. Rotation around partial double bonds. Winstein-Holness and Curtin-Hammet principle.

PC-(CB2)-23: NUCLEOPHILIC, ELECTROPHILIC AND FREE RADICAL REACTIVITY 15 Hrs

Bases, nucleophiles, Electrophiles and Catalysts. Acid-base dissociation. Electronic and structural effects, acidity and basicity. Acidity functions and their applications. Hard and soft acids and bases. Nuccleophilicity scales, Nucleofugacity. The α-effect.- Ambivalent nucleophiles. Acid-base catalysis. Specific and general catalysis. Bronstéd catalysis. .nucleophilic and electrophilic catalysis. Catalysis by non-covalent binding micellar catalysts. Nucleophilic and electrophilic Reactivity:Structural and electronic effects on SN1 and SN2 reactivity. Solvent effects,kinetic isotope effects. Intramolecular assistance. Electron transfer nature of SN2 reaction. Nuclcophilicity and S2 reactivity based on curve-crossing rnodel. Relationship between polar and electron transfer reactions. SRN1 mechanism. Electrophilic reactivity, general mechanism. Kinetics of SE2-Ar reaction, Structural effects on rates and selectivity. Curve crossing approach to electrophilic reactivity. ; Radical and pericyclic reactivity. (a)Radical stability, polar influences, solvent and steric effects. A curve crossing approach to radical addition, factors affecting barrier heights in additions, regioselectivity in radical reactions. Reactivity, specificity and periselectivity in pericyclic reactions.

PC-(CB2)-24: Chemical, Electrochemical and Bio Sensors 15hrs

Importance of Sensors, Biomolecular recognition elements, Artificial molecular-recognition materials, Molecular imprinted polymers, Electrode modification. Fluorescence, chemi and bio-luminescence sensors, Fluorescent tag molecules, Applications. Conductometric sensors, Coulometric sensors, Voltammetric sensors, Applications, Neurotransmitters, Amperometric sensors, Chronoamperometric analysis, Multichannel sensors, Microelectrode sensors, Electrochemical Impedance Sensors, Quartz crystal nanobalance sensors, Molecular recognition, Applications. Surface Plasmon resonance based sensors, Fiber optic sensors, Twodimensional microarray based sensors, Applications for Food Safety - Mycotoxins, adultrants, Biomedical diagnosis - Cancer markers.

Books suggested:

1. Molecular mechanics. By U.Bukert and N.L.Allinger, ACS Monograph 177,1982
2. Organic Chemistry book of Orbitals. L.Salem and W.L.Jorgenson
3. Mechanism and theory in Organic Chemistry, T.M.Lowry, K.C.Richardson, Harper and Row
4. Introduction to theoretical Organic Chemistry and molecular modeling by W.B.Smith, VCH, Weinhein.
5. Physical Organic chemistry, N.S.Isaaçs
6. Suprarnolecular Chemistry - concepts and perspectives by J M .Lehn,
7. The Physical basis of Organic Chemistry by H.Maskill.
8. Physical Organic Chemistry by Jack HineLaboratory course
9. Brian R. Eggins, Chemical Sensors and Biosensors, Analytical Techniques in the Sciences (ANTS), 2nd Edition, Wiley, 2002.
10. Gabor Harsanyi, Sensors in Biomedical Applications - Fundamentals, Technology and Applications, CRC Press, 2000.
11. Raluca-Ioana Stefan, Electrochemical Sensors in Bioanalysis, CRC Press, 2001.

ELECTIVE –4A (ID PAPER)

PAPER III CH(PC)- 403T(CB3): MOLECULAR MODELING AND IT'S APPLICATIONS

PC(CB3)-25: Molecular Modeling – I
PC(CB3)-26: Molecular Modeling – II
PC(CB3)-27: Drug Design Methods I - Ligand Based
PC(CB3)-28: Drug Design Methods II - Structure Based.

PC(CB3)-25: Molecular Modeling – I (15hrs)

Introduction to Molecular Modeling, Single molecule calculations, assemblies of molecules and reactions of molecules - Co-ordinate systems: Cartesian and Internal Co-ordinates, Z-matrix - Potential energy surface - Conformational search; Global minimum, Local minimum, Conformational analysis of ethane.

Force field ; Features of Molecular Mechanics, Bonded and Non-bonded interactions, Bond Stretching, Angle Bending, Torsional Terms (Improper Torsions, out of Plane Bending Motions, Cross Terms), Non Bonded Interactions (Electrostatic Interactions, Van-der Waals interactions), Hydrogen Bonding Interactions.

PC(CB3)-26: Molecular Modeling – II (15hrs)

Force Field Equation in Energy minimization (Energy as function of r, θ, ω) - Introduction to Derivative Minimization Methods (First Order Minimization), Types of energy minimization Methods ; Steepest Descent, Conjugate Gradient, Conformational Search procedures - Geometry optimization procedures - Molecular Dynamics: Introduction, description of Molecular Dynamics, basic elements of Monte-Carlo method, differences between Molecular Dynamics and Monte-Carlo method, Qualitative exposure to Molecular Dynamics Simulations.

PC(CB3)-27: Drug Design Methods I - Ligand Based (15hrs)

Lead Molecule - Structure Activity Relationship (SAR), Quantitative Structure Activity Relationship (QSAR), Distinguish between SAR and QSAR - Physicochemical parameters ; Electronic effects, Hydrophobicity, Steric Factors Taft's Steric function, Molar Refractivity, Verloop Steric factor - Molecular Descriptor analysis: Craig plot, Topliss scheme, Bioisosteres - Hansch model, Free-Wilson model for QSAR equations - Regression analysis: Multi Linear Regression and Partial Least Square (terms: n, SD, r, r^2, r^2%, F) - Examples for linear and non-linear equations - 3D QSAR: CoMFA and CoMSIA - Differences between 2D and 3D QSAR.

PC(CB3)-28: Drug Design Methods II - Structure Based. (15hrs)

Database similarity searches - Pair-wise alignment: Global sequence analysis (Needleman-Wunsch), Local Sequence Alignment (Smith Waterman), Multiple Sequence Alignment - Homology Modeling: Query sequence, Template selection, Alignment, Backbone Modeling, Loop Modeling, Side chain Modeling, Model optimization, Energy minimization - Model Evaluation: Ramachandran Plot, Verify 3D, Errata and ProSA - Active site Identification - Docking, Docking Algorithms: Genetic Algorithm, Incremental construction - Molecular Interactions, Scoring functions - Virtual Screening: Ligand Based and Structure Based. De novo ligand design and its limitations.

Books suggested:

1. Molecular Modelling: Principles and Applications, by Andrew Leach, Longman Publications.
2. Computational Chemistry, Guy H. Grant & W. Graham Richards, Oxford University Press.
3. Computational Chemistry: Introduction to the theory and Applications of Molecular and Quantum Mechanics, Errol Lewars, Springer Publications.
4. Recent advances in Bioinformatics by I. A. Khan and A Khanum Ukaaz publications, 2003.
5. Molecular modelling – Basic Principles and Applications by Hans Dieter Holtje and Gerd Folkers, Wiley-VCH, 1996
6. Introduction to Computational Chemistry by Jensen, Wiley Publishers, second edition
7. Bioinformatics – A Primer by P. Narayanan, New Age International, (PC) Ltd, 2005.
8. Introduction to Bioinformatics by Arthur M. Lesk, Oxford University Press (Indian. Edition), 2002
9. Principles of Medicinal Chemistry Vol. II by Dr. SS Kadam Pragati books Pvt. Ltd; 2007
10. An Introduction to Medicinal Chemistry by G L Patrick, Oxford University Press
11. Bioinformatics: Methods and Applications: Genomics, Proteomics and Drug Discovery. S.C. Rastog, Namita Mendiratta, Parag Rastogi, PHI Larning Pvt. Ltd; 2006
12. Pharmacy Practice Vol.I and II by Remington, Pharmaceutical Press
13. Burger's Medicinal Chemistry and Drug Discovery, 5th Edition, Wiley-Interscience, New York
14. Text book of Drug design and Vol.1 discovery 3rd Edition by POVL krogsgaard- Larsen Tommy liljefors and ULF Madsen.

ELECTIVE –4B (ID PAPER)

PAPER-IV CH(PC) 404T(CB4): Engineering Chemistry

PC(CB4) -29: Water And Waste Water Treatment
PC(CB4) -30: Corrosion And Its Control
PC(CB4) -31: Energy Sources
PC(CB4)- 32 Engineering Materials

PC(CB4) -29:Water and waste water treatment (15 hrs)

Review of Hardness: causes, measurement of hardness, units- types of hardness, estimation of temporary and permanent hardness, numerical problems. Boiler troubles- scales and sludge formation, caustic embrittlement, priming and foaming. Methods for boiler water treatment: Soda-lime process, zeolite process, ion exchange process. Treating saline water: distillation, electrodialysis, reverse osmosis. Municipal water supply: sedimentation, filtration, sterilization. Waste water treatment: physical, chemical and biological treatment. Sewage water , COD and BOD , numerical problems

PC(CB4) -30:Corrosion and its control: (15 hrs)

Magnitude of the problem, theories of corrosion, Chemical and electrochemical corrosion, corrosion reactions, factors affecting corrosion- nature of metal, purity of metal,electrochemical series, over voltage, nature of oxide film, nature of corrosion product, nature of environment, effect of temperature, effect of pH, effect of oxidant, humidity. Corrosion control methods-design and material selection, cathodic protection, sacrificial anode, impressed current cathode. Surface coating methods: Surface preparation, metallic coatings, application of metal coatings: hot dipping, galvanizing, tinning, cladding, electroplating, chemical conversion coatings. Organic surface coatings-paints, constituents of paints and their functions, methods of application of paints, failure of paint films, varnishes, enamels, lacquers.

PC(CB4) -31: Energy sources: (15 hrs)

Conventional energy resources: Chemical fuels, classification, (solids, liquids, gaseous) . Solid fuels: coal, analysis of coal , proximate and ultimate analysis and their significance. Liquid fuels: petroleum, refining of petroleum, cracking, reforming. Synthetic petrol - Bergius and Fischer-Tropsch's process, knocking, anti knocking agents, octane number. Diesel fuel: Cetane number. Other liquid fuels: LPG, biodiesel, kerosene, fuel oil, benzol, tar, power alcohol. Gaseous fuels: natural gas, coal gas, producer gas, oil gas, water gas, biogas, Combustion: Calorific value and its determination, bomb calorimeter. HCV and LCV values of fuels, problems. analysis of flue gas by Orsats method. Rocket fuels, solid propellants, liquid propellants, monopropellants, bipropellants.

Non conventional energy resources: Nuclear fuels- nuclear reactor, nuclear fission, nuclear fusion, sources of nuclear fuels, disposal of radio active wastes, reprocessing of nuclear fuels. solar, hydro, wind, tidal energies. Bio fuels, H_2 as a non polluting fuel.

PC(CB4) -32: Engineering materials. (15 hrs)

Cement: composition of Portland cement, analysis, setting and hardening of Portland cement (reactions), decay of cement concrete, lime, manufacture, types of lime, plaster of paris

Lubricants: Criterion of a good lubricant, classification of lubricants: petroleum oils, fixed oils, synthetic lubricants, semisolid lubricants, solid lubricants. Properties of lubricants: cloud point, pour point, flash and fire point, viscocity.

Refractories: Classification, characteristics of good refractory, failure of refractories. Glass, glass making oxides and their functions, manufacture of glass. Porcelain, enamels, abrasives.

Conductors and insulators: Classification of insulators, characteristics of thermal and electrical insulators and super conductors (Nb-Sn alloy, $YBa_2Cu_3O_{7-x}$) applications.

Composite materials: Advantageous properties of the composites, classification, mechanism of strengthening, mechanism of hardening of particle reinforcement, fabrication of the composites.

Liquid crystals: Characteristics of liquid crystal orders, physical properties of liquid crystals, classification of Liquid crystals, types of mesophases chemical nature of Liquid crystals, applications of Liquid crystals, future of liquid crystals.

Books suggested:

1.Text book of Engineering Chemistry by C.P. Murthy, C.V. Agarwal & A. Naidu: B.S. Publications, Hyderabad (2006).
2.Text book of Engineering Chemistry by S.S. Dara: S. Chand & Co. New Delhi (2006).
3.Engineering Chemistry by B. Siva Shanker : Mc-Graw Hill publishing Company Limited, New Delhi (2006)
4.Engineering Chemistry by J.C. Kuriocose &J. Rajaram,Tata McGraw Hill Co. NewDelhi (2004)
5.Engineering Chemistry by P.C. Jain & Monica Jain, Dhanpatrai publishing company, (2008)
6.Chemistry of Engineering Materials by C.V. Agarwal, C.P. Murthy & A. Naidu: BS publications
7.Chemistry of Engineering Materials by R.P. Mani & K.N. Mishra, CENGAGE learning
8.Applied Chemistry – A text book of engineering and Technology – Springar (2005)
9.Text book of Engineering Chemistry by Shasi Chawla: Dhanpatrai Publishing company, New Delhi (2008)
10. Engineering Chemistry by R. Gopalan, D. Venkatappayya & D.V. Sulochana Nagarajan – Vikas Publishers (2008).

ELECTIVE–4C (ID PAPER)

PAPER-IV CH(PC) 404T(CB5): Sugar Chemistry AND Sugar Technology

PC(CB5) -33: Advanced Sugar Chemistry
PC(CB5) -34: Sugar & Sugar byproducts
PC(CB5) -35: Methodology used in Sugar Analysis
PC(CB5)- 36: Sugar Technology and Management

PC(CB5) -33: Advanced Sugar Chemistry: (15 hrs)

Carbohydrate nomenclature. Fischer, Haworth and conformational structures of mono and oligo saccharides. Chemical reactivity of sugars. Reducing and non-reducing sugars. Chiral nature of sugars. R-S nomenclature, Fischer D-L nomenclature of sugars. Sugar enantiomers, diastereo isomers, epimers and enomers. Acyclic structure of sugars, determination of relative and absolute configuration of sugars. Cyclic forms of sugars. Conformational analysis of sugars. Hassel- Otter effect. Delta-two effect. Anomeric effect. Calculation of conformational free energies. Optical rotation, specific rotation and molecular rotation of sugars. General epimer rule. Relationship between rotation and conformation. Stereo chemical transformations. Mutarotation, enolization, isomerization, anhydride formation and reversion, pH stability of glucose and fructose, protection of sugar hydroxyls.

PC(CB5) -34: Sugar & Sugar byproducts: (15 hrs)

Structure determination of sucrose, synthesis of sucrose, biosynthesis of sucrose, chemical nature of sucrose. Oligo saccharide synthesis. Oligo saccharide optical rotating power (Hudson and Klyn rules). ^{13}C NMR spectroscopic data of glucose, fructose and sucrose. Uses of sugar chirons in organic synthesis. Sugar byproducts. Bagasse, molasses and press mud. Bagasse- characteristics and uses. Production of biogas, fiberboard and furfural. Press mud- extraction of cane wax, press mud and manure. Molasses- fermentation of molasses. Production of alcohol and rectified spirit.

PC(CB5) -35:Methodology used in Sugar Analysis: (15 hrs)

Sampling techniques. Determination of moisture in bagasse, molasses and cane sugar. Methods of estimation of total soluble solids in sugar and sugar house products. Optical methods of sugar analysis, sugar scales and normal weight. Estimation of reducing sugars and sugar present in cane juice by Eynon & Lane, Luff & Schoorl and Benedicts methods. Determination of sugars by Invertase method, Jackson- Gellis, Munsen- Walker's Cu_2O and De Whalleys' volumetric method. Determination of Ash by Carbonate- Ash and Cuitometeric (Conductometric) methods. Determination of various other constituents present in raw sugars. Estimation and chemical composition of cane and its juice.
Instrumental methods of sugar industry- Static characteristics and Dynamic characteristics. Gas, liquid, vapor thermometers. Bimetallic thermometers and thermocouples. Electronic panometer, cuitometer. Introduction to pneumatic control systems and elements. Working principle and instrumentation methodology of potentiometer, pH meter, polarimeter and cuitometer.

PC(CB5) -36: Sugar Technology and Basic Principles of Management: (15 hrs)
Sugar Technology: Cane juice interaction, maceration and imbibition. Principles of cane juice clarification, defecation and sulphitation. Juice heaters, filters and reaprovation vaccum pans. Centrifuges. Sugar driers and molasses. Introductory treatment of chemical control (i) Milling Control and (ii) Boiling house control.

Management: Concept and philosophy of management in major and small-scale industries. Location of factory site and Lay out of plant. Joint stock companies. Co-operative Societies. Production management and control. Personnel administration, purchases and sales, organization and control.

Books suggested:

1. Cane Sugar Hand Book, Maede & Chen, John Wiely & Sons
2. Determination of Food Carbohydrates, D. A. T. Southgate, Applied Science Publishers, London
3. Text Book of Sugar Chemistry and Sugar Technology, Mathur
4. Text Book of Sugar Byproducts, Morris Patrov
5. A Hand Book of Qualitative and Quantitative Organic Analysis, H. J. Clark, Orient Longman
6. Text Book of Biochemistry, Lehninger
7. Analysis of Sugars, Pleus
8. Text Book of Sugar Technology, Hugot
9. Instrumental Methods in Sugar Industry, Eckman
10. Principles of Instrumental Analysis, Skoog and West
11. Technical Methods of Analysis, Griffith, McGraw Hill
12. Advanced Sugar Chemistry, R. S. Shellaxberges
13. Sugar, John Yulkin, Jack Edelman, Liesel Hough
14. International Uniform Methods for Sugar Analysis, H. C. S. De Whelly

IV SEMESTER PRACTICALS

Note: The data obtained in all the experiments are to be analyzed by the students both *by the usual graphical methods and by regression (linear/nonlinear) techniques using a PC.*

CH (PC) 451P: Paper-V (Chemical Kinetics) 9hrs/week

- **Study of acetone-iodine reaction by spectrophotometry**
  1. Order w.r.t.[iodine]
  2. Order w.r.t. [acetone]
  3. Order w.r.t. [H^+]

- **Study of peroxydisulphate – iodide reaction by colorimetry**

- **Study of saponification of ethyl acetate by conductometry:**
  1. Overall order of the reaction
  2. Order w.r.t. [ethyl acetate]
  3. Order w.r.t. [NaOH]

♦ **Study of solvolysis of t-butylchloride by conductometry**:
effect of solvent dielectric constant/
polarizability (methanol/water mixture) on the rate of solvolysis

♦ **Study of oxidation of primary alcohols by dichromate by spectrophotometry**:
Application of Taft equation

CH (PC) 452P: Paper-VI (Instrumentation) 9 hrs/week

Spectrophotometry:

- Estimation of Cu(II) using EDTA
- Estimation of Fe(III) using thiocyanate
- Estimation of Fe(II) using 1,10-phenanthroline
- Estimation of Fe(III) in tap water using thiocyanate by standard addition method
- Simultaneous determination of dichromate and permanganate in a mixture
- Spectrophotmetric titrations: Cu(II) vs EDTA
  Fe(II) vs 1,10-phenanthroline
- Composition of Cu(II) – EDTA complex by Job's method
- Composition of Fe(II) – phenanthroline complex –Job's method, mole ratio, slope ratio method.
- Determination of composition and Gibbs energy of formation of Fe(III)–salicylic acid complex
- Determination of pK_a of methyl red indicator
- Estimation of Mn(II) by spetrophotometry using periodate.

Potentiometry:

- Potentiometric titrations:

1. Weak acids vs strong base and calculation of dissociation constants
2. Mixture of strong and weak acids vs strong base
3. Dibasic acid vs strong base
4. Fe(II) vs Ce(IV) and calculation of formal redox potential of Fe(II)/Fe(III)
   - Fe(II) vs MnO_4^-
   - Fe(III) vs EDTA
   - Mixture of halides vs $AgNO_3$
   - Mixture of KI and KSCN vs $AgNO_3$

Polarography:

- Estimation of Pb^{2+}, Cd^{2+} and Ni^{2+} separately and in a mixture.

Suggested books:

1. A textbook of practical organic chemistry by A I Vogel, Vol 1&2.
2. Senior practical physical chemistry. B. D. Khosla, V.C. Garg, Adarsh Gulati
3. Experimental Physical Chemistry: V. Athawale and P. Mathur.
4. Practical Physical Chemistry: B. Vishwanathan and P.S. Raghavan.
5. Practical in Physical Chemistry: P.S. Sindhu
6. Advanced Practical Physical chemistry: J.B.Yadav

M.Sc. CHEMISTRY

PHYSICAL ORGANIC CHEMISTRY SPECIALISATION
SYLLABUS OF III & IV SEMESTERS
REVISED AS PER NEW (CB) SYLLABUS

FOR STUDENTS ADMITTED FROM THE YEAR 2016 ONWARDS

M.Sc. CHEMISTRY (PHYSICAL ORGANIC CHEMISTRY SPECIALISATION)

Syllabus for III and IV Semesters

(for the batches admitted in academic year 2016 & later under CBCS pattern)

[Under Restructured CBCS Scheme]

Grand total marks and credits (all 4 semesters) 2400 marks – 96 credits

(Approved in the P.G.BOS meeting held on 01-07-2017)

Semester - III

	Instruction Hrs/week	Internal assessment marks*	Semester exam marks		Total marks	Credits
CH(PO) 301T	4	20	80		100	4
CH(PO) 302T	4	20	80		100	4
CH(PO) 303T(CB)	4	20	80		100	4
CH(PO) 304T (CB)	4	20	80		100	4
CH(PO) 351P	9	_	100	100	4	
CH(PO) 352P	9	_	100	100	4	
Total					**600**	**24**

Semester - IV

	Instruction Hrs/week	Internal assessment marks*	Semester exam marks		Total marks	Credits
CH(PO) 401T	4	20	80		100	4
CH(PO) 402T	4	20	80		100	4
CH(PO) 403T (CB)	4	20	80		100	4
CH(PO) 404T (CB)	4	20	80		100	4
CH(PO) 451P	9	_	100	100	4	
CH(PO) 452P	9	_	100	100	4	
Total					**600**	**24**

(**Choice based paper (CB) =** Paper offered by the same Department or other Department in the Science faculty)

*15 marks for written test and 5 marks for assignment

Grand total (all 4 semesters) 2400 marks and 96 credits

M.Sc. PHYSICAL ORGANIC CHEMISTRY SPECIALIZATION
Syllabus for III Semester
(For the batch admitted during the academic year 2016 onwards under the CBCS pattern)
[Under Restructured CBCS Scheme]

Paper I- CH(PO) 301T: Quantum Chemistry and Group Theory
PO- 09: Applications of Schrödinger equation
PO- 10: Angular momentum & approximate methods
PO- 11: Bonding in molecules
PO- 12: Group Theory

Paper II– CH (PO) 302T: Conformational Analysis, Asymmetric Synthesis, Synthetic Strategies and Advanced NMR spectroscopy
PO- 13: Conformational Analysis (Cyclic Systems) and ORD
PO- 14: Asymmetric synthesis
PO- 15: Synthetic Strategies
PO- 16: ^{13}C NMR and 2D NMR spectroscopy

Elective-3A
Paper-III-CH(PO) 301T(CB1): Spectroscopy, Photochemistry and Statistical Thermodynamics
PO-(CB1)1: Physical principles of spectroscopy & Vibrational spectroscopy
PO-(CB1)2: X-Ray Spectroscopy & Diffraction techniques
PO-(CB1)3: Chemical kinetics II
PO-(CB1)4: Statistical Thermodynamics

Elective–3B
Paper-III CH (PO) 303T(CB2):Biopolymer Chemistry
PO-(CB2)-5:Bioenergetics & physical properties of biopolymers
PO-(CB2)-6:Biological membranes & binding of ligands by biopolymers
PO-(CB2)-7: DNA, genes & cloning
PO-(CB2)-8: Bioinformatics

Elective-4A
Paper IV- CH(PO) 304(CB3)T: Modern Organic Synthesis
PO-(CB3)-9: Synthetic Reagents I
PO-(CB3)-10 Synthetic Reagents II
PO-(CB3)-11: New Synthetic reactions
PO-(CB3)-12: New techniques and concepts in organic synthesis

Elective–4B
Paper-IV CH(PO)304T(CB4): Organic materials, Dyes and Pigments
PO (CB4)-13: Organic Nanomaterials
PO (CB4)-14: Supramolecular Chemistry
PO (CB4)-15: Dyes – I
PO (CB4)-16: Dyes–II and Pigments

LABORATORY COURSES
Paper-V (Lab)-CH(PO) 351: Chemical Kinetics
Paper-VI(Lab)-CH(PO) 352: Synthesis of Organic compounds and Chromatography

M.Sc. PHYSICAL ORGANIC CHEMISTRY SPECIALIZATION
IV SEMESTER SYLLABUS
(For the batch admitted during the academic year 2016 under the CBCS pattern)
[Under Restructured CBCS Scheme]

PAPER-1 CH(PO) 401T:Non-equilibrium thermodynamics, NMR,NQR and Mossabaur Spectroscopy, Electrochemistry & Lasers
PO-17: Non-equilibrium Thermodynamics
PO-18: NMR , NQR and Mossbaur Spectroscopy
PO-19: Electrochemistry II
PO-20: Lasers in Chemistry

Paper-II CH(PO) 402T: Medicinal Chemistry and Biomolecules
PO-21: Principles of Drug design and drug discovery
PO-22: Lead modification and SAR Studies
PO-23: QSAR studies
PO-24: Biomolecules

Elective–3a
PAPER –III CH (PO) 403T(CB1) : Catalysis
PO(CB1)- 17 : Homogeneous catalysis
PO(CB1)- 18 : Surface Chemistry & Micellar catalysis
PO(CB1)- 19 : Heterogeneous catalysis
PO(CB1)- 20 : Phase transfer , Anchored & Photo catalysis

Elective –3b
PAPER-III CH(PO) – 403T(CB2) : Molecular modeling and It's Applications
PO(CB2)-21: Molecular Modeling – I
PO(CB2)-22: Molecular Modeling – II
PO(CB2)-23: Drug Design Methods I - Ligand Based
PO(CB2)-24: Drug Design Methods II - Structure Based.

Elective-4a(ID Paper)
Paper-IV CH (PO) 404T(CB3)T: Five and six membered heterocycles, Carbohydrates and Proteins, Structure determination of natural products and Green chemistry
PO-(CB3)- 25: Five and six membered heterocycles with two hetero atoms
PO-(CB3)- 26: Carbohydrates and proteins
PO-(CB3) - 27: Structure determination of natural products by chemical and spectral methods
PO-(CB3) - 28: Green chemistry

Elective-4b(ID Paper)
Paper IV- CH(PO) 404(CB4)T: Forensic Chemistry and Toxicology
PO-(CB4)29: Forensic Chemistry-I
PO-(CB4)30: Forensic Chemistry-II
PO-(CB4)31: Forensic Toxicology-I
PO-(CB4)32: Forensic Toxicology-II

LABORATORY COURSES
Paper-VII–(LAB)CH (PO) 451 P :Instrumentation
Paper-VIII–(LAB) CH (PO) 452P : Separation, identification and spectralanalysis of organic

compounds

M.Sc. PHYSICAL ORGANIC CHEMISTRY SPECIALIZATION
III SEMESTER SYLLABUS
(For the batch admitted during the academic year 2016 under the CBCS pattern)
[Under Restructured CBCS Scheme]

Paper I- CH(PO) 302T: Quantum Chemistry and Group Theory
PO- 09: Applications of Schrödinger equation
PO- 10: Angular momentum & approximate methods
PO- 11: Bonding in molecules
PO- 12: Group Theory

PO- 09: Applications of Schrödinger equation (15 hrs)

Systems with discontinuity in the potential field. A simple potential barrier. A potential barrier with a finite thickness. Quantum mechanical tunneling – examples - α-particle emission, inversion of NH_3, hydrogen transfer reactions.

The harmonic oscillator – detailed treatment. Wave functions and energies. Vibration of a diatomic molecule – harmonic oscillator model.

The rigid rotator – detailed treatment. Wave functions and energies. Spherical harmonics. Rigid rotator as model for a rotating diatomic molecule.

The hydrogen atom – detailed treatment. Angular and radial functions. Atomic orbitals. Measurability of the ground-state energy of hydrogen atom. Orthonormal nature of hydrogen-like wave functions. Probability calculations.

Atomic and molecular term symbols.
Atoms in external field, Zeeman and anomalous Zeeman effect.

PO- 10: Angular momentum & approximate methods (15 hrs)

Angular momentum operators. Commutation relations of angular momentum operators and their consequence. Eigen functions of L^2 and L_z and the eigen values. Magnitude and orientation of angular momentum vectors.

Electron spin. Spin operators. Pauli principle and the Pauli exclusion principle.

Approximate methods- The variation method. Construction of variation function by the method of linear combinations. H and He atom. Perturbation theory (first order and nondegenerate). Wave function and energy corrections. Application of perturbation theory to the helium atom.
Time- dependent perturbation theory. Interaction of radiation and matter. Allowed and forbidden transitions.
Multielectron atoms. The Hartree-Fock self-consistent field method. Basis functions. Slater-type orbitals (STOs).

PO- 11: Bonding in molecules (15 hrs)

Born-Oppenheimer approximation. MO theory of H_2^+ ion. Calculation of MOs and their energies. Evaluation of the overlap integral. Probability curves and enegy diagram. MO theory of H_2 molecule. Calculation of energy. MO theory of polyatomic molecules (general ideas). MO treatment of H_2O. Symmetry-adapted linear combinations. MOs of H_2O.

Concept of hybridization – sp, sp^2, and sp^3 hybrid orbitals.

Semiempirical MO methods. The Huckel theory of conjugated systems. HMO calculations on ethylene, allyl system, butadiene, cyclopropenyl system and benzene. π–electron charges and bond orders. Simplification of secular determinants of cyclopropenyl system, cyclobutadiene and benzene using molecular symmetry. Introduction to Extended Huckle Theory, extension of the Huckle's approach to molecules containing heteroatoms.

Orbital symmetry and reactivity: $H_2 + F_2 \rightarrow 2HF$ reaction. $2NO \rightarrow N_2 + O_2$ reaction.

PO-12: Group theory (15 hrs)

Matrices: Addition and multiplication of matrices. Diagonal matrix. Unit matrix. Transpose of a matrix. Adjoint of a matrix. Inverse of a matrix. The determinant of a square matrix. Expansion of a determinant. Properties of determinants.

Symmetry operations forming a group. Classes of symmetry operations. Matrix representation of symmetry operations and point groups. Generation of representations for point groups. Reducible and irreducible representations.

The Great Orthogonality theorem (proof not required) and its consequences. Relation between reducible and irreducible representations. Character tables. Construction of character tables for C_{2h}, C_{2v} and C_{3v} groups.

Quantum mechanics and group theory: Wave functions as bases for irreducible representations. The direct product – vanishing of integrals. Projection operators. Symmetries of vibrations. IR and Raman activity.

Books suggested:

1. Quantum Chemistry, Ira N. Levine, Prentice Hall
2. Introduction to Quantum Chemistry, A. K. Chandra, Tata McGraw Hill
3. Elementary Quantum Chemistry, F. L. Pilar, McGraw Hill
4. Molecular Quantum Mechanics, P. W. Atkins & R. S. Friedman, Oxford Univ. Press
5. Coulson's Valence, R. McWeeny, ELBS
6. The Chemical Bond, J. N. Murrel, S. F. A. Kettle & J. M. Tedder, John Wiley
7. Valency Theory, J. N. Murrel, S. F. A. Kettle & J. M. Tedder, ELBS
8. Chemical Applications of Group Theory, F. A. Cotton, John Wiley & Sons
9. Symmetry and Group Theory In Chemistry, Mark Ladd, Harwood Publishers, London
10. Symmetry Through the Eyes of a Chemist, I. Hargittai and M. Hargittai, 2nd Edition, Plenum Press, NY (1995).
11. Molecular Symmetry and Group Theory, Robert L. Carter, John Wiley & Sons (1998).
12. Group Theory for Chemists, G. Davidson, Macmillan Physical Science Series (1991).

Paper II– CH (PO) 302T: Conformational Analysis, Asymmetric Synthesis, Synthetic Strategies and Advanced NMR spectroscopy

PO- 13: Conformational Analysis (Cyclic Systems) and ORD
PO- 14: Asymmetric synthesis
PO- 15: Synthetic Strategies
PO- 16: ^{13}C NMR and 2D NMR spectroscopy

PO-13: Conformational analysis (Cyclic systems) and ORD 15 Hrs

Conformational analysis (Cyclic systems)

Study of conformations of cyclohexane, mono, di and tri substituted cyclohexanes, (1,3,5-trimethyl cyclohexanes and Menthols), cyclohexanone (2-alkyl and 3 -alkyl ketone effect), 2-halocyclohexanones, cycloheptane . Stereo chemistry of bicycle [3,3,0] octanes,hydrindanes, decalins and perhydroanthracenes. Conformational structures of piperidine, N-Methylpiperidine, tropane, tropine, pseudotropine, decahydroquinolineand quinolizidine. Factors governing the reactivity of axial and equatorial substituents in cyclohexanes.
(oxidation, S_N2 reaction, rearrangements, Ester hydrolysis) Stereochemistry of addition to the carbonyl group of a rigid cyclohexanone ring.

Optical Rotatory Dispersion (ORD) and CD Spectroscopy: Optical rotation, circular birefringence, circular dichroism and Cotton effect. Plain curves and anomalous curves. Empirical and semiempiricalrules-The axial haloketone rule, the octant rule, Helicity rule. Application of the rules to the study of absolute configuration and conformations of organic molecules.

PO-14: Asymmetric synthesis 15 Hrs

Introduction: Brief revision of classification of stereo selective reactions
Prostereoisomerism: Topicity in molecules Homotopic, stereoheterotopic (enantiotopic and diastereotopic) groups and faces- symmetry criteria.
Prochiral nomenclature: Pro chirality and Pro-R, Pro-S, Re and Si.
Conditions forstereoselectivity: Symmetry and transition state criteria, kinetic and thermodynamic control. Methods of inducing enantioselectivity.
Analytical methods: % Enantiomeric excess and diastereomeric excess. Determination of enantiomeric excess: specific rotation, Chiral NMR; Chiralderivatizing agents, Chiral solvent, Chiral shift reagents and Chiral HPLC.
Chiral Substrate controlled asymmetric synthesis: Nucleophilic additions to chiral carbonyl compounds. 1, 2- asymmetric induction, Cram's rule and Felkin-Anh model.
Chiral auxiliary controlled asymmetric synthesis: α-Alkylation of chiral enolates, Evan's oxazolidinone, 1, 4-Asymmetric induction and Prelog's rule.
Chiral reagent controlled asymmetric synthesis: Asymmetric reductions using BINAL-H. Asymmetric hydroboration using IPC_2 BH and $IPCBH_2$.
Chiral catalyst controlled asymmetric synthesis: Sharplessepoxidation. Asymmetric hydrogenations using chiral Wilkinson biphosphincatalyst.
Asymmetric aldol reaction: Diastereoselective aldol reaction (achiral enolate and achiral aldehydes) its explanation by Zimmerman-Traxelmodel.

PO-15: Synthetic Strategies15 Hrs

Introduction: Terminology, Target, synthon, synthetic equivalent, functional group interconversion (FGI), functional group addition. Criteria for selection of target. Linear and convergent synthesis. Retrosynthetic analysis and synthesis involving chemoselectivity, regioselectivity, reversal of polarity and cyclizations.

Order of events : S-Salbutamol, Propoxycaine.

One group C-C and C-X disconnections: Introduction .One group C-C disconnections in alcohols and carbonyl compounds. One group C-X disconnections in Carbonyl compounds, alcohols, ethers and sulphides.

Two group C-C and C-X disconnections : Introduction .Two group C-X disconnections in 1,1-difunctionalised, 1,2-difunctionalised and 1,3-difunctionalised compounds.

Two group C-C disconnections: Diels-Alder reaction, 1,3-difunctionalised compounds, 1,5-difunctionalised compounds, Michael addition and Robinson annulation.

Control in carbonyl condensations: oxanamide and mevalonic acid.

Strategic bond: definition, guidelines for disconnection; disconnection of C-X bonds, disconnect to greatest simplification, using symmetry in disconnection, disconnection corresponding to known reliable reaction, high yielding steps and recognizable starting materials. Retrosynthesis of Retronecene, Longifoline.

PO-16: ^{13}C NMR and 2D NMR Spectroscopy15 Hrs

i)^{13}C NMR spectroscopy: Introduction**,** Types of ^{13}Cnmr spectra: undecoupled, proton-decoupled and off-resonance decoupled (ORD) spectra. ^{13}C chemical shifts, factors affecting the chemical shifts, chemical shifts of organic compounds. Calculation of chemical shifts of alkanes, alkenes and alkynes. Homonuclear (^{13}C, ^{13}C J) and heteronuclear (^{13}C, ^{1}H J and ^{13}C, ^{2}H J) coupling. Applications of ^{13}C-NMR spectroscopy: Structure determination, stereochemistry, reaction mechanisms and dynamic processes in organic molecules. ^{13}C-NMR spectral editing techniques: principle and applications of APT, INEPT and DEPT methods.

ii) 2D-NMR spectroscopy: Principles of 2D NMR, Classification of 2D-experiments. Correlation spectroscopy (COSY) HOMOCOSY (^{1}H-^{1}H COSY) , TOCSY (Total Correlation Spectroscopy), HeteroCOSY (^{1}H,^{13}C COSY,HMQC), long range ^{1}H,^{13}C COSY (HMBC),Homonuclear and Heteronuclear 2D-J-resolved spectroscopy, NOESY and 2D-INADEQUATE experiments and their applications.

Recommended Books:

1. Stereochemistry of organic compounds — Principles & Applications by D Nasipuri
2. Stereochemistry of Carbon compounds by Ernest L Eliel & Samuel H. wilen
3. Stereochemistry: Conformation & Mechanism by P S Kalsi
4. The third dimension in organic chemistry, by Alan Bassendale
5. Stereo selectivity in organic synthesis by R S Ward.
6.Advanced organic chemistry. Part A Structure & Mechanism by Francis A. Corey and Richard J. Sundberg
7. Asymmetric synthesis by Nogradi
8. Asymmetric organic reactions by J D Morrison and H S Moschcr
9. Principles in Asymmetric synthesis by Robert E. Gawley&Jeffreyaube

10. Stereo differentiating reactions by Izumi
11. Some modern methods of organic synthesis by W Carruthers
12. Guidebook to organic synthesis, by R K Meckie, D M Smith & R A Atken
13. Organic synthesis by Michael B Smith
14. Organic Synthesis-The disconnection approach by S Warren
15. Organic Synthesis by C Willis and M Willis
16. Problems on organic synthesis by Stuart Warren
17.Organic chemistry Jonathan Clayden, Nick Greeves and Stuart Warren
18. The logic of chemical synthesis by Elias James Corey and Xue-Min Cheng
19. Spectroscopic identification of organic compounds by RM Silverstein, G C Bassler and T B Morrill
20. Organic Spectroscopy by William Kemp
21. Spectroscopic methods in Organic chemistry by DH Williams and I Fleming
22. Modern NMR techniques for chemistry research by Andrew B Derome
23. NMR in chemistry - A multinuclear introduction by William Kemp.
24. Spectroscopic identification of organic compounds by P S Kalsi
25. Introduction to organic spectroscopy by Pavia
26. Carbon-13 NMR for organic chemists by GC Levy and O L Nelson
27. Nuclear Magnetic Resonance Basic principles by Atta-ur-Rahman
28. Basic one and two-dimensional NMR spectroscopy by Horst Friebolin
29. NMR spectroscopy by H.Gunther

ELECTIVE-3A

Paper-III-CH(PO) 301T(CB1): Spectroscopy, Electrochemistry and Statistical Thermodynamics

PO-(CB1)1: Physical principles of spectroscopy & Vibrational spectroscopy
PO-(CB1)2: X-Ray Spectroscopy & Diffraction techniques
PO-(CB1)3: Electrochemistry – II
PO-(CB1)4: Statistical Thermodynamics

PO-(CB1)1:<u>Physical principles of spectroscopy & Vibrational spectroscopy</u> **(**15 Hrs)

Interaction of electromagnetic radiation with matter. Absorption and emission of radiation. Induced absorption, spontaneous emission and stimulated emission. Oscillator strength, transition moment integral. Selection rules, Spectrum of formaldehyde. Factors affecting width and intensity of spectral lines -Line width and natural line broadening, doppler broadening. Intensity of spectral lines.

Infrared spectroscopy- Anharmonic oscillator. Morse potential energy diagram.
Vibration – rotation spectroscopy, P, Q, R branches. Vibration – rotation spectra of polyatomic molecules – linear, symmetric top and asymmetric top molecules. Principles of FTIR.

Raman spectroscopy- Classical and quantum theories of Raman effect. Pure rotational, vibrational and vibrational – rotational Raman spectra. Selection rules. Depolarization factors of Raman lines and their relevance. Instrumentation. Typical applications of Raman spectroscopy – Strucure determination of XY_4 molecules, Phase transitions.

PO-(CB1)2:X-ray Spectroscopy and Diffraction techniques: (15 hrs)

X-ray fluorescence (XRF) : Experimental method, Processes in X-ray fluorescence, K-emission spectrum of tin, L-emission spectrum of gold.

X-ray absorption: Absorption techniques, Absorption edge fine structure (AEFS spectra) and extended X-ray absorption fine structure (EXAFS) spectra.

X-ray diffraction: Bragg condition. Miller indices, d-spacing formula, Lattice planes and number of d-spacings, experimental methods of X-ray diffraction. Laue method and Debye-Scherrer method. Primitive and non-primitive unit cells. Indexing the reflections. Identification of unit cells from systematic absences in diffraction pattern. Structure factor and its relation to intensity and electron density. Description of the procedure for an X-ray structure analysis. Typical examples.

Electron diffraction. Scattering intensity versus scattering angle. Wierl equation. Measurement technique. Elucidation of structure of simple gas phase molecules.

PO-(CB1)3: Chemical Kinetics II (15 hrs)

Reactions in solution: Factors affecting reaction rates in solution. Effect of pressure on rate of reaction. Diffusion controlled reactions. Influence of dielectric constant and ionic strength on ion-ion, ion-dipole and dipole-dipole reactions. Primary and secondary salt effects. Kinetic isotope effects: Primary and secondary isotope effects. Solvent isotope effects.

Fast reactions: Flow methods and the stopped-flow technique. The fluorescence technique. Shock tube method. Relaxation methods (T-jump and P- jump). Kinetic equations for chemical relaxation.

Enzyme kinetics: Michaelis - Menten mechanisms of enzyme catalyzed reactions involving one and two intermediates. Steady-state approximation. Derivation of kinetic equations. Evaluation of kinetic parameters. Enzyme- substrate complex: Fischer's lock and key and Koshland's induced fit hypothesis. Specificity of enzyme-catalyzed reactions. Discussion of the various types of forces involved in the formation of E-S complex. pH dependence of enzyme-catalyzed reactions – the kinetics and the equations involved.

PO-(CB1)4: Statistical Thermodynamics (15 hrs)

Concepts of distribution and probability. Estimation of probability and the most probable distribution. Systems composed of noninteracting particles. Derivation of Boltzmann distribution law. The molecular partition function. Systems composed of interacting particles.

The concept of ensemble and canonical ensemble. Canonical partition function and its relation to molecular partition function. The factorization of molecular partition function – translational, rotational, vibrational and electronic partition functions. Derivation of expressions for translational, rotational (diatomic) and vibrational partition functions. Relationship between partition functions and thermodynamic functions. The relationship between partition functions and thermodynamic functions. Law of equipartition energy.

Specific heats of solids – Einstein equation of heat capacity of solids – derivation. Explanation of heat capacity at very low and very high temperatures – Dulong and Petits Law. Debye theory.

The entropy of a monoatomic ideal gas. The Sackur-Tetrode equation- derivation. Mean translational and vibrational energies.

The relation between equilibrium constant and partition function- derivation.

Basic ideas of Bose-Einstein statistics and Fermi-Dirac statistics and comparison of these with Maxwell-Boltzmann statistics.

Books suggested:

1. Modern Spectroscopy, J. M. Hollas, John Wiley & sons
2. Fundamentals of Molecular Spectroscopy, Banwell&McCash
3. Introduction to Molecular Spectroscopy, G. M. Barrow, McGraw Hill
4. Molecular Spectroscopy, J. D. Graybeal, McGraw Hill
5. Basic principles of Spectroscopy, R. Chang, McGraw Hill
6. Physical Methods for Chemistry, R. S. Drago, Affiliated East West Press
7. Vibrational Spectroscopy: Theory and Applications, D. N. Sathyanarayana, New Age International
8. Introduction to Raman Spectroscopy, J. R. Ferraro & K. Nakamoto, Academic Press
9. Molecular structure and Spectroscopy, G.Aruldas, Eastern Economic Edition
10. X-ray diffraction procedures for polycrysralline and amorphous materials, H. P. Klug & L. E. Alexander, John Wiley
11. Physical Chemistry, Ira N. Levine, McGraw Hill
12. Chemical Kinetics, K. J. Laidler, McGraw Hill
13. Kinetics and Mechanism, A. A. Frost & R. G. Pearson, John Wiley & sons
14. Kinetics and Mechanism of Chemical Transformations, J. Rajaraman& J. Kuriacose, McMillan
15. Chemical Kinetics and Reaction Mechanisms, J. H. Espenson, McGraw Hill
16. Physical Organic Chemistry, N. S. Isaacs, ELBS
17. The Physical basis of Organic Chemistry, Howard Maskill, Oxford University Press
18. Atkin's Physical Chemistry, P. Atkins & Julio de Paula, Oxford University Press
19. Elements of Statistical Thermodynamics, L. K. Nash, Addison – Wesley
20. Introduction to Statistical Thermodynamics, T. L. Hill, Addison Wiley
21. Statistical Thermodynamics, M. C. Gupta, New Age International
22. Atkin's Physical Chemistry, P. Atkins & Julio de Paula, Oxford University Press

ELECTIVE –3B

Paper III CH(PO) 303T(CB2) : Biopolymer Chemistry

PO(CB2)-5: Bioenergetics & physical properties of biopolymers
PO (CB2)-6: Biological membranes & binding of ligands by biopolymers
PO (CB2)-7: DNA, genes & cloning
PO (CB2)-8: Bioinformatics

PO(CB2)-5: Bioenergetics & physical properties of biopolymers (15 hrs)

Bioenergetics. The standard state in biological processes. ATP – the currency of energy. Gibbs energy change in ATP hydrolysis, comparison with other phosphates. Principles of coupled reactions. Glycolysis and coupled reactions involving ATP. Biological oxidation-reduction reactions – transfer of H^+ ions and electrons. Synthesis of ATP in the mitochondria. The chemiosmotic theory. Gibbs energy change accompanying the proton movement.

Molecular weights of biopolymers. Viscometry,Use of viscometry in the study of ligand binding to DNA. Separation/molecular weight studies of biopolymers.Sedimentation: Sedimentation velocity.

Sedimentation coefficient. The Sverdberg equation. Sedimentation equilibrium analysis. Ultra centrifugation Molecular weights. Light scattering method.
Electrophoresis – principle involved. Gel electrophoresis. Electrophoretic mobility. Applications.

PO(CB2)-6: Biological membranes & binding of ligands by biopolymers (15 hrs)

Structure and function of cell membrane. Membrane equilibria and thermodynamics of membrane equilibria. Dialysis equilibrium. Osmotic pressure. Membrane potentials. Transport across membranes. Passive transport, facilitated transport and active transport

Sodium-potassium pump. Selective ion transport and membrane potential. The Goldman equation (derivation not required). Nerve cells. The transfer of information in the body. The action potential and the mechanism of action potential propagation. Signal transducing mechanism involving gated ion channels in the plasma membrane.

Binding of ligands and metal ions to macromolecules – one and n-euqivalent binding sites per molecule.Allosteric interactions – Oxygen binding to myoglobin and hemoglobin – Cooperative and non-cooperative binding. Hill equation and Hill plots. Transport of H^+ and CO_2 .Bohr effect.

PO(CB2)-7: DNA, Genes & Cloning (15 hrs)

Watson –Crick model of DNA. Types of DNA chains – linear, circular and supercoiled DNA. Types of RNA. Secondary structure of t-RNA.

Genes and genome: Gene expression. Transcription and translation (general principles only). Codons and the genetic code.

Sequence analysis of DNA by the Sanger chain-termination method.

Introduction to biotechnology and recombinant DNA technology. Molecular cloning. Restriction endonucleases and cloning vectors. Steps involved in the construction of recombinant DNA. DNA hybridization and hybridization probes.

Satellite DNAs – micro and mini satellites. Sequence polymorphisms – RFLPs. Principles of DNA finger printing technology.

PO(CB2)-8: Bioinformatics (15 hrs)

Introduction: Use of informatics and computers in biology. Homology as descendants of common ancestors, statistical analysis of sequence alignment.

General purpose Databases for Comparative Genomics: COGs, KEGG, MDGB -

Organism Specific Databases examples - E. Coli, Yeast, Oryza.

Introduction to Proteins - primary, secondary, tertiary and quaternary structures. Structure databases – PDB, MMDB, CSD. Homology modeling – Flow chart, structure refinement - Ramachandra Plot.

Books suggested:

1. Biophysical Chemistry, Cantor &Schimmel, W. H. Freeman and Company

2. Principles of Physical Biochemistry, Kensal E van Holde, W. Curtis Johnson & P. Shing Ho, Prentice Hall
3. Physical Biochemistry : Principles and Applications, David Sheehan, John Wiley
4. Physical Chemistry for the Chemical and Biological Sciences, Raymond Chang, University Science Books
5. Lehninger Principles of Biochemistry, D. L. Nelson & M. M. Cox, MacMillan
6. Biochemistry, L. Stryer, W. H. Freeman and Company
7. Concepts in Biochemistry, Rodney Boyer, Books/Cole Publishing Company
8. Modern Electrochemistry 2B, Bockris& Reddy, Kluwer Academic/ Plenum
9. Introduction to Bioinformatics by Arthur Lesk, Oxford University Press, Inc, New York
10. Bioinformatics , A practical guide to the Genes and Proteins. Edited by Andreas. D. Baxevanis and B. F. Francis Wiley Publishers

ELECTIVE –4A

Paper IV– CH (PO) 304T(CB3): Modern Organic Synthesis
PO-(CB3)-09: Synthetic Reagents I
PO-(CB3)-10: Synthetic Reagents II
PO-(CB3)-11: New Synthetic reactions
PO-(CB3)-12: New techniques and concepts in organic synthesis

PO-(CB3)-09: Synthetic Reagents I15 Hrs
i) Protecting groups: a) Protection of alcohols by ether, silyl ether and ester formation b) Protection of 1,2-diols by acetal, ketal and carbonate formation c) Protection of amines by benzyloxycarbonyl, t-butyloxycarbonyl, fmoc and triphenyl methyl groups. d) Protection of carbonyls by acetal, ketal and thiol acetal (Umpolung) groups. e) Protection of carboxylic acids by ester and ortho ester (OBO) formation.
ii) Organometallic Reagents: Preparation and application of the following in organic synthesis: 1) Organo lithium 2) Organo copper reagents 3) Organo boranes in C-C bond formation 4) Organo silicon reagents: reactions involving β-carbocations and α-carbanions, utility of trimethyl silyl halides, cyanides and triflates.
iii) Carbonyl methylenation: a) Phosphorous ylide mediated olefination 1) Witting reaction, 2) Horner-Wordsworth-Emmons reaction.b) Titanium- Carbene mediated olefination 1) Tebbe reagent, 2) Petasis reagent 3) Nysted reagent.
iv) Carbene insertions: Rh based carbene complexes, cyclopropanations.
v) C-H Activation: Introduction, Rh catalyzed C-H activation.

PO-(CB3)-10: Synthetic Reagents II15 Hrs

i)Oxidations: a) Oxidation of active C-H functions: DDQ and SeO_2. b) Alkenes to diols: Prevost and Woodward oxidation c) Alcohol to carbonyls: Cr^{VI} oxidants (Jones reagent, PCC, PDC) IBX, DMP, CAN, TEMPO, TPAP, Swern oxidation d) Oxidative cleavage of 1,2-diols: Periodic acid and Lead tetra acetate.

ii) Reductions: a) Catalytic hydrogenation: Homogenous (Wilkinsons's catalytic hydrogenation) and heterogeneous catalytic reduction. b) Non-metallic reductions: Diimide reduction c) Dissolving metal reductions: Birch reduction. d) Nucleophilic metal hydrides: $LiAlH_4$, $NaBH_4$, and

their modifications. e) Electrophilic metal hydrides: BH_3, AlH_3 and DIBAL. f) Use of tri-n-butyl tin hydride: Radical reductions.

PO-(CB3)-11: New Synthetic reactions 15 Hrs

1. Metal mediated C-C and C-X coupling reactions: Suzuki, Heck, Stille,Sonogishira cross coupling, Buchwald-Hartwig and Negishi-Kumada coupling reactions.

2. C=C Formation Reactions: Shapiro, Bamford-Stevens, McMurreyreactions, Julia-Lythgoeolefination and Peterson's stereoselective olefination.

3. Multicomponent Reactions: Ugi, Passerini, Biginelli, Bergman and Mannichreactions.

4. Ring Formation Reactions: Pausan-Khand reaction, Nazerov cyclisation.

5. Click Chemistry: Click reaction, 1,3-dipolar cycloadditions.

6.Metathesis: Grubb's 1st and 2nd generation catalyst, Olefin cross coupling metathesis (OCM), ring closing metathesis(RCM), ring opening metathesis(ROM), applications.

7. Other important synthetic reactions: Baylis-Hilman reaction,Eschenmoser-Tanabe fragmentation,Mitsunobu reaction,Stork-enamine reaction and Michael reactions.

PO-(CB3)-12: New techniques and concepts in organic synthesis15 Hrs

1. Techniques in peptide synthesis: Solid phase peptide synthesis, commonly used resins (Rink resin, Wang resin and Ellman resin, synthesis of cross linked Merrifield resin and drawbacks of solid phase synthesis.

2. Solid phase oligodeoxynucleotide synthesis: Phosphotriester, phosphitetriester and phosphoramidite pathway

3. Oligosaccharide synthesis: Glycosidation**:**cylicoxocarbenium ion, glycosyl donors and glycosyl acceptors, Kahneglycosidation, convergent and linear oligosaccharide synthesis.

4. Phase Transfer catalysis: Onium and crwon ethers as PTC.

5. Tandem synthesis: Tandem reactions; conjugate addition-aldol reaction, polymerization-cyclisation, elctrocylic-Diels Alder reaction.

6. Baldwin Rules: Exo and Endo cyclisation, tetrahedral, trigonal and diagonal systems, favoured and disfavouredcyclisations.

7.Chiron approach in organic synthesis: Nature's chiral pool, carbohydrates, amino acids, hydroxy acids, terpenes as chiral precursors. Synthesis of shikimic acid from D-arabinose, furanonycin from D-glucose, S-(-)-ipsenol from S-leucine.

8. Determination of absolute configuration: Mosher's method.

Recommended Books:

1. Some modern methods of organic synthesis by W. Carruthers.
2. Guidebook to organic synthesis, by R K Meckie, D M Smith & R A Atken.
3. Organic Synthesis by O House.
4. Organic synthesis by Micheal B Smith.
5. Reagents for organic synthesis, by Fieser&Fieser, Vol 1-11 (1984).
6. Organic synthesis by Robert E Ireland.
7. Organic Synthesis-The disconnection approach by S Warren.
8. Organic Synthesis by C Willis and M Willis.
9. Handbooks of reagents for organic synthesis by Reich and Rigby, Vol-I-IV.
10. Problems on organic synthesis by Stuart Warren.
11. Total synthesis of natural products: the Chiron approach by S. Hanesian.
12. Organic chemistry by Jonathan Clayden, Nick Greeves and Stuart Warren

13. Organic Reactions and their mechanisms by P.S.Kalsi
14. Organic reaction mechanisms by V.K.Ahulwalia and Rakesh Kumar Parashar

ELECTIVE –4B

Paper-IV CH(PO)304T(CB4): ORGANIC MATERIALS, DYES AND PIGMENTS

PO (CB4)-13: Organic Nanomaterials
PO (CB4)-14: Supramolecular Chemistry
PO (CB4)-15: Dyes – I
PO (CB4)-16: Dyes–II and Pigments

PO (CB4)-13: Organic Nanomaterials 15Hrs

Introduction: The 'top-down' approach, the 'bottom-up' approach and Nanomanipulation.
Molecular Devices: Photochemical devices, Liquid crystals, Molecular wires, Rectifiers, Molecular switches and Molecular Muscles.
New Carbon family: Types of Fullerenes, Types of Carbon nanotubes (Zig-Zag, Armchair and Chiral), Graphenes. Growth, Chemical Synthesis and optoelectronic properties of Fullerenes, CNTs (Zig Zag, Armchair and Chiral), singlewalled CNTs (SWCNTs) and multi walled MWCNTs)and Graphenes.
Structures of aromatics belts, nano car and molecular machines.
Optoelectronic molecules: OLEDs, Organic Solar Cells (Basic OLED mechanism and structures) Natural Benz heterazoles and their synthetic modifications as optoelectronic molecules.

PO (CB4)-14: Supramolecular Chemistry 15Hrs

I**ntroduction**: Supramolecular interactions (ion-ion, ion-dipole, H-bonding, cation-π, anion-π, π-π and Van der Walls interactions),Ionophore and molecular receptors.
Host-Guest Chemistry: Lock and key anology, Structures and applications of Cryptands,Spherands, Calixerenes, Cyclodextrins, Cyclophanes, Carcerands and hemicarcirands.
Self-assembly: Ladder, polygons, helices, rotaxanes, catanenes, Molecular necklace, dendrimers, self-assembly capsules their synthesis, properties and applications.
Enantioselective molecular recognition: Cyclodextrins, Crown ethers with chiral frame work, Chiral receptor from Kemp's triacid. Chiral receptors for tartaric acid.

PO (CB4)-15: Dyes – I15 Hrs

Synthetic and Natural dyes: Introduction, nomenclature and classification of synthetic dyes. Color and constitution - chromospheres and auxochromes with suitable examples, Witt's theory, Armstrong's theory, Baeyer's theory, Nietzki's theory, Waston's theory, Modern theories, Valence Bond Theory and Molecular orbital theory. Chemistry and synthesis of triphenyl methane dyes malachite green, rosaniline, para aniline blue, crystal violet methyl violet, hydroxytriphenyl methane dyes, Aurin, chrome violet], Azo dyes - types of azo dyes, synthesis of acidic and basic azo dyes, mono azo, di azo, tri azo and poly azo dyes. Chemistry and synthesis of cyanine dyes. Natural dyes – structure determination and synthesis of alizarine, Quinazarin and Indigo.

PO (CB4)-16: Dyes–II and Pigments 15 Hrs

a)**Introduction to Fluorescence dyes:** Interaction of organic molecules with electromagnetic radiation. Energy diagram. Activation and deactivation of organic molecules by light. Fluorescence and delayed fluorescence. Effect of molecular structure on fluorescence. General properties of fluorescent dyes and their requirements. Triplet-triplet absorption of organic molecules. Fluorescent quantum yields and factors affecting them. Synthesis of Fluorescent aromatic hydrocarbons. and Fluorescent heteroaromatic compounds.

b)**Introduction to laser dyes**. Synthesis of Oligophenylenes. Oxazoles and benzoxzoles. Stilbenoid compoundsCoumarin laser dyes, Rhodamine laser dyes.

c) **Pigments:** Introduction, Structures of Porphyrins , Bile pigments. Synthesis of Haemin and Chlorophyll. Synthetic pigments – preparation of phthalocyanines.

Recommended Books

1. Core Concepts in Supramolecular Chemistry and Nanochemistry by Jonathan W. Steed, David R. Turner and Karl J. Wallace; John-Wiley and Sons Publications
2. Supramolecular Chemistry by Jonathan W. Steed and Jerry L. Atwood, John-Wiley and Sons Publications
3. Supramolecular Chemistry-Concepts and Perspectives by J M. Lehn; Wiley-VCH (1995) Publications
4. Supramolecular Chemistry by P. D. Beer, P. A. Gale and D. K. Smith; Oxford University Press (1999)
5. Stereochemistry of organic compounds - Principles & Applications by D Nasipuri
6. Nanochemistry by G.B. Sergeev; Elsevier
7. Nanochemistry: A chemical approach to nano materials , G.A. Ozin& A.C. Arsenault; RSC publishers.
8. Organic Chemistry , Vol.1,2 by I.L.Finar
9. Color and constitution of organic molecules by J.Griffiths
10. Functional Dyes, Elsevier BV 2006, S H.KIM
11. Colorants for non-textile Applications, Elsevier BV 2000, H. S Freeman and A T Peters
12. Industrial Dyes-Chemistry, Properties, Applications. WILEY-VCH Verlag, 2003 Klaus Hunger
13. Introduction to Fluorescence Sensing, Springer 2009, by A P Demchenko
14. Natural Dyes and their Applications in Textiles by M. L. Gulrajani, IIT Delhi
15. Handbook on Natural Dyes for Industrial Applications by P. S. Vankar, National Institute of Industrial Research
16. Chemistry and Biochemistry of plant pigments, Vol. 2, by T.W.Goodwin
17. Contemporary Polymer Chemistry, H. R. Alcock& F. W. Lambe, Prentice Hall
18. Materials scince and engineering an introduction by William D Callister, Jr. Wiley Publishers

SEMESTER III LABORATORY COURSES

PAPER V (Lab)-CH(PO) 351P: Chemical Kinetics

1. Study of peroxydisulphate-iodide reactions;
   - Individual orders of the reactants by isolation and initial rate methods
   - Effect of temperature on reaction rate
   - Effect of ionic strength on reaction rate
   - clock reaction

2.Study of saponification of ethyl acetate by conductometry:
a). Overall order of the reaction b). Order w. r. to ethylacetate c).Order w.r. to NaOH

3.Study of acetone-iodine reaction by colorimetry/spectrophotometry
a).Order w.r.t. iodine b).Order w.r.t. acetone c). Order w.r.t. [H+]

4.Study of oxidation of primary alcohols using dichromate by spectrophotometry:
Application of Taft equation.

5.Study of solvolysis of t-butylchloride by conductometry: effect of solvent dielectric constant/polarizability (methanol/water mixture)on the rate of solvolysis.

Note: The Data obtained in all the experiments are to be analysed by the students both by the usual graphical methods and by regression (linear/nonlinear) techniques using a PC.

Suggested books:

1. A textbook of practical organic chemistry by A I Vogel, Vol 1&2.
2. Senior practical physical chemistry. B. D. Khosla, V.C. Garg, Adarsh Gulati
3. Experimental Physical Chemistry: V. Athawale and P. Mathur.
4. Practical Physical Chemistry: B. Vishwanathan and P.S. Raghavan.
5. Practical in Physical Chemistry: P.S. Sindhu
6. Advanced Practical Physical chemistry: J.B.Yadav

PAPERVI -CH(PO)352P: Synthesis of Organic compounds and Chromatography

1. Laboratory synthesis of the following compounds: 2-Phenyl indole (Fischer- Indole synthesis), 2,5-Dihydroxy acetophenone (Fries reaction), 7-hydroxy coumarin (Pechmann synthesis), Photo-dimerization of maleic anhydride, Benzanilide (Beckmann rearrangement), Benzilic acid from benzoin (rearrangement), Vanillylalchohol from vanillin (NaBH4 reduction), 4-Nitoacetanilide from acetanilide , Benzimidazoles and Benzimidazolines by reaction of o-phenylenediamine with aromatic aldehydes and carboxylic acids.

2.Thin layer chromatography :Thin layer chromatography: Determination of purity(All the above preparations) , monitoring the progress of chemical reactions (any of the four above preparations), identification of unknown organic compounds by comparing the Rf values of known standards.

3.Separation/Purification by column chromatography: Separation of a mixture of ortho and para-nitroanilines using silicagel as adsorbant and chloroform as the eluent. The column chromatography should be monitored by TLC. Purification of commercial sample of anthracene by column chromatography (using silica gel as adsorbant and n-hexane as eluent).

Suggested books:

1.A textbook of pracical organic chemistry by A I Vogel, Vol 1&2.
2.Unitized experiments in organic chemistry by R Q Brewster and others.
3.Handbook of organic analysis by H T C Clarke.
4.Practical Organic Chemistry by Mann and Saunders.

M.Sc. PHYSICAL ORGANIC CHEMISTRY SPECIALIZATION
IV SEMESTER SYLLABUS
(For the batch admitted during the academic year 2017 onwards under the CBCS pattern)
[Under Restructured CBCS Scheme]

PAPER-1 CH(PO) 401T:Non-equilibrium thermodynamics, NMR,NQR and Mossabaur Spectroscopy, Electrochemistry & Lasers

PO-17: Non-equilibrium Thermodynamics
PO-18: NMR , NQR and Mossbaur Spectroscopy
PO-19: Electrochemistry II
PO-20: Lasers in Chemistry

PC-17 Non-equilibrium Thermodynamics (15hrs)

Thermodynamic criteria for non-equilibrium states. Entropy production in irreversible processes. Entropy production in heat flow and entropy production in material flow.
Fluxes and forces. Linear flux-force relations. Phenomenonological equationsand coefficients. Microscopic reversibility. Onsager reciprocal relations. Application of Onsager relations to electrokinetic phenomena – electroosmotic pressure and streaming current. The Onsager relations and the principle of detailed balance. Liquid junction potentials – derivation of equation for liquid junction potential in terms of transport numbers using Onsager relations.
Steady states. Principle of minimum entropy production. Irreversible thermodynamics as applied to biological systems - examples.
Application to thermoelectric circuits. Seebeck and Peltier effect.

PC-18: NMR, NQR and MossbaurSpecroscopy. (15hrs)

Prnciple of nmr. Derivation of $h\ v = g\ \beta\ H$.Larmorprecessional frequency- spin-spin splitting (AX) - Qantitative treatment (proof for J= distance between two successive nmr spectral lines) – Instrumentation - CW instrument and FT instrument.

Two dimensional nmr spectroscopy: Principles of 2D nmr-Graphical representation of 2D nmrspecra – Homonuclear ^{1}H J, δ spectroscopy-its application for mixture analysis- (for instance mixture analysis of n-butyl bromide and n-butyl iodide) - The COSY experiment. Two dimensional ^{1}H, ^{1}H shift correlations. COSY spectra of an AX system, o-nitroaniline, alanine, glutamic acid and arginine.

The nuclear overhauser effect(NOE). wo dimensional nuclear overhauser spectroscopy(NOESY). Nuclear Quadrupole Resonance: Quadrupole nuclei and quadrupole moments-prolate and oblate nuclear charge distributions-energies of quadrupolar transitions-electric field gradient, coupling constants and splitting.

Mossbauer Spectroscopy - Mossbauer effect – Recoil energy, typical Mossbauer spectrum - isomer shift – quadrupole splitting – magnetic hyperfine interaction – ^{57}Fe – Mossbauer spectra of Fe^{2+} and Fe^{3+} (paramagnetic) and Fe^{3+} (magnetic) compounds.

PC –19: Electrochemistry – II (15 hrs)

The electrode-electrolyte interface: The electrical double layer. TheHelmholtz-Perrin parallel-plate model, the Gouy-Chapman diffuse-charge model and the Stern model. Quantum aspects of charge transfer at the interfaces. Tunneling.

Electrodics: Charge transfer reactions at the electrode-electrolyte interface. Exchange current density and overpotential. Derivation of Butler-Volmer equation. High field approximation. Tafel equation - low field - equilibrium, Nernst equation. The symmetry factor and its significance.

Corrosion: Electrochemical corrosion.Short-circuited energy producing cell. The definition and final expression of corrosion current and corrosion potential. Homogeneous theory of corrosion.Evans diagrams. Potential-pH (Pourbaix) diagrams of iron. Methods of corrosion rate measurement. Mechanism of anodic dissolution of iron. Protection against corrosion. Corrosion inhibition by organic molecules.

PC 20: Lasers in Chemistry: (15 hrs)

General principles of laser action. Stimulated emission. Rates of absorption and emission. Population inversion. Three-level and four-level laser systems. Pumping. Laser cavity – resonant modes. Characteristics of laser light. Laser pulses and their characteristics. Pulse production, Q-switching. Pulse modification, mode-locking.

Practical lasers. Solid-state lasers, gas lasers, chemical and excimer lasers. Examples.

Applications of lasers in chemistry: Femtochemistry. The pump-probe technique. Time-resolved spectroscopy. Photodissociation of ICN. Formation and dissociation of CO-hemoglobin complex. Conversion of ethylene to cyclobutane. Bond selectivity in chemical reactions – the reaction between hydrogen atoms and vibrationally excited HDO molecules.

Lasers and multiphoton spectroscopy – underlying principles. Two-photon spectra of diphenyloctatetraene. Lasers in fluorescence spectroscopy and Raman spectroscopy.

Books suggested:

1. Atkin's Physical Chemistry, P. Atkins & Julio de Paula, Oxford University Press
2. Molecular Thermodynamics, D. A. McQuarrie & J. D. Simon, University Science Books
3. Physical Chemistry: A molecular approach, McQuarie Simon, Viva Books Pvt. Ltd.
4. Text book of Biochemistry by Stryer.
5. Advanced physical chemistry by Gurtu and Gurtu.
6. Physical chemistry by Puri and Sharma.
7. NMR Spectroscopy: Basic principles, concepts and applications in chemistry, H. Gunther, John Wiley & sons
8. Introduction to Magnetic Resonance, A. Carrington & A.D. Maclachalan, Harper & Row
9. NMR, NQR, EPR and Mossbauer Spectroscopy in Inorganic Chemistry, R. V. Parish, Ellis Harwood
10. NMR basic principles - Atta-ur-Rahman, Springer publisher

11. Two dimensional NMR Spectroscopy-Applications for chemists and biochemists, edited by W. R. Croasmun& R. M. K. Carlson, VCH
12. Physical chemistry by Puri and Sharma.
13. Modern Electrochemistry 2B, Bockris& Reddy, Plenum.
14. Introduction to Electrochemistry, S. Glasstone.
15. Modern Electrochemistry, J. O. M. Bockris& A. K. N. Reddy, Plenum.
16. Introduction to Electrochemistry, S. Glasstone.
17. A Guide to Lasers in Chemistry, G. R. Van Hecke& K. K. Karukstis, Jones and Bartlett Publishers
18. Lasers in Chemical and Biological Sciences, S. Chopra & H. M. Chawla, Wiley Eastern Ltd

Paper-II CH(PO) 402T: Medicinal Chemistry and Biomolecules

PO-21: Principles of Drug design and drug discovery
PO-22: Lead modification and SAR Studies
PO-23: QSAR studies
PO-24: Biomolecules

PO-21: Principles of Drug design and drug discovery 15Hrs

Introduction to drug discovery. Folklore drugs, stages involved in drug discovery- disease, drug targets, bioassay. Discovery of a lead- screening of natural products and synthetic compound libraries. Existing drugs as leads (me too drugs). Pharmacokinetics (ADME), pharmacodynamics. Nature of drug – receptor interactions and their theories – Occupancy theory, Induced – fit theory, Macromolecular purturbation theory and Two-state model of receptor activation. Natural products as lead structures in drug discovery – Pharmacophore - structure pruning technique e.g. morphine.Discovery of lead structure from natural hormones and neurotransmitters.Principles of design of agonists (e.g.Salbutamol), antagonists e.g. cimitidine) and enzyme inhibitors (e.g. captopril). Drug discovery without lead – serendipity- Penicillin and Librium as examples. Principles of prodrug design. Introduction to drug patents and Clinical trials.

PO-22: Lead modification and SAR Studies 15 Hrs

SAR*:* Lead modification strategies, Bioisosterism, variation of alkyl substituents,chain homologation and branching, variation of aromatic substituents,extension of structure, ring expansion and ring contraction, ring variation, variation and position of hetero atoms, ring fusion, simplification of the lead, rigidification of lead.Discovery of oxaminquine, salbutamol, cimitidine and captopril Structure-Activity Relationship studies in sulfa drugs,benzodiazepines, and taxol analogs. Introduction of combinatorial chemistry, a brief outline of methods of parallel and mixed combinatorial synthesis.

PO-23: QSAR studies and computer aided drug design 15Hrs

QSAR: Introduction, physicochemical properties - pKa, electronic effects and Hammett constants(σ), lipophilicity constant(π), steric effects and Taft's constant, linear and nonlinear relationship between biological activityLipophilicity Substituent constants. Lipinski rule of five.

Hansch analysis, Craig's plot,Topliss scheme, Free Wilson approach, cluster significant analysis. Two case studies (QSAR study on pyranenamine, design of Crizotinib).

Computer aided drug design: Introduction, active site, allosteric binding site,use of grids in docking program - rigid docking, flexible docking of ligands. Basic principles and difference between structure and ligand based drug design, denovo drug design and utility to optimize the lead structure.

PO-24: Biomolecules **15 Hrs**

1. Enzymes: Definition. Classification based on mode of action. Mechanism of enzyme catalysis. Lock and Key model and Induced- Fit model. Enantiomer discrimination by Three-point Contact model. Factors affecting enzyme catalysis.Enzyme inhibition- reversible and irreversible inhibition. Enzymes in organic synthesis. Immobilised enzymes.

2. Nucleic acids: Primary, secondary and tertiary structure of DNA. Types of mRNA,tRNA and rRNA. Replication, transcription and translation. Genetic code. Protein biosynthesis. Chemical Synthesis of nucleosides and nucleotides.

3. Lipids: Lipid structure- acylglycerols, phosphoglyceridesand sphingolipids. Biosynthesis and chemical Synthesis of lipids.

Recommended books

1. Burger's medicinal chemistry and drug discovery by Manfred E. Wolf.
2. Introduction to Medicinal chemistry by Patrick.
3. Introduction to drug design by R Silverman
4. Comprehensive medicinal chemistry. Vol 1-5 by Hanzsch.
5. Principles of medicinal chemistry. by William Foye
6. Biochemical approach to medicinal chemistry. by Thomas Nogrady.
7. Pharmaceutical Chemistry and Drug synthesis by Roth and Kleeman
8. Drug design by E.J.Arienes
9. Principles of Medicinal Chemistty Vol I & II by Kadam et al
10. Medicinal chemistry An introduction by Garreth Thomas
11.Organic and Pharmaceutical chemistry By Delgrado
12. Organic Pharmaceutical chemistry By Harikishansingh
13. Medicinal Chemistry By Ashtoshkar
14. Medicinal Chemistry By Chatwal
15. Organic Drug synthesis By Ledneicer Vol 1-6
16.Strategies for organic drug synthesis and design By Daniel Ledneicer.
17.Top Drugs: Top synthetic routes By John Saunders
I8.Chirotechnoiogy By Roger A. Sheldon
19. Burger's Medicinal Chemistry and Drug Discovery: Principles and Practices. Vol. 1.
20. Medicinal Chemistry by G. Patricks.
21. Text book of Drug Design and Discovery, Edited by PovlKrogsgaard – Larsen Tommy Liljefors.
22. Structure Based Drug Design of Crizotinib (PF-02341066), a Potent and Selective Dual Inhibitor of Mesenchymal–Epithelial Transition Factor (c-MET) Kinase and Anaplastic Lymphoma Kinase (ALK) Martin P. Edwards, J. Med. Chem., 2011, 54 (18), pp 6342–6363. http://www.pfizer.com/news/featured_stories/featured_stories_martin_edwards.jsp

23. Enzyme structure and mechanism by Fersht and Freeman
24.Bio-Organic chemistry by HennanDugas
25.Nucleic acids in Chemistry and Biology by G M Blackbum MI Gait
26. LehningerPrinciples of Biochemistry by D L Nelson and M M Cox
27. Outlines of Biochemistry by ConnandStumpf
28. Biotransformations in Organic Chemistry by K Faber.

ELECTIVE –3A

PAPER III CH(P)- 403T(CB1): CATALYSIS

PC(CB1)-17: Homogeneous catalysis
PC(CB1)-18: Surface Chemistry & Micellar catalysis
PC(CB1)-19: Heterogeneous catalysis
PC(CB1)-20: Phase transfer , Anchored & Photo catalysis

PC(CB1)-17: Homogeneous catalysis. (15 hrs)

Introduction to catalysis. Types of catalysis, characteristics of catalyst, catalyst supports, promoters, general mechanism of catalysis, equilibrium treatment and steady state treatment. Activation energies of catalyzed reactions.

Acid-base catalysis, specific acid-base catalysis, general acid base catalysis, mechanism of acid – base catalysis, catalytic activity and acid-base strength- Bronsted relationships.
Acidity functions: Types of acidity functions. Hammett acidity function. Measurement of Hammett acidity function(Ho), usefulness of Hammett acidity function in understanding the mechanism of an acid catalyzed reactions. Zucker-Hammett hypothesis and its applications. Bunnett – Olson's criteria of acid-base catalyzed reactions with examples.

Catalysis by transition metal ions and their complexes. Use of Ziegler –Natta and metallocene catalysts as homogeneous catalysts for polymerization of olefins. Application of metal ion catalysis to the hydrogenation of alkenes, hydroformylation, oxidation and isomerization reactions. Asymmetric Catalysis–Introduction, Catalysts, Commercial Applications, Asymmetric Hydrogenation, Enantioselective Isomerization: L-Menthol, Asymmetric Epoxidation.

PC(CB1)-18: Surface Chemistry & Micellar catalysis (15hrs)

Surface tension. Curved interfaces. The Laplace equation. Capillary action. Thermodynamics of surface layers – Gibbs isotherm.

Adsorption. Types of adsorption, factors effecting adsorption, Chemistry and thermodynamics of adsorption. Determination of heats and entropies of adsorption.

Surface versus bulk structures. Adsorbate -induced restructuring of surfaces. Thermal activation of bond breaking on a surface. Co-adsorption. Chemisorption isotherms. Kinetics of chemisorption.

Surface films. Monometallic surfaces and bimetallic surfaces. Experimental techniques for the study of monolayer films. States and reaction in monomolecular films. Reaction between $H_2(g)$ and $N_2(g)$ catalyzed by surfaces to give $NH_3(g)$.

Micelles: Classification of surface active agents. Micellization and micellar interactions. Structure of micelles – spherical and laminar. Critical micellar concentration (CMC). Factors affecting the CMC of surfactants.

Counter ion binding to micelles. Thermodynamics of micellization. Phase separation and mass action models, solubilization, micro emulsion, reverse micelles. Reactions assisted by micelle formation. Examples of micelle-catalyzed reactions and their mechanisms.

PC(CB1)-19: Heterogeneous catalysis (15 hrs)

Heterogeneous catalysis. Broad categories of catalysts – metals, bimetals, semiconductors, insulators, zeolites, oxides, nano materials.

Preparation of metal catalysts, supported metal catalysts and non- metallic catalysts. Co-precipitation, Impregnation, sol-gel method, deposition-precipitation, hydrothermal synthesis, pulsed laser methods, plasma chemical methods, chemical vapor deposition methods

Steps in heterogeneous catalyzed reactions. Diffusion and adsorption. Mechanism of surface-catalyzed reactions. Adsorption isotherms - Langmiur Hinshelwood model, Rideal - Eley mechanism, Kinetics and thermodynamics of catalysed reactions. Catalytic activity – the determining factors. Structure sensitive and structure insensitive catalysts.

Characterization of catalysts: Surface area by BET method. Determination of pore volume and pore size distribution by BJH method. Pore size and specificity of catalysts. Surface acidity of catalysts- Determination of surface acidity by indicator method, IR spectroscopic method and TPD methods. Surface characterization by XRD, LEED, TEM& AFM, XPS, AES, techniques.

Auto exhaust emissions- catalytic converters. Catalytic hydrogenation and oxidation reactions.

Cracking and reforming. Fischer-Tropsch synthesis of methanol.

PC(CB1)-20: Phase transfer, Anchored & Photo catalysis **(**15 hrs)

Phase-transfer catalysis (PTC): Principles of phase-transfer catalysis. PTC classification.
Role of water in phase-transfer catalyzed reactions. Factors influencing the rate of PTC reactions.

Inverse phase transfer catalysis. Mechanism of nucleophilic displacement reactions.

Crown ethers: Crown ethers as phase transfer catalysts(PTC) in the reaction of alkyl halides with super oxide. Permanganate oxidation of alkenes and phenols in presence of PTC's viz., quarternary ammonium salts and crown ethers.

Anchored catalysis: Definition and examples of anchored catalysis- organic polymers, inorganic oxides and clays as supports. Structure of montmorillonite anchored catalysts- HEW structure and EF structure. Montmorillonite anchored catalysts- application of intercalated clay catalysts in hydrogenation reactions.

Photo catalysis: Photocatalytic effect, metal semiconductor systems as photo catalysts, nature of the metal loaded, extent of metal loading, nature of semiconductor, doped semiconductors, coupled Semiconductors. Application of photocatalysis for splitting of water by semiconductor particles, removal of organic and inorganic pollutants, for oxidation and reduction of organic compounds.

Books suggested:

1. Principles of Heterogeneous Catalysis in practice, G. C. Bond, Oxford Publishing
2. Heterogeneous Catalysis, C. Satterfield, McGraw Hill
3. Catalysis, Principles and applications, edited by B. Vishwanathan, S. Sivasanker& A. V. Rama Swamy, Narosa Publishing House
4. Catalysis, J. C. Kuriacose, Macmillan
5. Colloidal and surface chemistry , M. Satake, Y. Hayashi, Y.Mido, S.A.Iqbal and M.S.sethi, Discovery Publishing house.
6. " Physical Organic Chemistry" by L.P.Hammett, chapter 9 , McGraw Hill .
7. Chemical Review, **57,** 1935(1957), M.A. Paul and F.A. Long
8. Phase Transfer Catalysis, Fundamentals, Applications and Industrial perspective, C. M. Stark, C. Liotta & M. Halpern, Academic Press
9. Phase Transfer Catalysis, E. V. Dehmlow& S. S. Dehmlow, published by VerlagChemie, Weinheim, Berlin, Germany.
10. Phase Transfer Catalysis in Organic synthesis, W. P. Weber & G. W. Gokel, Springer
11. Hand book of phase transfer catalysis. Edited by Y. Sasson and R. Neumann, Springer.
12. Catalysis in Micellar and Macromolecular systems, J. H. Feudler& E. J. Feudler, Acad. Press
13. Reaction Kinetics in Micelles, E. H. Codes (ed), proceedings of ACS, Plenum Press.
14. Micelles – Theoretical and Applied aspects, V.Moroi, plenum press.
15. Physical Chemistry of surfaces, A.W.Adamson and A.P.gast, Wiley.
16. Polymer supported Catalysts, C. U. Pittman Jr, vol 8, Comprensive Organometallic Chemistry, Pergamon Press, Oxford.
17. Principles and Practice of Heterogeneous Catalysis, J. M.ThomasandW.J.Thomas, Wiley, VCH1997.
18. Spectroscopy in catalysis – An introduction by J. W. Niemantsverdriet, VCH publishing, 1993.
19. Modern methods of Organic Synthesis: Ahluwalia, Narosa Publishers.

ELECTIVE –3B

PAPER-3 CH(PO) – 403T(CB2) : Molecular modeling & It's Applications

PO(CB2)-21: Molecular Modeling – I
PO(CB2)-22: Molecular Modeling – II
PO(CB2)-23: Drug Design Methods I - Ligand Based
PO(CB2)-24: Drug Design Methods II - Structure Based.

PC(CB2)-21: Molecular Modeling – I (15hrs)

Introduction to Molecular Modeling, Single molecule calculations, assemblies of molecules and reactions of molecules - Co-ordinate systems: Cartesian and Internal Co-ordinates, Z-matrix - Potential energy surface - Conformational search; Global minimum, Local minimum, Conformational analysis of ethane.

Force field ; Features of Molecular Mechanics, Bonded and Non-bonded interactions, Bond Stretching, Angle Bending, Torsional Terms (Improper Torsions, out of Plane Bending Motions, Cross Terms), Non Bonded Interactions (Electrostatic Interactions, Van-der Waals interactions), Hydrogen Bonding Interactions.

PC(CB2)-22: Molecular Modeling – II (15hrs)

Force Field Equation in Energy minimization (Energy as function of r, θ, ω) - Introduction to Derivative Minimization Methods (First Order Minimization), Types of energy minimization Methods ; Steepest Descent, Conjugate Gradient, Conformational Search procedures - Geometry optimization procedures - Molecular Dynamics: Introduction, description of Molecular Dynamics, basic elements of Monte-Carlo method, differences between Molecular Dynamics and Monte-Carlo method, Qualitative exposure to Molecular Dynamics Simulations.

PC(CB2)-23:Drug Design Methods I - Ligand Based (15hrs)

Lead Molecule - Structure Activity Relationship (SAR), Quantitative Structure Activity Relationship (QSAR), Distinguish between SAR and QSAR - Physicochemical parameters ; Electronic effects, Hydrophobicity, Steric Factors Taft's Steric function, Molar Refractivity, Verloop Steric factor - Molecular Descriptor analysis: Craig plot, Topliss scheme, Bioisosteres - Hansch model, Free-Wilson model for QSAR equations - Regression analysis: Multi Linear Regression and Partial Least Square (terms: n, SD, r, r^2, r^2%, F) - Examples for linear and non-linear equations - 3D QSAR: CoMFA and CoMSIA - Differences between 2D and 3D QSAR.

PC(CB2)-24:Drug Design Methods II - Structure Based. (15hrs)

Database similarity searches - Pair-wise alignment: Global sequence analysis (Needleman-Wunsch), Local Sequence Alignment (Smith Waterman), Multiple Sequence Alignment - Homology Modeling: Query sequence, Template selection, Alignment, Backbone Modeling, Loop Modeling, Side chain Modeling, Model optimization, Energy minimization - Model Evaluation: Ramachandran Plot, Verify 3D, Errata and ProSA - Active site Identification - Docking, Docking Algorithms: Genetic Algorithm, Incremental construction - Molecular Interactions, Scoring functions - Virtual Screening: Ligand Based and Structure Based. De novo ligand design and its limitations.

Books suggested:

1. Molecular Modelling: Principles and Applications, by Andrew Leach, Longman Publications.
2. Computational Chemistry, Guy H. Grant & W. Graham Richards, Oxford University Press.
3. Computational Chemistry: Introduction to the theory and Applications of Molecular and Quantum Mechanics, Errol Lewars, Springer Publications.
4. Recent advances in Bioinformatics by I. A. Khan and A KhanumUkaaz publications, 2003.
5. Molecular modelling – Basic Principles and Applications by Hans Dieter Holtje and GerdFolkers, Wiley-VCH, 1996
6. Introduction to Computational Chemistry by Jensen, Wiley Publishers, second edition
7. Bioinformatics – A Primer by P. Narayanan, New Age International, (P) Ltd, 2005.
8. Introduction to Bioinformatics by Arthur M. Lesk, Oxford University Press (Indian. Edition), 2002
9. Principles of Medicinal Chemistry Vol. II by Dr. SS Kadam Pragati books Pvt. Ltd; 2007
10. An Introduction to Medicinal Chemistry by G L Patrick, Oxford University Press
11. Bioinformatics: Methods and Applications: Genomics, Proteomics and Drug Discovery. S.C. Rastog, NamitaMendiratta, Parag Rastogi, PHI Larning Pvt. Ltd; 2006
12. Pharmacy Practice Vol.I and II by Remington.
13. Burger's Medicinal Chemistry and Drug Discovery, 5th Edition.
14. Text book of Drug design and Vol.1 discovery 3rd Edition by POVL krogsgaard- Larsen Tommy liljefors and ULF Madsen.

Elective – 4A (ID Paper)

Paper-IV CH (PO) 404T(CB3): Five and six membered heterocycles , Carbohydrates and proteins,structure determination of natural products and Green chemistry

PO-(CB3)- 25: Five and six membered heterocycles with two hetero atoms
PO-(CB3)- 26: Carbohydrates and proteins
PO-(CB3) - 27: Structure determination of natural products by chemical and spectral methods
PO-(CB3) - 28: Green chemistry

PO-(CB3)- 25: Five and six membered heterocycles with two hetero atoms 15 Hrs

Synthesis, reactivity, aromatic character and importance of the following heterocycles: Pyrazole, Imidazole, Oxazole, Thiazole, Isoxazole, Isothiazole, Pyridazine, Pyrimidine. Pyrazine, Oxazine, thiazine, benzimidazole, benzoxazole and benzthiazole.

PO-(CB3)- 26:Carbohydrates and proteins 15 Hrs

Carbohydrates: Determination of the relative and absolute configuration in D(+)-glucose and D(-)-fructose. Proof for the ring size of D(+)-glucose. $^{4}C_{1}$ and $^{1}C_{4}$ conformations of D-glucose. Occurence, importance and synthesis of monosaccharides containing functional groups such as amino, halo and sulphur. Structure elucidation and synthesis of sucrose. Conformational structures of D(+)-ribose, 2-deoxyD-ribose, sucrose, lactose maltose and cellobiose. Structural features of starch, cellulose and chitin.

Proteins: Acid and enzymatic hydrolysis of proteins.Determination of the amino acid sequence in polypeptides by end group analysis.Chemical synthesis of di and tripeptides. Merrifield's solid phase synthesis.

PO-(CB3) - 27: Structure determination of natural products by chemical and spectral methods 15 Hrs

i) Determination of structure of morphine by chemical methods and spectral methods(IR, UV, ^{1}H-NMR, ^{13}C-NMR)
ii) Determination of structure of reserpine by chemical methods and spectral methods(IR, UV, ^{1}H-NMR, ^{13}C-NMR and Mass)
iii) Determination of structure of abeitic acid by chemical methods and spectral methods(IR, UV, ^{1}H-NMR, INEPT, DEPT, HOMOCOSY, HETEROCOSY and Mass)
iv) Determination of structure of geraneol by chemical methods and spectral methods(IR, UV, ^{1}H-NMR, INEPT, DEPT, HOMOCOSY, HETEROCOSY, 2D-INADEQUATE, NOE and Mass)

PO-(CB3) - 28: Green chemistry 15 Hrs

Introduction. Principles, atom economy and scope. Introduction to alternative approaches.
1.Solvent free reactions-principle, scope, utility of solvent free condition reactions.
Organic Synthesis in solid state (without using any solvent): Michael addition, Beckmann rearrangement, Synthesis of aziridines; solid supported organic synthesis: Synthesis of aziridines, pyridines, chromenes and flavones.
2. Aqueous Phase Reactions: Diels-Alder Reaction, Heck reaction, epoxidation,Dihydroxylation (Syn- & Anti-)

3.Microwave Technology: Microwaveequipment, activation-benefits, limitations, microwave effects.
a) Microwave Solvent free reactions (Solid state Reactions) - Deacetylation, deprotection, saponification of esters, alkylation of reactive methylene compounds, synthesis of nitriles from aldehydes, reductions.
b) Microwave assisted reactions in water — Hoffmann elimination, hydrolysis, oxidation, saponification reactions.
c) Microwave assisted reactions in organic solvents — Esterification reactions, Fries rearrangement, OrthoesterClaisen rearrangement, Diels- Alder reaction, decarboxylation.
d) Microwave assisted reactions under PTC conditions:
4.Ultrasound assisted reactions: introduction, substitution reactions, addition, oxidation, reduction reactions.
5.Organocatalysis: Aldol reactions, Acyl transfer reactions, nucleophilic N-heterocyclic carbenes in asymmetric organocatalysis, setter reaction and Baker's Yeast.
6. Ionic liquids: Introduction and applications in organic synthesis (illustrate with two examples).

Recommended Books:

1. Heterocyclic Chemistry, T.Gilchrist
2. An introduction to the Chemistry of heterocyclic compounds, R.M.Acheson
3. Heterocyclic Chemistry, J.A.Joule&K.Mills
4. Principles of Modern Heterocyclie Chemistry, A.Paquette
5. Heterocyclic Chemistry, J,A.Joule& Smith
6. Handbook of Heterocyclic Chemistry, A.R.Katritzky
7. Organic Chemistry Vol.I and Vol.II by I.L.Finar
8. Carbohydrate Chemistry by Barton Volumes
9. Carbohydrate chemistry by G.J.Boons
10. The chemistry of natural products: Vol.V - carbohydrates by S.F.Dyke
11. Organic Chemistry by McMurry.
12. Spectroscopic identification of organic compounds by RM Silverstein, G C Bassler and T B Morrill
13. NMR in chemistry - A multinuclear introduction by William Kemp
14. Introduction to organic spectroscopy by Pavia
15. Nuclear Magnetic Resonance Basic principles by Atta-ur-Rahman
16. Basic one and two-dimensional NMR spectroscopy by Horst Friebolin
17. NMR spectroscopy by H.Gunther
18. Textbook of organic chemistry, Vol II by I L Finar
19. Chemistry of natural products, Vol 12, by Atta-Ur-Rahman
20. An introduction to the chemistry of terpenoids and steroids, by William templeton
21. Steroids by Fieser arid Fieser
22. Alkaloids by Manske
23. Alkaloids by Bentley
24. The chemistry of terpenes by A Pinder
25. The terpenes by Simenson

26. Terpenoids by Mayo
27. Alkaloids by Pelletier
28. Total synthesis of Natural Products by Apsimon Vol 1-5
29. Principles of organic synthesis 3rdEd.R O C Norman and J M Coxen
30. One and two dimensional nmr spectroscopy by Atta Ur Rahman
31. Green chemistry, Theory and Practical, Paul T.Anastas and John C.Warner.
32. New trends in green chemistry By V.K.Ahulwalia and M.Kidwai.
33. Organic Synthesis: Special techniques. V.K.Ahulwalia and Renu Aggarwal.

ELECTIVE-4B(ID PAPER)

Paper-IV CH (PO) 404T (CB4): Forensic Chemistry & Toxicology

PO-(CB4)29: Forensic chemistry- I
PO-(CB4)30: Forensic chemistry- II
PO-(CB4)31: Forensic Toxicology-I
PO-(CB4)32: Forensic Toxicology-II

PO-(CB4)29:Forensic chemistry-I 15 Hrs

Forensic Chemistry - Introduction - Types of cases / exhibits - Preliminary screening - presumptive tests (colour and spot tests) - Examinations procedures involving standard methodsand instrumental techniques

Qualitative and quantitative forensic analysis of inorganic and organic material - Chemical fertilizers (N,P,K) _ Insecticides (Endosulfan, Malathion, Carbaryl) - Metallurgical analysis (Fe, Cu, Zn, Au, Ag) – Natural products (tobacco, tea, sugars, rubber) – Industrial chemicals - Sulphuric, Nitric and Hydrochloric acids, Sodium, Potassium hydroxide, Ammonium nitrate, Potassium chlorate, Organic solvents like Methanol, Ethanol, Acetone, Chloroform and Ether Organic chemicals like Acetanilide, P- Aminophenol, and Nitrobenzene etc. with reference to forensic work.

PO-(CB4)30:Forensic chemistry-II 15 Hrs

Examination of petroleum products - Distillation and fractionation - various fractions and theircommercial uses - Standard method of analysis of petroleum products – Analysis of petroleumproducts for adulteration and arson residues. Chemistry of fire - Investigation and evaluation of fires – Causes of fire - Analysis of arsonresidues by conventional and instrumental methods. Analysis of trace evidence - Cosmetics, Dyes, Trap related evidence materials, Paints, Pigments,Fibres, Oils fats, Greases, Industrial dusts, Chemicals and Plant materials.

PO-(CB4)31:Forensic Toxicology-I 15 Hrs

Toxicology- Introduction- History- Scope- Areas of Toxicology- Role of forensic toxicologist- Poisons- Classification of poisons- Types of poisoning- Sample collection and preservation oftoxicological exhibits in fatal and survival cases- Storage of samples- Signs and symptoms ofpoisoning- Toxicological investigation/examination of poisoned death- Interpretationoftoxicologicaldata- Courtroom testimony in toxicological cases.Case Histories.

PO-(CB4)32:Forensic Toxicology-II 15 Hrs

Principles of Toxicology- Introduction – Pharmacokinetics - Methods of transportation oftoxicant- Absorption- Distribution- Storage of toxicants- Redistribution - Metabolism- Oxidation– Reduction – Hydrolysis – Conjugation - Excretion- Other routes of elimination- Toxicokinetics- one and two compartmental model – Toxicodynamics- Spectrum of undesired(toxic) effects- Interaction of chemicals- Tolerance- Dose response relationship- Developmentaland reproductive toxicity- Mutagenicity- Toxicity testing.

Recommended books:

1. James, S. H. and Nordby, J. J. Forensic Science: An Introduction to Scientific and Investigative Techniques, 2003.
2. Saferstein, R Criminalistics - An Introduction to Forensic Science, Prentice Hall,1995.
3. Sarkar, S Fuels and Combustion, Orient Longman, 1990
4. Verma, R. M Analytical Chemistry – Theory and Practice, CBS Pub., 1994
5. Svehla, G. Ed. Vogel's Qualitative Inorganic Analysis, Longman, 1998.
6. Bassett: Vogel's Text Book of Quantitative Inorganic Analysis, Longman, 1978
7. Vogel, A. I Text Book of Practical Organic Chemistry including Qualitative OrganicAnalysis, ELBS, 1971.
8. Narayanan, T. V Modern Techniques of Bomb Detection and Disposal, R. A. Security System, 1995.
9. Almirall, J. R. and Furton, K. G Analysis and Interpretation of Fire Scene Evidence, CRC Press, 2004.
10. Bogusz, M. J Handbook of Analytical Separations Vol. 2 ,Forensic Science, Elsevier, 2000.
11. Bureau of Indian Standards: Specifications and Methods of Analysis for PetroleumProducts.
12. Wilson and Wilson's Comprehensive Analytical Chemistry Volumes
13. Standard Methods of Chemical Analysiss
14. AOAC Official Methods of Analysis
15. Daeid, N.N. Fire Investigation: Theory and Practice, Taylor and Francis, 2003
16. Klaassen, C. D., Casarett and Doull's Toxicology: The Basic Science of Poisons, 5thed, McGraw-Hill, 1995.
17. Moffat, A.C.,Osselton, D. M. Widdop, B. Clarke's Analysis of Drugs and Poisons in Pharmaceuticals, body fluids and postmortem material, 3rd ed., Pharmaceutical Press2004.
18. Bogusz, M. J., Hand Book of Analytical Separations, Vol. 2, Forensic Science, 1st ed., Elsevier Science ,2000.
19. Siegel, J.A., Saukko, P. J., Knupfer, G.,: Encyclopedia of Forensic Sciences (Vol3),
20. Academic Press, 2000.
21. Paranjape, H.M., Bothara, G.K., Jain, M.M. Fundamentals of Pharmacology, 1st ed.,Nirali Prakashan,1990.
22. Budhiraja, R.D. Elementary Pharmacology and Toxicology, Popular Prakashan, 2nd ed. 1999.
23. Laboratory procedure Manual, Forensic Toxicology DFS, 2005
24. Cravey, R.H; Baselt, R.C.: Introduction to Forensic Toxicology , Biochemical
25. Publications, Davis, C.A. (1981)
26. Stolmen, A. Progress in Chemical Toxicology Academic Press, New York (1963)
27. Modi, Jaisingh, P. Textbook of Medical Jurisprudence& Toxicology, M.M. TripathiPublication (2001)
28. Eckert; An Introduction to Forensic Science, CRC Press

SEMESTER IV LABORATORY COURSES

PAPER VII (Lab)-CH(PO) 451P: Instrumentation

I. Conductometry:

Conductometric titrations :

a) Mixture of strong and weak bases vs strong acid
b) Mixture of strong and weak bases vs weak base
c) Mixture of strong acid, weak acid and CuSO4 vs strong base
d) Formic acid, acetic acid, chloro acetic acid, dichloro acetic acid and trichloro acetic acid and their mixtures vs strong base
e) Precipitation titration: K_2SO_4 vs $BaCl_2$
2. Dissociation constant of weak acids
3. Effect of solvent dielectric constant on dissociation constant of a weak acid
4. Verification Onsager equation

II. pH – metry:

1.Preparation of a) phosphate b) acetate and c) borate buffers
2. pH-metric titrationsof
   a) monobasic acids vs strong base
   b) dibasic acids vs strong base
   c) tribasic acids vs strong base
   d) mixture of strong and weak acids vs strong base
3.Determination of dissociation constant of monobasic/dibasic acids by Alber-Serjeant method.
4. Determination of dissociation constant of acetic acid in DMSO, acetone and dioxane.
5. Determination of pKa and pKb of glycine (calculation using a computer program)

III. Spectrophotometry:

1.Estimation of a) Cu(II) using EDTA
b) Fe(III) using thiocyanate
c) Fe(II) using 1,10-phenanthroline
d) Fe(III) in tap water using thiocyanate by standard addition method
e) dichromate and permanganate simultaneously in a mixture
2. Spectrophotometric titrations:
   a) Cu(II) vs EDTA
   b) Fe(II) using 1,10-phenanthroline
   c) Mixture of Cu(II) and Bi(III) vs EDTA
3. Determinaton of composition of
   a) Cu(II)-EDTA complex by Job's method
   b) Fe(II)-phenanthroline complex- by Job's method or mole ratio /slope ratio method
4.Determination of pKa of methyl red indicator

IV Potentiometry:

1.Potentiometric titrations:
a) Weak acid vs strong base and calculation of dissociation constants
b) Mixture of strong and weak acids vs strong base

c) Dibasic acid vs strong base
d) Fe(II) vs Ce(IV) and calculation of formal redox potentials of Fe(II)/Fe(III)
e) Fe(II) vs MnO4-
f) I – vs MnO4-
g) Fe(II) vs EDTA
h) Mixture of halides vs $AgNO_3$
i) Mixture of KI and KSCN vs $AgNO_3$
2. Determination of temperatue dependence of e.m.f of a cell
3. Determination of formation constant of silver-ammonia complex
4. Determination of solubility product
5 .Determination of mean ionic activity coefficient of HCl

Suggested Books:

1. Senior Practical Physical Chemistry: B.D. Khosla, V.C. Garg and A. Khosla
2. Experimental Physical Chemistry: V. Athawale and P. Mathur.
3. Practical Physical Chemistry: B. Vishwanathan and P.S. Raghavan.
4. Practical in Physical Chemistry: P.S. Sindhu
5. Advanced Practical Physical chemistry: J.B.Yadav
6. Vogel Text book of Quantitative Analysis, 6th edition, Pearson education Ltd. 2002.

Paper VIII –(LAB) CH (PO) 452P : Separation, identification and spectralanalysis of organic compounds

1. Separation of two component mixtures by chemical methods and their identification by chemical reactions – separation by using solvent ether, dil. hydrochloric acid, 5% aqueous sodium bicarbonate and sodium hydroxide solutions, checking the purity of the two components by TLC, identification of the compounds by a systematic study of the physical characteristics (mp/bp), extra elements (nitrogen , halogens and sulfur), solubility, functional groups, preparation of crystalline derivatives and identification by referring to literature. A minimum of 6 mixtures should be separated and analyzed by these procedures.
2. Separation of three component mixtures by chemical method. A minimum of 2 mixtures should be separated.
3. Identification of unknown organic compounds by interpretation of IR, UV, 1H nmr, 13C nmr and mass spectra. A minimum of **15** representative examples should be studies.

Suggested Books:

1. The systematic identification of organic compounds by R L Shriner, R C Fusion and D Y Curtin
2. A textbook of practical organic chemistry by A I Vogel, Vol I & II
3. Unitized experiments in organic chemistry by R Q Brewster and others
4. Handbook of organic analysis by HTC Clarke
5. Practical Organic Chemistry by Mann and Saunders
6. Spectroscopic identification of organic compounds by Silverstein , Bassler& Morrel.

FIVE YEAR INTEGRATED COURSE (FYIC)

SYLLABUS FOR IX NAD X SEMESTER

Semester IX

Subject Code	Subject	Instruction Hrs /Week	Internal Assessment. Marks	Max Marks Sem. Exams	Duration of Sem. Exam. Hrs
	THEORY				
FYIC-T901	Inorganic Chemistry	4 Hrs	20	80	3
FYIC-T902	Organic Chemistry	4 Hrs	20	80	3
FYIC-T903	Physical Chemistry	4 Hrs	20	80	3
FYIC-T904	Analytical techniques, spectroscopy and green chemistry	4 Hrs	20	80	3
	Seminar	2 Hrs			
	PRACTICALS				
FYIC-P905	Inorganic Chemistry Lab	6 Hrs		100	6
FYIC-P906	Organic Chemistry Lab	6 Hrs		100	6
FYIC- P 907	Physical Chemistry Lab	6 Hrs		100	6
	Total	**34+2 hrs**	**80**	**620**	

Semester X

Subject Code	Subject	Instruction Hrs /Week	Internal Assessment. Marks	Max Marks Sem. Exams	Duration of Sem. Exam. Hrs
	PROJECT				
FYIC -Project					
Project Seminar				100	
Project Pre-Viva				100	
Project Dissertation				400	
	Total			**600**	

SEMESTER –IX

Paper-I FYIC 901 INORGANIC CHEMISTRY

(Bonding, Group Theory and its Applications)

IC-01: Group Theory, Normal mode analysis and Spectral Activity

IC-02: MOT of Metal Complexes

IC-03: Electronic Spectroscopy of Metal Complexes

IC-04: IR and Raman Spectroscopy

Paper II FYIC 902 ORGANIC CHEMISTRY

OC- 01: New synthetic reactions

OC- 02: Pericyclic reactions

OC- 03: Photochemistry

OC- 04: ^{13}C NMR spectroscopy

Paper III FYIC 903 PHYSICAL CHEMISTRY

PC-01: Applications of Schrödinger equation

PC-02: Chemical Kinetics-II

PC- 03: Electrochemistry -II

PC-04: Bonding in molecules

Paper-IV FYIC 904 GENERAL CHEMISTRY

(ANALYTICAL TECHNIQUES, SPECTROSCOPY and GREEN CHEMISTRY)

GC-01: Atomic Spectroscopy

GC-02: CD, ORD and 2D NMR techniques

GC-03: Diffraction Methods

GC-04: Green Chemistry

SEMSETER-IX

PAPER I: FYIC 901: Bonding, Group Theory and its Applications

IC-01: Group Theory, Normal mode analysis and Spectral Activity
IC-02: MOT of Metal Complexes
IC-03: Electronic Spectroscopy of Metal Complexes
IC-04: IR and Raman Spectroscopy

IC-01: Group Theory, Normal Mode Analysis and Spectral Activity (15 hours)
Group Multiplication Tables – Properties of a Group-Subgroups-Classes of Symmetry Elements. Representation of Symmetry Elements: Simple Matrices, Block-Factorization, Matrix Representation of *E, Cn, Sn, i and* σ Elements –Matrix Representation of C_2,C_3,C_{2v},C_{3v} and C_{2h}point groups. Character of a Matrix and a Representation,Reducible and Irreducible Representations, Properties of Irreducible Representations, Construction of Character Tables for some simple Point Groups:C_{2V},C_{3V} and C_{2h} – Mulliken Symbolism for Irreducible Representations - Standard Reduction Formula – Direct Products.

Normal Modes analysis & Spectral Activity: Number, Type and Symmetry – Symmetry of Normal Modes of Molecules: Cartesian and Internal Coordinate Methods of Analysis – Normal Mode Analysis of Molecules with Cnv (n=2,3), C2h, D2h, Td and Oh Point Groups – Internal Coordinates and Redundancy (Qualitative concept) – Infrared and Raman Activity of Normal Modes (Infinite Groups Excluded)

IC-02: Molecular Orbital Theory of Metal Complexes (15 hours)
Symmetry Classification of Metal and Ligand Orbitals in Cubic and Non-Cubic Environments: Octahedral, Tetrahedral, Square Planar, Square Pyramidal, Trigonal Bipyramidal Geometries – Concept of Ligand Group Orbitals – Construction of Molecular Orbital Energy Level Diagrams for Octahedral, Tetrahedral and Square Planar Metal Complexes with Sigma (σ) and Pi (π) Bonding Contribution from the Ligands.

IC-03: Electronic Spectroscopy of Metal Complexes (15 hours)
Orgel Diagrams, Strong Field Configurations: The Method of Descending Symmetry, Correlation Diagrams and Tanabe-Sugano Diagrams for d^2 and d^8 Configurations. Classification of Electronic Spectra for Metal Complexes - Electric Dipole Transitions – Magnetic Dipole Transitions – Selection Rules: Orbital Selection Rules and Spin Selection Rules – Relaxation in Selection Rules – Nature of Electronic Spectral Bands: Band Widths, Band Intensities and Factors Influencing Band Shapes – Jahn-Teller Effect – Spectrochemical Series – Nephelauxetic Effect – Crystal Field Spectra of Oh and Td Metal Complexes of 3d Metals – Calculation of 10Dq Values, Racah Parameter (B) and Nephelauxetic Ratio ( ) – Charge Transfer Spectra.

IC-04: Infrared and Raman Spectroscopy (15 hours)
Conditions for Infrared and Raman Spectroscopies – Symmetry Based Selection Rules of Infrared and Raman. Symmetry Requirements for Overtone, Binary and Ternary Combination Bands – Prediction of Diagnostic Fundamentals in Isomers of Metal Complexes – Structure Fitting: Determination of Coordination Sites and Linkage Isomers, Distinguishing Isomers of Metal Complexes - Effect of Coordination on Ligand Vibrations: Examples involving Mono, Bi and/or Polydentate Ligands of Oxygen, Sulfur, Nitrogen, Phosphorous, Arsenic, Carbon and Halogen Donors. Application of Resonance Raman Spectroscopy to Structural Elucidation of the active Sites of Heme and Non-Heme Oxygen Carriers.

SUGGESTED BOOKS

1. Symmetry and Spectroscopy of Molecules, K. Veera Reddy, Second Edition, New Age International (P) Limited Publishers (2009)
2. Chemical Applications of Group Theory, F. A. Cotton, 3rd edition, Wiley NY (1990)
3. Symmetry and Group Theory In Chemistry, Mark Ladd, Harwood Publishers, London (2000)
4. Symmetry Through the Eyes of a Chemist, I. Hargittai and M. Hargittai, 2nd Edition, Plenum Press, NY (1995)
5. Molecular Symmetry and Group Theory, Robert L. Carter, John Wiley & Sons (1998)
6. Group Theory for Chemists, G. Davidson, Macmillan Physical Science Series (1991)
7. Molecular Symmetry, Schoenland
8. Electronic Spectroscopy, A. B. P. Lever
9. Introduction to Ligand fields, B. N. Figgis
10. Infrared and Raman Spectroscopy of Inorganic and Coordination Compounds, K. Nakamoto
11. Infrared spectroscopy of Inorganic Compound, Bellamy

PAPER II: FYIC 902 ORGANIC CHEMISTRY

OC 01- New synthetic reactions
OC 02- Pericyclic reactions
OC 03-Photochemistry
OC 04- ^{13}C NMR spectroscopy

OC-01: New synthetic reactions: (15 hours)

1. Metal mediated C-C and C-X coupling reactions: Suzuki, Heck, Stille, Sonogishira cross coupling, Buchwald-Hartwig and Negishi-Kumada coupling reactions.

2. C=C Formation Reactions: Shapiro, Bamford-Stevens, McMurrey reactions, Julia-Lythgoe olefination and Peterson's stereoselective olefination.

3. Multicomponent Reactions: Ugi, Passerini, Biginelli, Bergman and Mannich reactions.

4. Ring Formation Reactions: Pausan-Khand reaction, Nazerov cyclisation.

5. Click Chemistry: Click reaction, 1,3-dipolar cycloadditions.

6.Metathesis: Grubb's 1st and 2nd generation catalyst, Olefin cross coupling metathesis (OCM), ring closing metathesis(RCM), ring opening metathesis(ROM), applications.

7. Other important synthetic reactions: Baylis-Hilman reaction, Eschenmoser-Tanabe fragmentation, Mitsunobu reaction, Stork-enamine reaction and Michael reactions.

OC-02: Pericyclic reactions (15hours)

Introduction, Classification of pericyclic reactions,

Electrocyclic reactions: con rotation and dis rotation. Electrocyclic closure and opening in 4n and 4n+2 systems.

Cycloaddition reactions: suprafacial and antara facial additions in 4n and4n+2 cycloadditions.

Sigmatropic reactions: [i, j] shifts- suprafacial and antarafacial shifts, Cope and Claisen rearrangement reactions.

Approaches for the interpretation of mechanism of pericyclic reactions: Aromatic Transition States (ATS)/Perturbation Molecular Orbitals (PMO) approach-Concept of Huckel –Mobius aromatic and antiaromatic transition states. Framing Woodward-Hofmann selection rules for all the pericyclic reactions by ATS approach. Solving problems based on ATS approach.

Molecular orbitals: ethylene, 1, 3-butadiene, 1, 3, 5-hexatriene, allyl cation, allyl radical, pentadienyl cation, pentadienyl radical.

Frontier Molecular Orbital (HOMO-LUMO) approach-concept: Framing Woodward-Hofmann selection rules for all the pericyclic reactions by Frontier Molecular Orbital (FMO) approach. Solving problems based on FMO approach.

Conservation of orbital symmetry: (Correlation Diagrams) approach- for electrocylic and cycloadditions & cycloreversions.

OC-03: Photochemistry (15 hours)

Photochemistry: Photochemistry of π-π^* transitions: Excited states of alkenes, cis-trans isomerisation, and photo stationary state. Photochemistry of 1,3-butadiene Electrocyclisation and sigmatropic rearrangements, di-π methane rearrangement. Intermolecular reactions, photocycloadditions, photodimeriastion of simple and conjugated olefins. Addition of olefins to α, β-unsaturated carbonyl compounds. Excited states of aromatic compounds, Photoisimerisation of benzene.

Photochemistry of (n-π*) transitions: Excited states of carbonyl compounds, homolytic cleavage of α- bond, Norrish type I reactions in acyclic and cyclic ketones and strained cycloalkane diones.
Intermolecular abstraction of hydrogen: photoreduction-influence of temperature, solvent, nature of hydrogen donor and structure of the substrate.
Intramolecular abstraction of hydrogen: Norrish type II reactions in ketones, esters and 1,2 diketones, Addition to carbon-carbon multiple bonds, Paterno-Buchi reaction,
Photochemistry of nitrites-Barton reaction

OC-04: ^{13}C NMR spectroscopy (15 hours)

CW and PFT techniques. Types of ^{13}C nmr spectra: undecoupled, proton- decoupled and offresonancedecoupled (ORD) spectra. ^{13}C chemical shifts, factors affecting the chemical shifts, chemical shifts of organic compounds. Calculation of chemical shifts of alkanes, alkenes and alkynes. Homonuclear (^{13}C, ^{13}C J) and heteronuclear (^{13}C, ^{1}H J and ^{13}C- ^{2}H J) coupling. Applications of ^{13}C-NMR spectroscopy: Structure determination, stereochemistry, reaction mechanisms and dynamic processes in organic molecules. ^{13}C-NMR spectral editing techniques: principle and applications of APT, INEPT and DEPT methods.

Recommended Books:

1. Some modern methods of organic synthesis by W Carruthers
2. Guidebook to organic synthesis, by R K Meckie, D M Smith & R A Atken
3. Organic synthesis by O House
4. Organic synthesis by Michael B Smith
5. Molecular Reactions and Photo chemistry by Depuy and Chapman
6. Organic synthesis by Robert E Ireland
7. Organic Synthesis - The disconnection approach by S Warren
8. Organic Synthesis by C Willis and M Willis
9. Handbook of reagents for organic synthesis by Reich and Rigby, Vo I, IV
10. Problems on organic synthesis by Stuart Warren
11. Total synthesis of natural products: the Chiron approach by S.Hanessian
12. Organic chemistry Claydon and others 2005
13. Name Reactions by Jie Jack Li
14. Reagents in Organic synthesis by B.P.Mundy and others.
15. Tandem Organic Reactions by Tse-Lok Ho
16. Spectroscopic identification of organic compounds by RM Silverstein, G C Bassler and T B Morrill
17.Organic Spectroscopy by William Kemp
18. Spectroscopic methods in Organic chemistry by DH Williams and I Fleming
19. Carbon-13 NMR for organic chemists by GC Levy and O L Nelson
20. Nuclear Magnetic Resonance Basic principles by Atta-ur-Rahman
22. Advanced organic chemistry. Part A Structure & Mechanism by Francis A. Corey and Richard J. Sundberg
23. Modern NMR techniques for chemistry research by Andrew B Derome
24. NMR in chemistry - A multinuclear introduction by William Kemp
25. Spectroscopic identification of organic compounds by P S Kalsi
26. Introduction to organic spectroscopy by Pavia
27. Carbon-13 NMR for organic chemists by GC Levy and O L Nelson

29. Photochemistry by C W S Wells
30. Organic Photochemistry by Turro
31. Molecular Photochcmistry by Gilbert & Baggo
32. Organic Photochemistty by D Coyle
33. Optical rotatory cispersion by C Djerassi
34. Optical rotatory dispersion and circular dichroism by P Crabbe
35. Mechanism and Structure in Organic chemistry by S Mukherjee
36. Advanced Organic Chemistry: Reactions, Mechanisms & Structure by Jerry March
37. Pericyclic Reactions by Mukherjee
38. Conservation of Orbital Symmetry by Woodward and Hoffmann
39. Organic Reactions and Orbital Symmetry, Gilchrist and Storr
40. Pericyclic Reactions — a problem solving approach, Lehr and Merchand
41. The Nature of Chemistry — Units 17-19 - Aromaticity — Open University, U K. Publications

Paper III: FYIC 903 Physical Chemistry

PC-01: Applications of Schrödinger equation

PC-02: Chemical Kinetics-II

PC- 03: Electrochemistry -II

PC-04: Bonding in molecules

PC – 01: Applications of Schrödinger equation (15 hours)

Systems with discontinuity in the potential field. A simple potential barrier. A potential barrier with a finite thickness. Quantum mechanical tunneling – examples – α -particle emission, inversion of NH_3, hydrogen transfer reactions.

The harmonic oscillator – detailed treatment. Wave functions and energies. Vibration of a diatomic molecule – harmonic oscillator model.

The rigid rotator – detailed treatment. Wave functions and energies. Spherical harmonics. Rigid rotator as model for a rotating diatomic molecule.

The hydrogen atom – detailed treatment. Angular and radial functions. Atomic orbitals. Measurability of the ground-state energy of hydrogen atom. Orthonormal nature of hydrogen like wave functions. Probability calculations. Atomic and molecular term symbols.

Atoms in external field, Zeeman and anomalous Zeeman effect.

PC- 02: Chemical kinetics – II (15 hours)

Reactions in solution: Factors affecting the reaction rates in solution. Effect of pressure on rate of reaction. Diffusion controlled reactions. Influence of dielectric constant and ionic strength on ion-ion, ion-dipole and dipoledipole reactions. Kinetic isotope effects: Primary and secondary isotope effects. Solvent isotope effects.

Fast reactions: Flow methods and the stopped-flow technique. The fluorescence technique. Shock tube method Relaxation methods (T-jump andP- jump). Kinetic equations for chemical relaxation.

Enzyme kinetics: Michaelis - Menten mechanisms of enzyme catalyzed reactions involving one and two intermediates. Steady-state approximation. Derivation of kinetic equations. Evaluation of kinetic parameters. Enzyme- substrate complex: Fischer's lock and key and Koshland's inducedfit hypotheses. Specificity of enzyme-catalyzed reactions. Discussion of the various types of forces involved in the formation of E-S complex. pH dependence of enzyme-catalyzed reactions the kinetics and the equations involved.

PC –03: Electrochemistry – II (15 hours)

The electrode-electrolyte interface: The electrical double layer. The Helmholtz-Perrin parallelplate model, the Gouy-Chapman diffuse-charge model and the Stern model. Quantum aspects ofcharge transfer at the interfaces. Tunneling.

Electrodics: Charge transfer reactions at the electrode-electrolyte interface. Exchange current density and overpotential. Derivation of Butler-Volmer equation. High field approximation. Tafel equation - low field - equilibrium, Nernst equation. The symmetry factor and its significance.

Corrosion: Electrochemical corrosion. Short-circuited energy producing cell. Homogeneous theory of corrosion. The corrosion current and the corrosion potential. The basic electrodics of corrosion. Potential-pH (Pourbaix) diagrams of iron and gold. Methods of corrosion rate

measurement. Mechanism of anodic dissolution of iron. Protection against corrosion. Corrosion inhibitors.

PC – 04: Bonding in molecules (15 hours)

Born-Oppenheimer approximation. MO theory of H_2^+ ion. Calculation of MOs and their energies. Evaluation of the overlap integral. Probability curves and enegy diagram. MO theory of H_2 molecule. Calculation of energy. Atomic and molecular term symbols. MO theory of polyatomic molecules (general ideas). MO treatment of H_2O. Symmetry-adapted linear combinations. MOs of H_2O.

Concept of hybridization – sp, sp^2, and sp^3 hybrid orbitals.

Semiempirical MO methods. The Huckel theory of conjugated systems. HMO calculations on ethylene, allyl system, butadiene, cyclopropenyl system and benzene. π–electron charges and bond orders. Simplification secular determinants of cycloprenyl system, cyclobutadiene and benzene using molecular symmetry. Extension of the Huckel approach to molecules containg heteroatoms.

Orbital symmetry and reactivity: $H_2 + F_2 \rightarrow 2HF$ reaction. $2NO \rightarrow N_2 + O_2$ reaction.

Reference Books

1. Quantum Chemistry, Ira N. Levine, Prentice Hall
2. Introduction to Quantum Chemistry, A. K. Chandra, Tata McGraw Hill
3. Elementary Quantum Chemistry, F. L. Pilar, McGraw Hill
4. Molecular Quantum Mechanics, P. W. Atkins & R. S. Friedman, Oxford UniversityPress
5. Quantum Chemistry by R. K. Prasad
6. Chemical Kinetics, K. J. Laidler, McGraw Hill
7. Kinetics and Mechanism, A. A. Frost & R. G. Pearson, John Wiley & sons
8. Kinetics and Mechanism of Chemical Transformations, J. Rajaraman & J. Kuriacose, McMillan
9. Chemical Kinetics and Reaction Mechanisms, J. H. Espenson, McGraw Hill
10. Physical Organic Chemistry, N. S. Isaacs, ELBS
11. The Physical basis of Organic Chemistry, Howard Maskill, Oxford University Press
12. Rates and Equilibriums of Organic Reactions, J. E. Leffler & E. Grunwald, Dover publications
13. Reaction Dynamics, edited by N. Sathyamurthy, Narosa Publishing House
14. Modern Electrochemistry, J. O. M. Bockris & A. K. N. Reddy, Plenum
15. Advanced Physical Chemistry, J.N.Gurtu and H. Snehi, Pragati Prakashan, Meerut.
16. Physical Chemistyr: A molecular approach, McQuarie Simon, Viva Books Pvt. Ltd. New Delhi.
17. Atkin's Physical Chemistry, P. Atkins & Julio de Paula, Oxford University Press
18. The Chemical Bond, J. N. Murrel, S. F. A. Kettle & J. M. Tedder, John Wiley

Paper IV:FYIC 904 GENERAL CHEMISTRY
(ANALYTICAL TECHNIQUES, SPECTROSCOPY and GREEN CHEMISTRY)

GC-01: Atomic Spectroscopy
GC-02: CD, ORD and 2D NMR techniques
GC-03: Diffraction Methods
GC-04: Green Chemistry

GC-01: Atomic Spectroscopy (15 hours)

Atomic Absorption Spectroscopy (AAS): Principles of AAS, Instrumentation – flame AAS and furnace AAS, resonance line sources, sensitivity and detection limits in AAS, interferences – chemical and spectral, evaluation methods in AAS and application in qualitative and quantitative analysis.
Atomic Emission Spectroscopy (AES): Principles of AES, Instrumentation, Interferences, evaluation methods, Application in quantitative analysis.
Inductively Coupled Plasma - Atomic Emission Spectroscopy (ICP-AES): Limitations of AES, Principles of plasma spectroscopy, plasma as an excitation source. Inductively coupled plasma source, ICP-AES – Instrumentation. Application of ICP-AES, Comparison with AAS.

GC – 02: CD, ORD and 2D NMR techniques (15 hours)
Optical Rotatory Dispersion (ORD) and CD Spectroscopy: Optical rotation, circular birefringence, circular dichroism and Cotton effect. Plain curves and anomalous curves. Empirical and semiempirical rules-The axial haloketone rule, the octant rule, Helicity rule, Exciton chirality method-Exciton coupling between identical chromophores. Benzene sector and chirality rule. Application of the rules to the study of absolute configuration and conformations of organic molecules.

2D-NMR techniques: Principles of 2D NMR, Classification of 2D-experiments. Correlation spectroscopy (COSY) HOMO COSY (^{1}H-^{1}H COSY) , TOCSY (Total Correlation Spectroscopy), Hetero COSY (^{1}H, ^{13}C COSY, HMQC), long range ^{1}H, ^{13}C COSY (HMBC), Homonuclear and Heteronuclear 2D-J-resolved spectroscopy, NOESY and 2D-INADEQUATE experiments and their applications.

GC-03: Diffraction Methods (15 hours)
X-ray Diffraction: Bragg's Law - Miller Indices - Photographic and Counter Methods of Measurement of Intensity - Deduction of Structure Amplitude from Intensity Measurements - Extinction and Absortion - Structural Analysis of Crystals - Laue's, Bragg's and Debye Scherror Methods - Interpretation of NaCl and KCl Crystal Structures - Electron Density Studies by Xrays - Platinum Phthalocyanine Complex, Silyl acetate, Tetraalkyl biphosphate – Advantages and Limitations of X-ray Diffraction.
Electron Diffraction by Gases: Principles - Radial Distribution Curves - Interpretation of Results
for $PBrF_2S$, PF_3S, PF_2HS, $HClO_4$, Silyl monothioacetate and Germyl monothioacetate and HgCl2 molecules - Advantages and Limitations.
Neutron Diffraction: Principles - Application in Hydrogen Bonding Studies - Combined use of X-ray and Neutron Diffraction Studies - Advantages and Limitations.

GC-04 : Green Chemistry (15 hours)

Introduction. Principles, atom economy and scope. Introduction to alternative approaches.

1. Solvent free reactions-principle, scope, utility of solvent free condition reactions.

Organic Synthesis in solid state (without using any solvent): Michael addition, Beckmann rearrangement, Synthesis of aziridines; solid supported organic synthesis: Synthesis of aziridines, pyridines, chromenes and flavones.

2. Aqueous Phase Reactions: Diels-Alder Reaction, Heck reaction, epoxidation, Dihydroxylation (Syn- & Anti-)

3. Microwave Technology: Microwave equipment, activation-benefits, limitations, microwave effects.

a) Microwave Solvent free reactions (Solid state Reactions) - Deacetylation, deprotection, saponification of esters, alkylation of reactive methylene compounds, synthesis of nitriles from aldehydes, reductions.

b) Microwave assisted reactions in water — Hoffmann elimination, hydrolysis, oxidation, saponification reactions.

c) Microwave assisted reactions in organic solvents — Esterification reactions, Fries rearrangement, Orthoester Claisen rearrangement, Diels- Alder reaction, decarboxylation. d) Microwave assisted reactions under PTC conditions:

4. Ultrasound assisted reactions: introduction, substitution reactions, addition, oxidation, reduction reactions.

5. Organocatalysis: Aldol reactions, Acyl transfer reactions, nucleophilic N-heterocyclic carbenes in asymmetric organocatalysis, setter reaction and Baker's Yeast.

6. Ionic liquids: Introduction and applications in organic synthesis (illustrate with two examples).

SUGGESTED BOOKS

1. Progress in Inorganic Chemistry Vol 30 ed :S.J.Lippard.
2. Coordination Chemistry Reviews Vol 39 1981,p121
3. Principles of Instrumental Analysis, Skoog, Holler and Nieman.
4 . Instrumental Techniques for Analytical Chemistry, Frank Settle.
5. Principles of Analytical Chemistry, M. Valcarcel.
6. Solid State Chemistry and its Applications, *West.*
7. Introduction to Solids, Azaroff.
8. Solid State Chemistry, D.K. Chakrabarthy
9. Physical Methods in Chemistry, R. S. Drago
10. Physical Methods in Advanced Inorganic Chemistry, Hill and Day.
11. Instrunmental Methods of Analysis, Sixth edition, CBS Publishers, Willard, Merrit, Dean, and Settle.
12. Chemical structure and Bonding, R.L. Decock and H.B. Gray.
13.Green chemistry, Theory and Practical, Paul T.Anastas and John C.Warner.
14. New trends in green chemistry By V.K.Ahulwalia and M.Kidwai.
15.NMR in chemistry - A multinuclear introduction by William Kemp
16. Spectroscopic identification of organic compounds by P S Kalsi
17. Introduction to organic spectroscopy by Pavia
18. Carbon-13 NMR for organic chemists by GC Levy and O L Nelson
19. Nuclear Magnetic Resonance Basic principles by Atta-ur-Rahman
20.Organic Spectroscopy by William Kemp
21. Spectroscopic methods in Organic chemistry by DH Williams and I Fleming

22. Carbon-13 NMR for organic chemists by GC Levy and O L Nelson
23. Optical rotatory dispersion and circular dichroism by P Crabbe
24. Optical rotatory dispersion by C Djerassi
25. Modern NMR techniques for chemistry research by Andrew B Derome

Laboratory Courses

PAPER 905 Inorganic Chemistry Practicals: **6 hrs/week**

Instrumental Methods of Analysis

I Potentiometry:

i. Determination of Fe^{2+} in Iron wire usng $K_2Cr_2O_7$ and $KMnO_4$
ii. Determination of Ferrous and Vanadyl in a mixture by Ceric Ammonium Nitrate.
iii. Assay of sulphanilamide in sample.

II pHmetry:

i. Determination of CO_3^{2-} and HCO_3^- in a mixture
ii. Determination of the dissociation constants of Glycine (HL)
iii. Determination of binary constants of Ni(II) – Gly Systems

III Conductometry:

i. Determination of the Composition of Cu(II)-Oxine Complex
ii. Determination of the Composition of Cu(II)-EDTA Complex

IV Spectrophotometry

i. Estimation of manganese in steel
ii. Estimation of chromium.
iii. Determination of composition of Complex by Job's Method and Mole ratio Method in Cu(II)-EDTA

V Colorimetry

i. Determination of blood sugar
ii. Determination of blood cholesterol
iii. Determination of Paracetamol

VI Fluorimetry

i. Determination of Riboflavin
ii. Determination of Quinine Sulphate.

VII Flame photometry

i. Determination of Na
ii. Determination of K

VII Atomic Absorption Spectroscopy (Demonstration): Determination of Mg and Pb.

Suggested Books

1. Chemistry Experiments for Instrumental Methods, Donald T Sawyer William R.Hememan etal John Wiley & Sons 1984.
2.Analytical Chemistry by Gary D.Christian 6th Edition John Wiley&Sons Inc New York 1994.
3.A Text Book of Quantitative Inorganic Analysis by A.I. Vogel 3rEdition Elbs Publication 1969.
4.Vogel's Text Book Of Quantitative Inorganic Analysis Jeffery etal 4th edition Elbs Publications 1988.
5.Vogel's Text Book of Quantitative Chemical Analysis, 6th edition. Pearson Education Ltd 2002.
6.Analytical Chemistry Thoery and Practice by R.M. Verma 3rd Edn.CBS Publishers & Distrbutors1994.
7.Comprehensive Experimental Chemistry by V.K. Ahluwalia etal New Age Publications 1997.
8.Laboratory hand Book of Instrumental Drug Analysis.by B.G. Nagavi 2nd edn. 1996

Paper-906 ORGANIC CHEMISTRY Practicals: **6 hrs/week**

Spectroscopic identification of organic compounds, Chromatography and Isolation of Natural Products

1. Identification of unknown organic compounds by interpretation of IR, UV, 1H -NMR, 13C NMR and mass spectral data. A minimum of 10 representative examples should be studied.
2. Separation by column chromatography: Separation of a mixture of ortho and paranitroanilines using silicagel as adsorbant and chloroform as the eluent. The column chromatography should be monitored by TLC.
3. Isolation of the following natural products:
   Caffeine from tea leaves (solvent extraction), Piperine from pepper (Soxhlet extraction), Eucalyptus oil from leaves (steam distillation), Lycopene from tomatoes.

Recommended books:

1. Practical organic chemistry by Mann & Saunders
2. Text book of practical organic chemistry by Vogel
3. The systematic identification of organic compounds by Shriner et.al
4. Analytical chemistry by G N David Krupadanam et.al
5. Advanced practical medicinal chemistry by Ashutoshkar
6. Pharmaceutical drug analysis by Ashutoshkar
7. Quantitative analysis of drugs in pharmaceutical formulations by P D Sethi
8. Practical pharmaceutical chemistry part-1 and part-2 by A H Beekett and J B Stenlake
9. Spectroscopic identification of organic compounds by R M Silverstein and F X Webster

Paper-907 Physical Chemistry Practiccals (Instrumentation -II) 06 hrs per week

Spectrophotometry:

1. Estimation of Cu(II) using EDTA
2. Estimation of Fe(III) using thiocyanate
3. Estimation of Mn(II) by spetrophotometry using periodate
4. Spectrophotmetric titration of Cu(II) vs EDTA
5. Spectrophotmetric titration of Fe(II) vs 1,10-phenanthroline
6. Determination of composition and Gibbs energy of formation of Fe(III) – salicylic acid complex
7. Simultaneous determination of dichromate and permanganate in a mixture
8. Composition of Fe(II) – phenanthroline complex –by Job's method, by mole ratio method.

Potentiometry:

1. Titration of strong acid(HCl) vs strong base (NaOH)
2. Titration of weak acid vs strong base(NaOH) & calculation of dissociation constants
   [**Weak acids:** Acetic acid, Chloro acetic acid, Dichloro acetic acid, Trichloro acetic acid, Propinoic acid and butyric acid]
3. Titration of a mixture of strong(HCl) and weak acids vs strong base(NaOH)
   [**Weak acids:** Acetic acid, Chloro acetic acid, Dichloro acetic acid, Trichloro acetic acid, Propinoic acid and butyric acid]
4. Dibasic acid(Oxalic acid) vs strong base (NaOH)& determination of pK_{a1} and pK_{a2}
5. Redox titrations:

a) Fe(II) vs Ce(IV) and calculation of formal redox potential of Fe(II)/Fe(III)

b) Fe(II) vs MnO_4^-

c) Fe(II) and V (v) vs Ce (IV)

d) I^- vs MnO_4^-

6. Precipitation titrations

a) Mixture of halides (KCl & KI) vs $AgNO_3$

b) Mixture of KSCN & KI vs $AgNO_3$

7. Fe (III) vs EDTA (Complexometric titration)

Suggested Books

1. Senior Practical Physical Chemistry, B.D. Khosla,V.C Garg.
2. Experimental Physical Chemistry, Athawale,V.D., New Age International

Semester X

Subject Code	Subject	Instruction Hrs /Week	Internal Assessment. Marks	Max Marks Sem. Exams	Duration of Sem. Exam. Hrs
	PROJECT				
FYIC -Project					
Project Seminar				100	
Project Pre-Viva				100	
Project Dissertation				400	
	Total			**600**	