FIVE YEAR INTEGRATED M.Sc. COURSE (CHEMISTRY) SYLLABUS

Semester-VII

Subject code	Subject	Instruction Hrs/week	Internal Assessment Marks	Max. Marks Sem. Exam.	Duration of Sem.Exam.Hrs
	THEORY				
FYIC-T701	Group theory and Spectroscop	4 Hrs	20	80	3
FYIC-T702	Organic Chemistry	4 Hrs	20	80	3
FYIC-T703	Physical Chemistry	4 Hrs	20	80	3
FYIC-T704	Analytical Chemistry	4 Hrs	20	80	3
	Seminar	2 Hrs			
	PRACTICALS				
FYIC-P705	Inorganic Chemistry Lab	6 Hrs		100	6
FYIC-P706	Organic Chemistry Lab	6 Hrs		100	6
FYIC-P707	Physical Chemistry Lab	6 Hrs		100	6
	Total	**34+2 Hrs**	**80**	**620**	

Semester-VIII

Subject code	Subject	Instruction Hrs/week	Internal Assessment Marks	Max. Marks Sem. Exam.	Duration of Sem.Exam.Hrs
	THEORY				
FYIC-T801	Bioinorganic Chemistry	4 Hrs	20	80	3
FYIC-T802	Organic Chemistry	4 Hrs	20	80	3
FYIC-T803	Physical Chemistry	4 Hrs	20	80	3
FYIC-T804	Physical-Organic Chemistry	4 Hrs	20	80	3
	Seminar	2 Hrs			
	PRACTICALS				
FYIC-P805	Inorganic Chemistry Lab	6 Hrs		100	6
FYIC-P806	Organic Chemistry Lab	6 Hrs		100	6
FYIC-P807	Physical Chemistry Lab	6 Hrs		100	6
	Total	**34+2 Hrs**	**80**	**620**	

FIVE YEAR INTEGRATED M.Sc. COURSE(CHEMISTRY) SYLLABUS
SEMESTER - VII

Paper I FYIC 701 (Group Theory and Spectroscopy)

IC 01: Group Theory
IC 02: Molecular Orbital Theory – Bonding in Molecules and Metal Complexes
IC 03: Electron Spectroscopy of Metal Complexes
IC 04: Nuclear Quadrupole Resonance and Mossbauer Spectroscopy

Paper II FYIC 702 (Organic Chemistry)

OC-01- Conformational Analysis (cyclic systems)
OC-02- Principles of Asymmetric synthesis
OC-03- Methodology of asymmetric synthesis
OC-04: Synthetic Strategies

Paper III FYIC 703 (Physical Chemistry)

PC-01: Chemical kinetics – II
PC-02: Supramolecular Chemistry - I
PC-03: Electrochemistry – II
PC- 04: Lasers in Chemistry

Paper IV FYIC 704 (Analytical Chemistry)

GP 01: High Performance Liquid Chromatography
GP 02: Atomic Spectroscopy
GP 03: Diffraction Methods
GP 04: Thermal analysis& Radiochemical methods and Process Instruments
-Automated analysis

FIVE YEAR INTEGRATED M.Sc.(CHEMISTRY) COURSE
SEMESTER VII

Paper- I FYIC 701 (Group Theory and Spectroscopy)

IC 01: Group Theory
IC 02: Molecular Orbital Theory – Bonding in Molecules and Metal Complexes
IC 03: Electron Spectroscopy of Metal Complexes
IC 04: Nuclear Quadrupole Resonance and Mossbauer Spectroscopy

IC 01: Group Theory

Representation of Symmetry Elements: Simple Matrices, Block-Factorization, Matrix Representation of E, C_n, S_n, i and σ. Elements - Representation of Point Groups: Reducible and Irreducible Representations, Character of a Matrix and Representation, Properties of Irreducible

Representations, Construction of Character Tables for some simple Point Groups – Mulliken Symbolism for Irreducible Representations - Standard Reduction Formula – Direct Products – Symmetry Properties of Atomic Orbitals and Terms.
Normal Modes: Number, Type and Symmetry – Symmetry of Normal Modes of Molecules: Cartesian and Internal Coordinate Methods of Analysis – Normal Mode Analysis of Molecules with C_{nv} (n=2,3,4), C_{nh} (n=2,3), D_{nh} (n=2,3,4), T_d and O_h Point Groups – Internal Coordinates and Redundancy (Qualitative concept).

IC 02: <u>Molecular Orbital Theory – Bonding in Molecules and Metal Complexes</u>

Born-Oppenheimer approximation. MO theory of H_2^+ ion. Calculation of Ψ for MOs and their energies. Evaluation of the overlap integral. Probability curves and energy 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, Construction (Only) of Ψ using LCAO method.

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: <u>Electronic Spectroscopy of Metal Complexes</u>

Strength of Crystal Fields – Effect of Weak Crystal Fields on Terms – Ligand Field Term Diagrams: Orgel Diagrams for d^1-d^9 Configurations, 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 of 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 O_h and T_d Metal Complexes of 3d Metals – Calculation of 10Dq Values, Racah Parameter (B) and Nephelauxetic Ratio (β) – Charge Transfer Spectra

IC 04: Nuclear Quadrupole Resonance and Mossbauer Spectroscopy

<u>Nuclear Quadrupole Resonance Spectroscopy</u>

Electrostatic Field Gradiant (EFG) at Nuclei - Interaction with Nuclear Quadrupole Moments - Experimental Considerations - Quadrupole Coupling Constants - Nuclear Quadrupole Energy Levels and Transitions for Nuclei of different Spins - Effect of Magnetic Field - Interpretation of e^2Qq_{mol} Values for Diatomic Halides – Determination of Nuclei in different chemical environments - Determination of isomers and - Determination of bond ionicities from QCC values.

<u>Mossbauer Spectroscopy</u>

Principles, 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.

SUGGESTED BOOKS

1. Symmetry and Spectroscopy of Molecules, K. Veera Reddy**,** New Age International (P) Limited, Publishers (1998)
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. Electronoc Spectroscopy, A. B. P. Lever
9. Intorduction to Ligand fields, B. N. Figgis
10. Structural Methods in Inorganic Chemistry, E. A. V. Ebsworth, D. W. H. Rankin and S. Craddock, ELBS.
11. Physical Methods in Chemistry, R. S. Drago, W.B. Saunders Co., 1977.
12. NMR, NQR, EPR and Mossbauer Spectroscopy in Inorganic Chemistry, by R.V. Parish, Ellis Horwood.
13. Inorganic Spectroscopic Methods, Alan K. Brisdon, Oxford Science Publication, 1998.
14. Physical Methods for Inorganic Biochemistry, Wright, Hendrickson, Osaki and James, 1986.
15. Chemical Structure and Bonding, R.L. Decock and H.B. Gray.
16. Physical Methods for Chemists, Russell S. Drago Second edition, Saunders College Publishing, 1992.
17. Principles of Mossbauer spectroscopy, T. C. Gibb, Chapman and Hall, London, 1976.
18. Mossbauer Spectroscopy, N. N. Greenwood and T. C. Gibb, Chapman and Hall, London, 1971.

Paper- II FYIC 702 (Organic Chemistry)

OC-01- Conformational Analysis (cyclic systems)
OC-02- Principles of Asymmetric synthesis
OC-03- Methodology of asymmetric synthesis
OC-04: Synthetic Strategies

OC 01- Conformational analysis (Cyclic systems) 15 Hrs

Study of conformations of cyclohexane, mono, di and polysubstituted cyclohexanes, cyclohexene, cyclohexanone (2-alkyl and 3 -alkyl ketone effect), 2-halocyclohexanones, cyclopentane, cyclobutane, cycloheptane, cyclooctane. Stereo chemistry of decalins, bicyclo[3,3,O]octane and hydrindanes, perhydroanthracene.

Conformational structures of piperidine, N-Methylpiperidine, tropane, tropine, pseudotropine, decahydroquinoline and quinolizidine.
Conformaijonal effects on the stability and reactivity of diastereomers in cyclic molecules - steric and stereo electronic factors - examples
Factors governing the reactivity of axial and equatorial substituents in cyclohexanes.
Stereochemistry of addition to the carbonyl group of a rigid cyclohexanone ring.

OC 02- Principles of asymmetric synthesis 15 Hrs

Introduction and terminology: Topocity in molecules Homotopic, stereoheterotopic (enantiotopic and diastereotopic) groups and faces- symmetry, substitution and addition criteria.Prochirality nomenclature: Pro-R, Pro-S ,Re and Si.
Selectivity in synthesis: Stereospecific reactions (substrate stereoselectivity). Stereoselective reactions (product stereoselectivity) :Enantioselectivity and diastereoselectivity.
Conditions for stereoselectivity: Symmetry and transition state criteria, kinetic and thermodynamic control. Methods for inducing enantio and diastereoselectivity.
Analytical methods: % Enantiomer excess, % enantioselectivity , optical purity, % diastereomeric excess and % diastereoselectivity. Techniques for determination of enantioselectivity: Specific rotation, Chiral ^{1}H nmr, Chiral lanthanide shift reagents and Chiral HPLC.

OC 03- Methodology of asymmetric synthesis: 15 Hrs

Classification of asymmetric reactions into l.substrate controlled, 2. chiral auxiliary controlled, 3. chiral reagent controlled and 4. chiral catalyst controlled.
1. Substrate controlled asymmetric synthesis: Nucleophilic additions to chiral carbonyl compounds. 1,2- asymmetric induction, Cram's rule and Felkin-Anh model.
2. Chiral auxiliary controlled asymmetric synthesis: α-Alkylation of chiral enolates, azaenolates, imines and hydrazones. Chiral sulfoxides. 1, 4-Asymmetric induction and Prelog's rule. Use of chiral auxiliaries in Diels-Alder and Cope reactions.
3. Chiral reagent controlled asymmetric synthesis: Asymmetric reductions using BINAL-H. Asymmetric hydroboration using IPC_2 BH and $IPCBH_2$.Reductions with CBS reagent.
4. Chiral catalyst controlled asymmetric synthesis: Sharpless, Jacobsen and Shi asymmetric epoxidations. Sharpless asymmetric dihydroxylation and amino hydroxylation. Asymmetric hydrogenations using chiral Wilkinson biphosphine and Noyori catalysts. Chiral catalyst controlled Diels- Alder reactions, Enzyme mediated enantioselective synthesis:
5. Asymmetric aldol reaction, Diastereoselective aldol reaction and its explanation by Zimmerman-Traxel model. Auxiliary controlled aldol reaction. Double diastereoselection-matched and mismatched aldol reactions.

OC-04 - Synthetic Strategies: 15 Hrs

Synthetic Strategies, Terminology: target, synthon, synthetic equivalent, functional group interconversion (FGI), functional group addition, functional group elimination. Crieteria for selection of target. Linear and convergent synthesis. Retrosynthetic analysis and synthesis involving chemoselectivity, regioselectivity, reversal of polarity and cyclizations. Strategic bond: Criteria for disconnection of strategic bonds. One group and two group C-X disconnections. One

group C-C disconnections. Alcohol and carbonyl compounds. Two group C-C disconnections; DielsAlder reaction, 1,3-difunctionalised compounds, 1,5- difunctionalised compounds, Michael addition and Robinson annulation, synthesis of (+) Disparlure by retro synthetic approach.

Recommended Books:

1. Stereochemistry of organic compounds — Principles & Applications by D Nasipuri
2. The third dimension in organic chemistry, by Alan Bassendale
3. Stereochemistry: Conformation & Mechanism by P S Kalsi
4. Stereochemistry of Carbon compounds by Ernest L Eliel
5. Stereoselectivity in organic synthesis by R S Ward.
6. Asymmetric synthesis by Nogradi
7. Asymmetric organic reactions by it) Morrison and HS Moschcr
8. Stereo differentiating reactions by Izumi
9. Some modern methods of organic synthesis by W Carruthers
10. Guidebook to organic synthesis, by R K Meckie, D M Smith & R A Atken
11. Organic synthesis by Michael B Smith
12. Enzyme structure and mechanism by Fersht and Freeman
13. Bio-Organic chemistry by Hennan Dugas
14. Nucleic acids in Chemistry and Biology by G M Blackbum MI Gait
15. Lehninger Principles of Biochemistry by D L Nelson and M M Cox
16. Outlines of Biochemistry by Conn and Stumpf
17. Biotransformations in Organic Chemistry byK Faber.

Paper- III FYIC 703 (Physical Chemistry)

PC-01: Chemical kinetics – II
PC-02: Supra molecular Chemistry - I
PC-03 : Electrochemistry – II
PC- 04: Lasers in Chemistry

PC-01: Chemical kinetics – II **(15hrs)**

Review of the transition-state theory. Application to reaction between atoms and molecules. Limitations of the transition-state theory.

Unimolecular reactions: Modification of Lindemann's theory. Hinshelwood treatment, RRK treatment and RRKM treatment.Reactions in solution: Factors affecting reaction rates in solution. Diffusion controlledr eactions. 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.

Electron transfer reactions: Inner sphere and outer sphere redox reactions. Marcus theory, the physical model. Marcus cross relation and calculation of rate constant of a bimolecular reaction.

Chain reactions: Decomposition of N_2O_5. Hydrogen-oxygen reaction and the explosion limits. Decomposition of ethane and acetaldehyde – the Rice-Herzfeld mechanisms.Fast reactions: Flow methods and the stopped-flow technique. Relaxation methods (T-jump and P-jump). Kinetic equations for chemical relaxation.

PC-02:Supramolecular Chemistry - I **(15 hrs)**

Basic Concepts of Host-Guest Complexation(Ionophore Chemistry).

General Principles of Molecular Recognition, Complex Formation and Host Design- Thermodynamics of Multi-Site Host-Guest Complexation: Macrocycles, Clefts and Open-chain Host Structures- Ionophores for Cations: Chelate, Macrocyclic and Cryptate Effects- Complexation Selectivity: the Hole-Size Concept and its Limitations- Enthalpy and Entropy Contributions and compensations- Heat Capacity Changes and Pre-organization- Ionophores for Anions: Macrocycles with secondary binding sites- Lariat Ethers, Ditopic Receptors, Co-complexation and Second-sphere Coordination- Conformational Coupling Between binding sites: Cooperativily, Allosteric Effects and Induced Fit.

PC –03 : 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. 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: Lasers in Chemistry: **(15 hrs)**

General principles of laser action. Stimulated emission. Rates of absorption and emission. Einstein coefficients. 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.

References

1. Chemical Kinetics, K. J. Laidler, McGraw Hill
2. Kinetics and Mechanism, A. A. Frost & R. G. Pearson, John Wiley & sons

3. Kinetics and Mechanism of Chemical Transformations, J. Rajaraman & J. Kuriacose, McMillan
4. Chemical Kinetics and Reaction Mechanisms, J. H. Espenson, McGraw Hill
5. Physical Organic Chemistry, N. S. Isaacs, ELBS
6. The Physical basis of Organic Chemistry, Howard Maskill, Oxford University Press
7. Rates and Equilibriums of Organic Reactions, J. E. Leffler & E. Grunwald, Dover publications
8. Reaction Dynamics, edited by N. Sathyamurthy, Narosa Publishing House
9. Modern Electrochemistry, J. O. M. Bockris & A. K. N. Reddy, Plenum
10. Advanced Physical Chemistry, J.N.Gurtu and H. Snehi, Pragati Prakashan, Meerut.
11. Physical Chemistyr: A molecular approach, McQuarie Simon, Viva Books Pvt. Ltd. New Delhi.
12. Atkin's Physical Chemistry, P. Atkins & Julio de Paula, Oxford University Press
13. A Guide to Lasers in Chemistry, G. R. Van Hecke & K. K. Karukstis, Jones and Bartlett Publishers
14. Lasers in Chemical and Biological Sciences, S. Chopra & H. M. Chawla, Wiley Eastern Ltd

Paper- IV FYIC 704 (Analytical Chemistry)

GP 01: High Performance Liquid Chromatography
GP 02: Atomic Spectroscopy
GP 03: Diffraction Methods
GP 04: Thermal analysis& Radiochemical methods and Process Instruments
-Automated analysis

GP 01: High Performance Liquid Chromatography

Theoretical considerations- retention time (t_R), retention volume (V_R), Distribution coefficient (K_D). Plate theory- Column efficiency, Height Equivalent to Theoretical Plate (HETP), number of theoretical plates(n). Rate theory- Van Deemter's equation.

HPLC: Theory, instrumentation (block diagram), pumps, isocratic and gradient systems, columns, separation modes-stationary phases (adsorption, bonded phase, reverse phase, ion exchange, affinity, ion pair, ion exchange and chiral - stationary phases), properties of mobile phases. Detectors- UV, Fluorescence, refractive index, elcrochemical, multipurpose detectors. Derivatization techniques. Quantitation- External and internal standard methods.

Hyphenated technique: HPLC-MS - Introduction to Interfaces – Moving belt interface, particle beam interface, electrospray method, thermospray method and atmospheric pressure chemical ionization method.

GP 02: Atomic Spectroscopy

Atomic Absorption Spectroscopy (AAS): Principles and Instrumentation of AAS – Flame and Furnace AAS - Resonance Line Sources, Sensitivity and Detection Limits - Interferences – Chemical and Spectral Evaluation Methods - Applications in Qualitative and Quantitative Analysis.

Atomic Emission Spectroscopy (AES) and Inductively Coupled Plasma (ICP-AES)
Principle of AES – Instrumentation - Evaluation Methods - Application in Quantitative Analysis - 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.
ICP-MS- Principle, Instumentation – applications.

Atomic Fluorescence spectroscopy- Principle, instrumentation – applications.
X-ray fluorescence: Introduction, instrumentation, applications.

GP 03: Diffraction Methods

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 Absorption - Structural Analysis of Crystals - Laue's, Bragg's and Debye Scherror Methods - Interpretation of NaCl and KCl Crystal Structures - 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 - Radial Distribution Curves - Interpretation of Results for $PBrF_2S$, PF_3S, PF_2HS, $HClO_4$, Silyl monothioacetate and Germyl monothioacetate and $HgCl_2$ molecules - Advantages and Limitations.
Neutron Diffraction: Principles - Application in Hydrogen Bonding Studies - Combined use of X-ray and Neutron Diffraction Studies - Advantages and Limitations.

GP 04: Thermal analysis & Radiochemical methods and Process Instruments -Automated analysis

Thermal analysis: Differential Scanning calorimetry and differential analysis, Thermogravimetry- evolved gas detection and analysis. Methodology of thermogravimetry, Differntial scanning calorimetry and differential thermal analysis. Thermomechanical analysis, Dynamical mechanical analysis, thermometric titrimetry and direct – injection enthalpies – problems.
Radiochemical methods: Nuclear reactions and radiations, measurement of radioactivity, Neutron activation analysis, isotope dilution analysis, Liquid scintillation systems.

Process instruments and automated analysis: Introduction, Automation strategy – Production of high quality drinking water and the treatment of waste water. Industrial process analyzers, Chemical sensors, Laboratory robots.

Recommended Books:

1. Vogel's Text Book of Quantitative Chemical Analysis, 6th edition.
2. Modern Analytical Chemistry, David Harvey, Mc Graw Hill Publication 2000.
3. Analytical Chemistry, Skoog and West, 6th Edition.
4. Instrumental methodology in Chemical Analysis, Galen W. Ewing.
5. Mass Spectrometry for Chemists and Bio-chemists, Robert A.W. Johnstone
6. and Malcolm. E. Rose, 2nd Edition.

7. Principles of Instrumental Analysis, Skoog, Holler & Neiman
8. Structural Methods in Inorganic Chemistry, E.A.V. Ebsworth, David B.H. Rankin and Stephen Cradock.
9. Analytical NMR Ed. Ld. Field and S. Stern hill, John Wiley and Sons Ltd, 1989.
10. Mass Spectrometry- Principles & Applications, Hoffman & Stroobant, 2nd Ed. (Wiley) 2003.
11. Mass Spectrometry for Chemists and Bio-chemists, Robert A.W. Johnstone and Malcolm. E. Rose, 2nd Edition.
12. Principles of Instrumental Analysis, Skoog, Holler & Neiman

Semester - VII

Laboratory Papers

FYIC – 705 : Inorganic Chemistry Lab - (Paper -V) 6 hrs/week

I. Laboratory preparation and Characterization of 3d metal Complexes.

1. $VO(acac)_2$
2. $[Co(NH_3)_6][Co(NO_2)_6]$
3. Prussian Blue and Turnbull Blue.

Analysis:

II. Spectrophotometry

1. Estimation of manganese
2. Estimation of Chromium
3. Determination of composition Fe(II) - o-Phen complex by Job's Method and Mole ratio method.

III. Conductometry

Determination of the composition of Cu(II) oxine and Cu(II) EDTA complexes

SUGGESTED BOOKS:

1. Practical Inorganic Chemsitry, G. Marr and B. W. Rockett.
2. Experimental Inorganic/Physical Chemistry, M.A. Malati.
3. Chemistry Experiments for Instrumental Methods, Donald T. Sawyer William. etal
4. Analytical Chemistry by Gary D. Christian.
5. A Text Book of Quantitative Inorganic Analysis by A.I. Vogel
6. Vogel's Text Book of Quantitative Inorganic Analysis, Jeffery etal.
7. Vogel's Text Book of Quantitative Chemical Analysis.
8. Analytical Chemistry Theory and Practice by R.M. Verma.
9. Determination and use of Stability Constants – Martell and Motekaitis.
10. Metal Complexes in Aqueous Solution A.E. Martell and R.D. Handcock.

FYIC – 706: Organic Chemistry Lab - (Paper -VI) 6 hrs/week

Synthesis, Separation and identification of organic compounds:

1. **Synthesis of organic molecules :** 2-Phenyl indole (Fischer indole synthesis), 2,5-Dihydroxy acetophënone (Fries reaction)), Benzilic acid from benzoin (rearrangement), Photo-dimerization of maleic anhydride, benzophenone (Friedel-Crafts reaction), Benzanilide (Beckmann rearrangement), Vanillyl alcohol from vanillin ($NaBH_4$ reduction), Phenytoin, benzocaine, antipyrine.

1. **Separation of two component mixtures by chemical methods and their identification by chemical reactions** — separation by using solvent ether, 5% aq. hydrochloric acid, 5 % aq sodium bicarbonate and 5% sodium hydroxide solutions, checking the purity of the two components by TLC, identification of the compounds by a systematic study of the physical characteristics (m p / b p), 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. **Thin layer chromatography**: Determination of purity of a given sample, monitoring the progress of chemical reactions, identification of unknown organic compounds by comparing the R_f values of known standards.

Recommended Books.

1. The systematic identification of organic compounds by R L Shriner, R C Fusion and D Y Curtin . I
2. A textbook of practical organic chemistry by A I Vogel, Vol I and II
3. Unitized experiments in organic chemistry by R Q Brewster and others
4. Practical Organic Chemistry by Mann and Saunders

FYIC – 707: Physical Chemistry Lab (Paper- VII) 6 hrs/week

Chemical Kinetics

- Study of peroxydisulphate – iodide reaction:
  Individual orders of the reactants by initial rate methods
  Effect of temperature on reaction rate
  Effect of ionic strength on reaction rate
- Study of peroxydisulphate – iodide reactions, uncatalyzed and Cu(II)-catalyzed reactions.
- Study of acetone – iodine reaction by Spectrophotometry
  Order w.r.t.[iodine]
  Order w.r.t. [acetone]
  Order w.r.t. $[H^+]$

SUGGESTED BOOKS:

1. Junior Practical Physical Chemistry By Khosla and Gard.

2. Senior Practical Physical Chemistry By Khosla and Gard.
3. Text Book of Practical Chemistry By Vogel

FIVE YEAR INTEGRATED M.Sc. COURSE(CHEMISTRY)

SEMESTER- VIII

Paper- I FYIC 801(Bioinorganic Chemistry)

IC 01: Metal Ion Interactions with Nucleic Acids and their Constituents
IC 02: Transport of Oxygen, Electrons and Metal Ions
IC 03: Metalloenzymes of Iron, Zinc and Nickel
IC 04: Metalloenzymes of Cobalt, Copper and Molybdenum

Paper- II FYIC 802 (Organic Chemistry)

OC 01- Pericyclic reactions
OC 02- Photochemistry
OC 03- New synthetic reactions
OC 04- Introduction to Drug design and drug discovery

Paper- III FYIC 803(Physical Chemistry)

PC – 01 : Applications of Schrödinger equation
PC -02: Statistical Thermodynamics
PC - 03. Non-equilibrium Thermodynamics
PC-04: Nanoparticles and their applications

Paper- IV FYIC 804 (Physical-Organic Chemistry)

POO 1: MO and VB theory of reactivity
POO 2: Kinetic, isotopic, structural, solvent, steric and conformatlonal effects
POO 3: Nucleophilic, electrophilic and free radical reactivity
POO 4: Supramolecular chemistry - II

FIVE YEAR INTEGRATED M.Sc. COURSE(CHEMISTRY)
SEMESTER- VIII

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IC 03: Metalloenzymes of Iron, Zinc and Nickel
IC 04: Metalloenzymes of Cobalt, Copper and Molybdenum

IC 01: Metal Ion Interactions with Nucleic Acids and their Constituents

Proton Binding Sites of Nucleic Acid Constituents: Purine and Pyrimidine Bases, Nucleosides and Nucleotides - 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 Sites in Nucleosides, Nucleotide - Metal Ion Interactions - Intramolecular Equilibrium Constant K_I, 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 – Concept of T_M.

IC 02: Transport of Oxygen, Electrons and Metal Ions

Transport of Electrons: Iron-Sulphur Proteins: Rubredoxins and Ferredoxins (2Fe, 3Fe, 4Fe, 8Fe Proteins) - High Potential Iron-Sulphur Proteins – Structural and Spectral features of Iron-Sulphur Proteins - Electron-transport by Cytochromes, Azurin and Plastocyanin - Importance of Structures of Azurin and Plastocyanin in facilitating Rapid Electron Transport.

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 03: Metalloenzymes of Iron, Zinc and Nickel

Iron Enzyme: Structural and Mechanistic Aspects of Cytochrome P_{450}, Cytochrome oxidase, Catalase and Peroxidase - Role of the Metal Ion.
Zinc Enzymes: Structural and Mechanistic Aspects of Carbonic Anhydrase, Carboxy Peptidase, Alcohol Dehydrogenase - Role of Zinc.
Nickel Enzyme: Urease, Hydrogenase and Factor F_{430}: Reactions Catalysed , Mechanistic Aspects.

IC 04: Metalloenzymes of Cobalt, Copper and Molybdenum

Cobalt Enzymes: Cobalt in Vitamin B_{12} - Structural Features of Vitamin B_{12} with reference to coordination of Cobalt - Different Oxidation States of Cobalt - Various forms of Vitamin B_{12} and Active Enzyme forms - Types of Reactions Catalysed by i) Methyl Cobalamin ii) Deoxyadenosyl Cobalamin - Mechanism of the Methyl Malonyl CoA conversion to Succinyl CoA - Role of the Apoenzyme - Unique features of Cobalt to suit Vitamin B_{12}.

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, Xanthine oxidase and Sulfite oxidase.

SUGGESTED BOOKS

1. Bioinorganic Chemistry, Bertini, Gray, Lippard and Valentine, University Science Books, California USA 1994.
2. Principles of Bioinorganic Chemistry, S.J. Lippard and M.Berg University Science Books, Calfornia 1994.
3. Biological Chemistry of Elements, J.J.R. Franstodasilva and R.J.P. Williams Oxford University Press 1991.
4. Metal Ions in Biological Systems (Series), Ed. H. Sigel Marcel Dekkar, New York
5. Inorganic Biochemistry, J.A. Cowan, VCH publishers 1993.
6. Advances in Inorganic Biochemistry, edited by G.L.Eichorn & Marzilli
7. Bioinorganic Chemistry, Vol-I edited by G.L.Eichorn.
8. J.Chem.Edn 52(1975) 754, Earl. Frieden. (**For Unit 2**)
9. Helmut Sigel: **(For Unit 2)**
   Angew. Chem. Inter. Edit, 14(1975) 394; J. Am.Chem.Soc, 99(1977) 4489; J.Am.Soc. 102(1980) 2998; Inor. Chem. 22(1983) 925; J.Am.Soc. 98 (1976) 730; Chemical Society Reviews (1993) 255; J.Am.Soc. 103(1981) 248; J.Am.Soc 99 (1977) 3142.

Paper- II FYIC 802 (Organic Chemistry)

OC 01- Pericyclic reactions
OC 02- Photochemistry
OC 03- New synthetic reactions
OC 04- Introduction to Drug design and drug discovery

OC-01: New synthetic reactions: 15 Hrs

Baylis-Hillman reaction, RCM olefm metathesis, Grubb catalyst, Mukayama aldol reaction, Mitsunobu reaction, McMurrey reaction, Julia-Lythgoe olefination, and Peterson's stereoseleetive olefination, Heck reaction, Suziki coupling, Stille coupling and Sonogishira coupling,Buchwald-Hartwig coupling, Eishenmosher-Tanabe fragmentation and Shapiro reaction, Aza-Cope and Aza-Wittig reaction, BINAL and BINAP assisted reactions. Ugi reaction,Click reaction
Mannich reaction, Robinson annulations, . Stork-enamine reaction and . Umpolung use of dithio acetals,

OC-02: Pericyclic reactions 15 Hrs

Characteristics — Types of pericyclic reactions — Electrocyclic, cycloaddition — cycloreversion and sigmatropic reactions — examples — 4n and 4n+2 electron type — stereospecif,city. Theories involved in understanding pericyclic reactions.
1) Aromatic Transition states theory — concept — Woodward-Hoffmarn se1ection rules for electrocyclic reactions, cycloaddition — cycloreversions and sigmatropic reactions based on ATS aromatic transition state (Huckel-Mobius)approach. Examples.

2) Frontier Molecular Orbital Theory concept — Woodward-Hoffmann selection rules for electrocyclic, cycloaddition — cycloreversion and sigmatropic reactions based on FMO approach. Examples .
3) Conservation of Molecular Orbitals Theory concept — Framing of Woodward-Hoffmantn selection rules for electrocyclie, cycloaddition and cycloreversions based on Conservation of Molecular Orbitals approach.

OC-03: Photochemistry **15 Hrs**

Photochemistry of π,π* transitions: Excited states of alkenes, cis-trans isomerisation, photostationary state, electrocyclisation and sigmatropic rearrangements, di-π methane rearrangement. Intermolecular reactions, photocycloadditions, photodimerisation ofsimple and conjugated olefins.Photoisimerisation of benzene

Photochemistry of n,π* transitions:Excited states of carbonyl compounds, hemolytic cleavage of α- bond Norrish type I reaction in acyclic and cyclic ketones and strained cycloalkanediones.

Intermolecular abstraction of hydrogen: photoreduction and influence of temperature, solvent and nature of hydrogen donor and structure of the substrate

Intramolecular abstraction of hydrogen:Norrish type II reaction, Addition to carbon-carbon multiple bonds, Paterno-Buchi reaction, Photochemistry of nitrites-Barton reaction

OC-04: Introduction to Drug design and drug discovery **15 Hrs**

Introduction to drug discovery. Folklore drugs. Natural products as lead structures in drug discovery.Structure pruning technique in lead modification e.g. morphine. Serendipitious discovery of leads e.g.Penicillin and Librium. Drug targets and receptor theory. Nature of drug-receptor interactions. Pharmacodynamics and pharmacokinetics (ADME) of drugs. Agonists, antagonists and enzyme inhibitors. Discovery of lead structure from natural harmones and neurotransmitters. Existing drugs as leads (me too drugs). Principles of design of agonists (e.g.Salbutamol), antagonists e.g. cimitidine) and enzyme inhibitors (e.g. captopril). Principles of prodrug design. Molecular graphics based lead discovery. Introduction to drug patents and Clinical trials.

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
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

Recommended Books for photochemistry

1. Molecular Reactions and Photo chemistry by Depuy and Chapman
2. Photochemistry by C W S Wells
3. Organic Photochemistry by Turro
4. Molecular Photochcmistry by Gilbert & Baggo
5. Organic Photochemistty by D Coyle
6. Optical rotatory cispersion by C Djerassi
7. Optical rotatory dispersion and circular dichroism by P Crabbe
8. Mechanism and Structure in Organic chemistry by S Mukherjee
9. Advanced Organic Chemistry: Reactions, Mechanisms & Structure by Jerry March
10. Pericyclic Reactions by Mukherjee
12. Conservation of Orbital Symmetry by Woodward and Hoffmann
13. Organic Reactions and Orbital Symmetry, Gilchrist and Storr
14. Pericyclic Reactions — a problem solving approach, Lehr and Merchand
15. The Nature of Chemistry — Units 17-19 - Aromaticity — Open University, U K. Publications

Recommended Books for spectroscopy:

1. Spectroscopic identification of organic compounds by RM Silverstein, G C Bassler and T B Morrill
2. Organic Spectroscopy by William Kemp
3. Spectroscopic methods in Organic chemistry by DH Williams and I Fleming
4. Modern NMR techniques for chemistry research by Andrew B Derome
5. NMR in chemistry - A multinuclear introduction by William Kemp
6. Spectroscopic identification of organic compounds by P S Kalsi
7. Introduction to organic spectroscopy by Pavia
8. Carbon-13 NMR for organic chemists by GC Levy and O L Nelson

Recommended Books for Drug design

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

Paper- III FYIC 803(Physical Chemistry)

PC – 01 : Applications of Schrödinger equation
PC -02: Statistical Thermodynamics
PC - 03. Non-equilibrium Thermodynamics
PC-04: Nanoparticles and their applications

PC – 01 : 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.
Atoms in external field, Zeeman and anomalous Zeeman effect.

PC -02: 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 - 03. 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.

PC-04: Nanoparticles and their applications (15hrs)

Introduction to nano particles. Preparation of nano particles –various methods- RF plasma, chemical methods, thermolysis, pulsed laser methods, optical and electrical properties of nanoparticles. Characterization of nano particles-experimental methods-powder X-ray diffraction, transmission electron microscopy (TEM), scanning electron microscopy (SEM) and atomic force microscopy(AFM).
Reduced dimensionality in solids – zero dimensional systems, fullerenes, quantum dots. Optical properties of quantum dots. One dimensional systems, carbon nano tubes, electric, mechanical and other properties.
Applications of nano particles in – photocatalysis, laser and light emitting diodes, optical filters, optical band gap materials. Use of carbon nano tubes in fuel cells and catalysis.

References for paper

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. Elements of Statistical Thermodynamics, L. K. Nash, Addison – Wesley
6. Introduction to Statistical Thermodynamics, T. L. Hill, Addison Wiley
7. Statistical Thermodynamics, M. C. Gupta, New Age International
8. Atkin's Physical Chemistry, P. Atkins & Julio de Paula, Oxford University Press

9. Molecular Thermodynamics, D. A. McQuarrie & J. D. Simon, University Science Books

Paper- IV FYIC 804 (Physical-Organic Chemistry)

PO-01: MO and VB theory of reactivity
PO-02: Kinetic, isotopic, structural, solvent, steric and conformatlonal effects
PO-03: Nucleophilic, electrophilic and free radical reactivity
PO-04: Supramolecular chemistry

PO-0 1- 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.

PO-0 2: 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.

PO-0 3: 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.

PO-0 4: Supramolecular chemistry-II **15 Hrs**

Properties of covalent bonds- bond length, inter-bond angles, force constant, bond and molecular dipole moments. Molecular and bond polarisability, bond dissociation enthalpy, entropy. Intermolecular forces, hydrophobic effects. Electrostatic, induction, dispersion and resonance energy, magnetic interactions, magnitude of interaction energy, forces between macroscopic bodies, medium effects, Hydrogen bond. Principles of molecular association and organization as exemplified in biological macromolecules like enzymes, nucleic acids, membranes and model systems like micelles and vesicles. Molecular receptors and design principles. Cryptands, cyclophanes, calixeranes, cyclodextxins. Supramolecular reactivity and catalysis. Molecular channels and transport processes. Molecular devices and nanotechnology.

References

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

Semester – VIII
Laboratory Papers

FYIC – 805: Inorganic Chemistry Lab (Paper-V) 6 hrs/week

Instrumental Methods:

I. **Potentiometry:**

(i) Determination of Fe^{2+}in Iron wire usng $KMnO_4$
(ii) Determination of Ferrous and Vanadyl in a mixture by Ceric Ammonium Nitrate.
(iii) Determination of Halides (Cl^-& I^-) in a mixture using Silver ion Electrode.

II. pH metry:

1. Determination of Dissociation Constants
   i) Glycine
   ii) Ethylene diamine
2. Determination of Stability Constants of Binary Complexes
   i) Glycine : Ni
   ii) Glycine : Cu
   iii) Ethylene diamine - Ni
3. Determination of Stability Constants of Ternary Complexes
   i) Glycine : Ethylene diamine : Ni

SUGGESTED BOOKS:

1. Chemistry Experiments for Instrumental Methods, Donald T. Sawyer William. etal
2. Analytical Chemistry by Gary D. Christian.
3. A Text Book of Quantitative Inorganic Analysis by A.I. Vogel
4. Vogel's Text Book of Quantitative Inorganic Analysis, Jeffery etal.
5. Vogel's Text Book of Quantitative Chemical Analysis.
6. Analytical Chemistry Theory and Practice by R.M. Verma.
7. Determination and use of Stability Constants – Martell and Motekaitis.
8. Metal Complexes in Aqueous Solution A.E. Martell and R.D. Handcock.

FYIC – 806: Organic Chemistry Lab (Paper-VI) 6 hrs/week

Spectroscopic identification of organic compounds, drug analysis and Isolation of Natural products.

1. Identification of unknown organic compounds by interpretation of IR., UV, ^{1}H-NMR, ^{13}CNMR and Mass spectra. A minimum of 20 representative examples should be studied
2. Estimation of the following drugs: Aspirin (titrimetry), Chloride in Ringer's lactate (argentometry), - Ca+ 2 ions (complexometry, Riboflavin (Colorimetry).
3. Isolation of the following natural products: Caffeine from tea leaves (solvent extraction), Piperine from pepper (Soxhlet extraction).

Recommended books:

1. Textbook of practical organic chemistry by Vogel
2. Practical organic chemistry by Mann and Saunders

FYIC – 807: Physical Chemistry Lab (Paper-VII) 6 hrs/week

Conductometry:

- Conductometric titrations:

  Mixture of strong acid, weak acid and $CuSO_4$ vs strong base
  Mixture of halides (chloride + iodide) vs $AgNO_3$
  Precipitation titration: K_2SO_4 vs $BaCl_2$

- Dissociation constants of weak acids
- Effect of solvent on dissociation constant of a weak acid
- Verification of Onsager equation

pH metry:

- pH – metric titrations:
  Monobasic acids vs strong base Malonic acid Vs NaOH.
  Dibasic acid vs strong base Oxalic acid Vs NaOH.
  Tribasic acid vs strong base H_3PO_4 Vs NaOH.
  Mixture of strong and weak acids vs strong base.
  Determination of dissociation constants of monobasic/dibasic acids by Albert – Serjeant Method.

SUGGESTED BOOKS:

1. Junior Practical Physical Chemistry By Khosla and Gard.
2. Senior Practical Physical Chemistry By Khosla and Gard.
3. Text Book of Practical Chemistry By Vogel.