Course Structure & Syllabus For Integrated M.Sc. Chemistry (Session 2018-2023)

ADAMAS UNIVERSITY DEPARTMENT OF CHEMISTR , Int. M.Sc. SEMESTER-I							
Type of the Paper	**Paper Code**	**Theory / Practical**	**Contact Hour Per Week**	**L**	**T**	**P**	**Credit**
CORE	**Theory**	**Engineering Mathematics-I**	**4**	**3**	**1**	**0**	**4**
CORE	**Theory**	**Engineering Physics - I**	**3**	**3**	**0**	**0**	**3**
CORE	**Theory**	**Computer Programming**	**3**	**3**	**0**	**0**	**3**
CORE	**Theory**	**HSS –I**	**3**	**3**	**0**	**0**	**3**
CORE	**Theory**	**HSS–II (Economics For Engineers)**	**3**	**3**	**0**	**0**	**3**
CORE	**Practical**	**Engineering Physics - I Lab**	**3**	**0**	**0**	**3**	**2**
CORE	**Practical**	**Computer Programming Lab**	**3**	**0**	**0**	**3**	**2**
CORE	**Practical**	**Engineering Drawing and CAD**	**3**	**0**	**0**	**3**	**2**
TOTAL			**25**	**15**	**1**	**9**	**22**

Engineering Mathematics-I: Calculus & Differential Equations
Engineering Mathematics–II: Linear Algebra, PDE, Complex Analysis
HSS-I: From a list of Language related topics
HSS-II: From a list of Economics and Finance related topics
Total Credits (First Year): 48

Course Structure & Syllabus For Integrated M.Sc. Chemistry (Session 2018-2023)

ADAMAS UNIVERSITY DEPARTMENT OF CHEMISTRY , Int. M.Sc. SEMESTER-II							
Type of the Paper	**Paper Code**	**Theory / Practical**	**Contact Hour Per Week**	**L**	**T**	**P**	**Credit**
CORE		**Engineering Mathematics–II**	**3**	**3**	**0**	**0**	**3**
CORE	**Theory**	**HSS – III**	**3**	**3**	**0**	**0**	**3**
CORE	**Theory**	**Engineering Chemistry**	**3**	**3**	**0**	**0**	**3**
CORE	**Theory**	**Electrical and Electronics Technology**	**3**	**3**	**0**	**0**	**3**
CORE	**Theory**	**Life Sciences**	**3**	**3**	**0**	**0**	**3**
CORE	**Theory**	**Engineering Mechanics**	**3**	**3**	**0**	**0**	**3**
CORE	**Practical**	**Engineering Chemistry Lab**	**3**	**0**	**0**	**3**	**2**
CORE	**Practical**	**Electrical and Electronics Technology Lab**	**3**	**0**	**0**	**3**	**2**
CORE	**Practical**	**Engineering Workshop**	**3**	**0**	**0**	**3**	**2**
CORE	**Practical**	**Computing Lab**	**3**	**0**	**0**	**3**	**2**
TOTAL			**30**	**18**	**0**	**12**	**26**

Course Structure & Syllabus For Integrated M.Sc. Chemistry (Session 2018-2023)

ADAMAS UNIVERSITY								
DEPARTMENT OF CHEMISTRY – Int. M.Sc. PROGRAMSEMESTER-III								
Type of the Paper		**Theory / Practical**	**Brief Contents**	**Contact Hour Per Week**	**L**	**T**	**P**	**Credit**
CORE		**Theory** **(Physical I)**	Kinetic theory of gases Advanced thermodynamics Theory of Rate Process and Reaction dynamics Transport Phenomena	**4**	**3**	**1**	**0**	**4**
CORE		**Practical** **(Physical Lab I)**	List of experiments will be provided separately	**3**	**0**	**0**	**2**	**3**
CORE		**Theory** **(Inorganic I)**	Atomic Structure Chemical Bonding Chemical periodicity Nuclear chemistry	**4**	**3**	**1**	**0**	**4**
CORE		**Practical** **(Inorganic Lab I)**	List of experiments will be provided separately	**3**	**0**	**0**	**2**	**3**
CORE		**Practical** **(Inorganic Lab II)**	List of experiments will be provided separately	**3**	**0**	**0**	**2**	**3**
CORE		**Theory** **(Organic I)**	Bonding features in Organic Molecules Organic Reaction Mechanism –I : Mechanistic Classification Organic Reaction Kinetics Nucleophilic Substitution at sp^3center Elimination reaction	**4**	**3**	**1**	**0**	**4**
FOUNDATION (Skill Enhancement Course **SEC)**		**Choice Based** (List of options will be provided separately)		**2**	**2**	**0**	**0**	**2**
GENERIC ELECTIVE III		**Theory**	Engineering Physics II/Engineering Chemistry II	**4**	**3**	**1**	**0**	**3**
		Practical	Engineering Physics II Lab. /Engineering Chemistry II Lab.	**3**	**0**	**0**	**2**	**2**
Total				**30**				**25**

Course Structure & Syllabus For Integrated M.Sc. Chemistry (Session 2018-2023)

ADAMAS UNIVERSITY								
DEPARTMENT OF CHEMISTRY – Int. M.Sc. PROGRAMSEMESTER-IV								
Type of the Paper		**Theory / Practical**	**Brief Contents**	**Contact Hour Per Week**	**L**	**T**	**P**	**Credit**
CORE		**Theory** **(Physical II)**	Quantum Mechanics I and II Colligative properties	**4**	**3**	**1**	**0**	**4**
CORE		**Practical** **(Physical Lab II)**	List of experiments will be provided separately	**3**	**0**	**0**	**2**	**3**
CORE		**Theory** **(Inorganic II)**	Precipitation and Red-ox reactions Coordination Chemistry-I and Chemistry of s- and p- Block Elements Theory of acid-bases	**4**	**3**	**1**	**0**	**4**
CORE		**Theory** **(Organic II)**	Stereochemistry and Conformation Organic Reaction Mechanism –II Substitution at sp^2 carbon) Carbonyl System) Aromatic Substitution (Nucleophilic and Electrophilic), Radical Substitution Addition Reaction	**4**	**3**	**1**	**0**	**4**
CORE		**Practical** **(Organic Lab I)**	List of experiments will be provided separately	**3**	**0**	**0**	**2**	**3**
ELECTIVE (Discipline Specific)		**Theory** **(Material Science)**	Solid state chemistry Nano Science Polymer Chemistry	**4**	**4**	**0**	**0**	**4**
ELECTIVE (Discipline Specific)		**Material Science Lab I**	List of experiments will be provided separately	**3**	**0**	**0**	**2**	**2**
Total				**30**				**24**

Course Structure & Syllabus For Integrated M.Sc. Chemistry (Session 2018-2023)

ADAMAS UNIVERSITY

FACULTY OF SCIENCE

DEPARTMENT OF CHEMISTRY – Int. M.Sc. PROGRAM SEMESTER - V

Type of the Paper		Theory / Practical	Brief Contents	Contact Hour Per Week	L	T	P	Credit
CORE		**Theory** **(Physical III)**	Chemical Equilibrium and Ionic equilibrium Phase Rule Statistical Thermodynamics Colloid and Surface Sciences	**4**	**3**	**1**	**0**	**4**
CORE		**Theory** **(Organic III)**	Pericyclic Reactions Organometallic Chemistry, Nitrogen Compounds Spectroscopy including Fourier Transform methodology Organic Reaction : Reaction to carbon- heteroatom multiple bonds, Rearrangements	**4**	**3**	**1**	**0**	**4**
CORE		**Practical** **(Organic Lab II)**	List of experiments will be provided separately	**3**	**0**	**0**	**2**	**3**
CORE		**Theory** **(Inorganic III)**	Coordination Compounds-II Magnetism and Spectra of Coordination Complexes Chemistry of d- and f- Block Elements Organometallic Chemistry	**4**	**3**	**1**	**0**	**4**
CORE		**Practical** **(Inorganic Lab II)**	List of experiments will be provided separately	**3**	**0**	**0**	**2**	**3**
ELECTIVE (Discipline Specific)		**Theory** **(Biomolecules: Structure and function)**	Chemistry of Bio molecules : Structure and Function Biochemistry: Bioenergetics	**4**	**4**	**0**	**0**	**4**
ELECTIVE (Discipline Specific)		**Biomolecules Lab I**	List of experiments will be provided separately	**3**	**0**	**0**	**2**	**2**
FOUNDATION (Skill Enhancement Course **SEC)**		**Choice Based** **(**List of options will be provided separately**)**		**2**	**2**	**0**	**0**	**2**
		Industrial Interaction/Internship		**6**	**0**	**0**	**6**	**2**
Total				**28**				**28**

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ADAMAS UNIVERSITY								
FACULTY OF SCIENCE **DEPARTMENT OF CHEMISTRY – Int. M.Sc. PROGRAM SEMESTER – VI**								
Type of the Paper		**Theory / Practical**	**Brief Contents**	**Contact Hour Per Week**	**L**	**T**	**P**	**Credit**
CORE Theory		**Theory** **(Physical IV)**	Molecular Properties Spectroscopy I : Molecular & Electronic Spectroscopy. Spectroscopy II : Magnetic resonance spectroscopy Photochemistry	**4**	**3**	**1**	**0**	**4**
CORE		**Theory** **(Inorganic IV)**	Analytical Chemistry: Statistical Methods in Chemical Analysis and Environmental Analysis Analytical Chemistry: Analytical Separation, Bio-inorganic Chemistry	**4**	**3**	**1**	**0**	**4**
CORE Theory		**Theory (Organic IV)**	Retro Synthetic Strategy, Organic Spectroscopy: UV, IR, NMR and ESI-MS	**4**	**3**	**1**	**0**	**4**
ELECTIVE (Discipline Specific)		**Theory** **(Instrumentation)**	Basic electronics and Instrumentation. Instrumental Methods of Analysis: Electrochemical and Spectral Methods, Instrumental Methods Analytical Chemistry: Chemical Methods and Analysis, Thermodynamics of Dissolution	**4**	**4**	**0**	**0**	**4**
ELECTIVE **(Discipline Specific)**		**Instrumentation Lab I**	List of experiments will be provided separately	**3**	**0**	**0**	**2**	**2**
ELECTIVE (Discipline Specific)		**Project**		**9**	**6**	**0**	**0**	**6**
SCY5370		**Seminar on Contemporary Chemistry**		**3**	**3**	**0**	**0**	**3**
Total				**31**				**27**

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ADAMAS UNIVERSITY								
FACULTY OF SCIENCE **DEPARTMENT OF CHEMISTRY– Int. M.Sc. PROGRAM SEMESTER-VII**								
Type of the Paper		**Theory / Practical**	**Brief Contents**	**Contact Hour Per Week**	**L**	**T**	**P**	**Credit**
CORE		**Theory** **(Physical V)**	Equilibrium Thermodynamics and Surface Phenomena, Statistical Mechanics, Chemical Kinetics, Electrochemistry	**4**	**3**	**1**	**0**	**4**
CORE		**Theory** **(Inorganic V)**	Nature of Chemical Bonding, Coordination Chemistry: Structure , Stability and Function	**4**	**3**	**1**	**0**	**4**
CORE		**Theory** **(Organic V)**	Stereochemistry, Pericyclic Reaction, Organic photo-chemistry	**4**	**3**	**1**	**0**	**4**
CORE		**Practical** **(Physical Lab III)**	List of experiments will be provided separately	**6**	**0**	**0**	**4**	**4**
CORE		**Practical** **(Organic Lab III)**	List of experiments will be provided separately	**6**	**0**	**0**	**4**	**4**
CORE		**Theory** (Non-renewable Energy Resources: principles and applications)		**3**	**2**	**0**	**0**	**3**
Total				**28**				**23**

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ADAMAS UNIVERSITY								
FACULTY OF SCIENCE **DEPARTMENT OF CHEMISTRY – Int. M.Sc. PROGRAM SEMESTER-VIII**								
Type of the Paper		**Theory / Practical**	**Brief Contents**	**Contact Hour Per Week**	**L**	**T**	**P**	**Credit**
CORE		**Theory** **(Physical VI)**	Quantum Mechanics, Atomic Structure, Molecular Spectroscopy and Molecular Interaction	**4**	**3**	**1**	**0**	**4**
CORE		**Theory** **(Inorganic VI)**	Chemistry of d-Block and f-Block Elements, Organometallic Chemistry, Instrumental Methods of Analytical Chemistry	**4**	**3**	**1**	**0**	**4**
CORE		**Theory** **(Organic VI)**	Synthetic Chemistry Strategy and Methodology, Heterocyclic Chemistry and Chemistry of Natural Products	**4**	**3**	**1**	**0**	**4**
CORE		**Practical III** **(Inorganic Lab I)**	List of experiments will be provided separately	**6**	**0**	**0**	**4**	**4**
CORE		**Practical IV** **(Analytical Lab I)**	List of experiments will be provided separately	**6**	**0**	**0**	**4**	**4**
Total				**26**				**20**

Course Structure & Syllabus For Integrated M.Sc. Chemistry (Session 2018-2023)

ADAMAS UNIVERSITY								
FACULTY OF SCIENCE **DEPARTMENT OF CHEMISTRY – Int. M.Sc. PROGRAM SEMESTER- IX**								
Type of the Paper		**Theory / Practical**	**Brief Contents**	**Contact Hour Per Week**	**L**	**T**	**P**	**Credit**
CORE		**Theory** **(Group Theory and Spectroscopy I)**	Symmetry and Group theory in Chemistry, Absorption Spectroscopy Photochemistry, Photophysics	**4**	**3**	**1**	**0**	**4**
CORE		**Theory** **(Polymers and Molecules of Life)**	Polymer Chemistry, Molecules of Life, Biophysical Chemistry	**4**	**3**	**1**	**0**	**4**
CORE		**Theory** **(Spectroscopy II)**	Magnetic Resonance Spectroscopy: NMR, ESR: Basics and Application, Photoelectron Spectroscopy, Mass Spectrometry, Mossbauer, FTIR, FTNMR, 2D NMR, Basic Electronics and Instrumentation	**4**	**3**	**1**	**0**	**4**
CORE		**Practical V** **(Computational Chemistry Lab I)**	List of experiments will be provided separately	**6**	**0**	**0**	**4**	**4**
CORE		**Choice based paper I**		**4**	**3**	**1**	**0**	**4**
CORE		**Project I**		**4**	**0**	**0**	**4**	**4**
FOUNDATION		**Interaction with Industries and National Research Laboratories**	Interaction with Industries and National Research Laboratories	**2**	**0**	**0**	**2**	**2**
Total				**30**				**25**

Course Structure & Syllabus For Integrated M.Sc. Chemistry (Session 2018-2023)

ADAMAS UNIVERSITY								
FACULTY OF SCIENCE **DEPARTMENT OF CHEMISTRY – Int. M.Sc. PROGRAM SEMESTER - X**								
Type of the Paper		**Theory / Practical**	**Brief Contents**	**Contact Hour Per Week**	**L**	**T**	**P**	**Credit**
CORE		**Theory** **(Supramolecular Chemistry and Nano Science)**	Molecular Recognition, Chemical Sensor, Solid State chemistry and Crystallography, Nano Materials	**4**	**3**	**1**	**0**	**4**
CORE		**Theory** **Choice based paper II**	Advanced Paper I	**4**	**3**	**1**	**0**	**4**
CORE		**Theory** **Choice based paper III**	Advance Paper II	**4**	**3**	**1**	**0**	**4**
CORE		**Project II**	Advanced Lab Experiments	**6**	**0**	**0**	**5**	**4**
CORE		**Project/Dissertation and Comprehensive viva**	Project Completion	**12**	**0**	**0**	**8**	**10**
Total				**30**				**26**

Course Structure & Syllabus For Integrated M.Sc. Chemistry (Session 2018-2023)

LIST OF 'SKILL ENHANCEMENT' SUBJECTS OFFERED BY THE DEPT. OF CHEMISTRY*:

1. Pharmaceutical Chemistry
2. Chemistry of Cosmetics & Perfumes
3. Green Chemistry
4. Fuel Chemistry
5. Computational Chemistry
6. Advanced Level Environmental Chemistry

*Offering of subjects will vary from year to year

LIST OF 'Discipline Specific Elective Papers' OFFERED BY THE DEPT. OF CHEMISTRY*:

1. Instrumentation
2. Chemistry of Nano Materials
3. Bio-Chemistry: Bio energetic
4. Dissertation

*Offering of subjects will vary from year to year

Course Structure & Syllabus For Integrated M.Sc. Chemistry (Session 2018-2023)

SEMESTER I & II (SAME AS PHYSICS)

SEMESTER III
CHEMISTRY : PHYSICAL CHEMISTRY-I
(Credits: 4)
Theory: 60 Lectures

Unit 1 - Kinetic theory of gasses (13L)

Concept of pressure and temperature. Nature of distribution of velocities in one, two and three dimensions. Maxwell's distribution of speeds. Kinetic energy distribution in one, two and three dimensions, calculations of average, root mean square and most probable values in each case; calculation of number of molecules having energy $\geq \varepsilon$, Principle of equipartition of energy and its application to calculate the classical limit of molar heat capacity of gases. Basic idea about beta, gamma and error functions. Collision of gas molecules; collision diameter; collision number and mean free path; frequency of binary collisions (similar and different molecules); wall collision and rate of effusion.

Unit 2 – Advanced Thermodynamics (14L)

Importance and scope, definition of system and surroundings: type of systems (isolated, closed and open); extensive and intensive properties; steady state versus equilibrium state; concept of thermal equilibrium and the zeroth law of thermodynamics; thermodynamic coordinates, state of a system, equation of state, state functions and path functions; partial derivatives and cyclic rule; concept of heat and work (IUPAC convention); graphical explanation of work done during expansion and compression of a ideal gas; reversible and irreversible processes and work done; first law of thermodynamics, internal energy (U) as a state function; enthalpy as a state function; energy conservation in the living organism; heat changes at constant volume and constant pressure; relation between C_p and C_v using ideal gas and van der Waals equations; joule‘s experiment and its consequence; explanation of term $(\delta U/\delta V)_T$; isothermal and adiabatic processes; thermo chemistry: heat changes during physicochemical processes at constant pressure/volume; Kirchhoff‘s relations; bond dissociation energies; changes of thermodynamic properties in different chemical changes.

Unit 3- Chemical kinetics II (13L)

Phenomenological kinetics: degree of advancement of a reaction, reaction rate, rate constant, order and molecularity of a reaction, determination of order of a reaction by half-life and differential method: zero, first, second and fractional order reactions, pseudo first order reaction; solutions of elementary differential equations, complex reaction: opposing, parallel and consecutive reactions (all step of first order), kinetic and thermodynamic control of reaction; idea of rate determining step; steady-state approximation; kinetics and mechanism of reaction; kinetics of chain reaction; temperature dependence of rate constant, Arrhenius equation, energy of activation.

Course Structure & Syllabus For Integrated M.Sc. Chemistry (Session 2018-2023)

Unit 4- Transport Phenomena (20L)

Flows under the influence of mechanical, chemical and electrical forces: General features offluid flow (streamline turbulent flows, Reynold's number); nature of viscous drag forstreamline motion, Newton's equation, viscosity coefficient, Poisuille equation (with derivation),Viscosity of gas, temperature dependence of viscosity coefficient of liquid and comparison withthat for gases; Stokes law and terminal velocity; experimental determination of viscosity ofandliquids. Molecular motions in liquids including electrolytic conduction: Electronic versuselectrolytic conduction, measurement of conductance, cell constant; specific, equivalent andmolar conductance; variation of specific and equivalent conductance with dilution for strong andweak electrolytes; Kohlrausch's law of independent migration of ions, ion conductance and ionicmobility; Walden's rule; equivalent conductance at infinite dilution and its determination forstrong and weak electrolytes; Ostwald dilution law and determination of ionization constants forweak electrolytes from conductance measurements; applications of conductance measurement:determination of solubility product and ionic product of water, conductometric titration; transportnumber, Hittorf's rule, determination of transport number by the moving boundary method.

Reference Books:

- Atkins, P. W. & Paula, J. de *Atkin's Physical Chemistry* 10th Ed., Oxford University Press (2014).
- Ball, D. W. *Physical Chemistry* Thomson Press, India (2007).
- Castellan, G. W. *Physical Chemistry* 4th Ed. Narosa (2004).
- Mortimer, R. G. *Physical Chemistry* 3rd Ed. Elsevier: NOIDA, UP (2009).
- Engel, T. & Reid, P. Physical Chemistry 3rd Ed. Pearson (2013).

Chemistry: SCY 52201,PHYSICAL LAB I (Credit: 3)

1. **Surface tension measurements.**
   a. Determine the surface tension by (i) drop number (ii) drop weight method.
   b. Study the variation of surface tension of detergent solutions with concentration.
2. **Viscosity measurement using Ostwald's viscometer**.
   a. Determination of viscosity of aqueous solutions of (i) polymer (ii) ethanol and (iii) sugar at room temperature.
   b. Study the variation of viscosity of sucrose solution with the concentration of solute.
3. **Indexing of a given powder diffraction pattern of a cubic crystalline system.**
4. **pH metry**
   a. Study the effect on pH of addition of HCl/NaOH to solutions of acetic acid, sodium acetate and their mixtures.
   b. Preparation of buffer solutions of different pH
      i. Sodium acetate-acetic acid
      ii. Ammonium chloride-ammonium hydroxide
   c. pH metric titration of (i) strong acid vs. strong base, (ii) weak acid vs. strong base.
   d. Determination of dissociation constant of a weak acid.

Any other experiment carried out in the class.

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Reference Books

- Khosla, B. D.; Garg, V. C. & Gulati, A. *Senior Practical Physical Chemistry,* R. Chand & Co.: New Delhi (2011).
- Garland, C. W.; Nibler, J. W. & Shoemaker, D. P. *Experiments in Physical Chemistry8th Ed.*; McGraw-Hill: New York (2003).
- Halpern, A. M. &McBane, G. C. *Experimental Physical Chemistry 3rdEd.;* W.H. Freeman & Co.: New York (2003).

INORGANIC-I

Credit:4 (Contact hours: 60)

Unit-1: Atomic structure: (12L) Why study quantum mechanics, Bohr's model, Sommerfeld's extension, de Broglie's wave particle duality; Heisenberg's uncertainty principle and Schrödinger's equation (qualitative); significance of ψ and ψ^2;Hydrogenicwavefunctions, radial density, angular probability, introduction to the concept of atomic orbitals; shapes, radial and angular probability diagrams of s, p and d orbitals (qualitative idea). Many electron atoms and ions, Aufbau principle, Pauli's exclusion, Hund's rules, Slater's rules, Term symbolsof atoms and ions for atomic numbers.

Unit-2:Chemical Bonding (20 L): Ionic Bonding: Size effects, radius ratio rules and their limitations. Packing of ions in crystals, lattice energy, Born- lande equation and its applications, Born-Haber cycle and its applications.Solvation energy, polarizing power and polarizability, ionic potential, Fajan's rules.Defects in solids (elememetary idea).

Covalent Bonding: Lewis structures, formal charge. Valence Bond Theory, directional character of covalent bonds, hybridizations, equivalent and non-equivalent hybrid orbitals, Bent's rule, VSEPR theory, shapes of molecules and ions containing lone pairs and bond pairs (examples from main group chemistry), Partial ionic character of covalent bonds, bond moment, dipole moment and electronegativity differences. Concept of resonance, resonance energy, resonance structures, Molecular orbital theory of homo and heterodiatomic molecules (B_2, C_2, N_2, O_2, CO and HF).

Unit-3: Chemical periodicity(18L): Periodic table, group trends and periodic trends in physical properties.Classification of elements on the basis of electronic configuration.Modern IUPAC Periodic table.General characteristic of s, p, d and f block elements.Position of hydrogen and noble gases in the periodic table. Effective nuclear charges, screening effects, Slater's rules, atomic radii, ionic radii (Pauling's univalent), covalent radii, ionization energy, electron affinity, electronegativity and its different scales, orbital/group electronegativity, ionic potential, diagonal relationship,inert pair effect, catenation

Unit-4: Nuclear Chemistry(10L): Various radioactive disintegration modes, nature of radiations, theory of radioactive disintegration, different types of radioactive equilibria, half life/average life period; different natural/artificial radioactive series, group displacement law, units/measurements of radioactivity. Nuclear stability and nuclear binding energy. Nuclear forces: meson exchange theory. Nuclear models (elementary idea): Concept of

nuclear quantum number, magic numbers. Nuclear Reactions: Artificial radioactivity, transmutation of elements, fission, fusion and spallation, neutron activation analysis Radio chemical methods: principles of determination of age of rocks and minerals, radio carbon dating, hazards of radiation and safety measures.

Reference Books:

- Lee, J.D. *Concise Inorganic Chemistry* ELBS, 1991.
- Douglas, B.E. and McDaniel, D.H. *Concepts & Models of Inorganic Chemistry* Oxford, 1970
- Atkins, P.W. & Paula, J. *Physical Chemistry*, 10th Ed., Oxford University Press, 2014.
- Day, M.C. and Selbin, J. *Theoretical Inorganic Chemistry*, ACS Publications, 1962.

Inorganic Lab I (Credit: 2)

Section A: Inorganic Chemistry - Volumetric Analysis

1. Titrimetric Analysis

(i) Calibration and use of apparatus
(ii) Preparation of solutions of titrants of different Molarity/Normality

2. Acid-Base Titrations
Principles of acid-base titrations to be discussed.
(i) Estimation of sodium carbonate using standardized HCl.
(ii) Estimation of carbonate and hydroxide present together in a mixture.
(iii) Estimation of carbonate and bicarbonate present together in a mixture.

Section B: Inorganic Qualitative-Detection of acid and basic radicals, group separation

Cation radicals derived from:

Na, K, NH_3, Mg, Ca, Sr, Ba, Al, Pb, Bi, Cr, Mn, Fe, Co, Ni, Cu, Zn, Cd

Anion radicals:

F^-, CI^-, Br^-, I^-, NO_3^-, NO_2^-, SCN^-, S^{2-}, SO_4^{2-}, $S_2O_3^{2-}$, PO_4^{3-}, BO_3^{3-}, CrO_4^{2-}, BrO_3^-, IO_3^-, $[Fe(CN)_6]^{4-}$, $[Fe(CN)_6]^{3-}$

Detection and confirmation of four radicals by macro, semi- micro tests and assignment of probable composition of the mixtures.

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Reference text:

- Mendham, J., A. I. Vogel's *Quantitative Chemical Analysis 6th Ed.,* Pearson, 2009
- Vogel's Qualitative Inorganic Analysis (7th Edition): G. Svehla

ORGANIC I (60 Lectures)

Unit 1 - General Introduction and Bonding Features in Organic Molecules (10L)

Functional group based classification and nomenclature. Sources/ origin of different compounds. Molecular formula and IHD / DBE.

Valence bond theory: Concept of hybridization, resonance (including hyper conjugation), inductive effect, steric effect, steric inhibition of resonance.

Orbital pictures of bonding (sp^3, Sp^2, sp: C-C, C-N & C-O system).

MO theory: Sketch and energy levels of MOs of i) acyclic π orbital system (C=C, conjugated diene and allyl systems) ii) cyclic π orbital system (neutral system: [4], [6] annulenes; charged system: 3, 4, 5-membered ring system); Frost diagram, Huckel's rules for aromaticity, antiaromaticity; homoaromaticity.

Physical properties: Melting point, boiling point; solubility; dipole moment; acid and base strength.

Unit 2- Mechanistic Classification (10 L)

Mechanistic classification: Ionic, radical and pericyclic; representation of mechanistic stepsusing arrow formalism. Reactive intermediates: carbocations (carbenium and carbonium ions), carbanions, carbon radicals, carbenes - structure using orbital picture, electrophilic / nucleophilic reactivity, stability, generation and fate. Reaction thermodynamics: free energy and equilibrium, enthalpy and entropy factor, intermolecular &intramolecular reactions. Application of thermodynamic principles in tautomericequilibria (keto-enoltautomerism). Composition of the equilibrium in different systems (simple carbonyl, 1,3- and 1,2- dicarbonyl systems, phenols and related system; substituent and solvent effect).

Unit 3 – Reaction Kinetics (5L)

Reaction kinetics: Rate const and free energy of activation, free energy profiles for one step and multi step reactions, catalyzed reactions, kinetic control and thermodynamic control, kinetic isotopic effect, principle of microscopic reversibility, Hammond postulate.

Unit 4 –Stereochemistry and Conformation of Acyclic Molecules (15L)

Stereochemistry: Symmetry, chirality, optical activity, optical purity. Stereogenic units i) stereocentres: systems involving 1, 2, 3 centres, stereogenicity, chirotopicity. pseudo asymmetric (D/ Land R/S descriptor, threo / erythro and syn / anti nomenclatures (for aldols) ii) stereoaxis: chiral axis in allenes& biphenyls, R / S descriptor; cis / trans, syn / anti, E / Z descriptors (for C=C, C=N). Topicity of ligands and faces (elementary idea) and descriptors.

Conformation: Conformational nomenclature; factors affecting stability of conformations, conformational analysis of ethane, propane, butane, haloethane, 1,2-haloethane, 1,2-glycol, 1,2-halohydrin; invertomerism of trialkylamines.

Unit 5 – Nucleophilic Substitution at sp^3centre (20L)

Nucleophilic substitution at sp^3centre: Mechanism: S_N1, S_N2, S_Ni mechanisms, effect ofsolvent, substrate structure, leaving group, nuc1eophiles including ambident nucleophiles, substitution involving NGP; relative rate &stereochemical features [systems: alkyl halides, allyl halides, alcohols, ethers, epoxides]

Unit 6-Elimination reaction: Acyclic and cyclic system:

Elimination - Mechanisms: El, E2 and ElcB; reactivity, orientation (Saytzeff / Hofmann) and stereoselectivity; substitution vs elimination.

Reference Books:

- Morrison, R. N. & Boyd, R. N. *Organic Chemistry*, Dorling Kindersley (India) Pvt.Ltd. (Pearson Education).
- Carrey, F. A. &Sundberg, R. J.*Advanced Organic ChemistryPart A: Structure and Mechanisms,* Springer.
- Ernest L. Eliel. *Stereochemistry of Organic Compounds*. Wiley VCH
- D. Nasipuri. *Stereochemistry of Organic Compounds. Principles and Applications*. New Age.
- Sykes, P. A Guidebook to Mechanism in Organic Chemistry, Orient Longman, New Delhi (1988).
- Clayden, J.; Greeves, N.; Warren, S.; Wothers, P.; *Organic Chemistry,* Oxford University Press.

Engineering Chemistry Theory

Code: CY1107

Contact hours: 45

Credits:3

Unit-1

Thermodynamics: Thermodynamics of Chemical Processes: Review of 1st law, Concept of entropy, Chemical potential, Equilibrium conditions for closed systems, Phase and reaction equilibria, Maxwell relations.

Unit-2

Reaction Dynamics, Catalysis & Electrochemistry: Rate laws, 1st Order reaction & 2nd order reaction, Arrhenius equation, Mechanism and Theories of reaction rates,Characteristics and Types of Catalyst, Theories of Catalysis, Electrode potential, Redox reaction & Nernst Equation.

Course Structure & Syllabus For Integrated M.Sc. Chemistry (Session 2018-2023)

Unit-3

Molecules & Solid State: Homonuclear and Heteronuclear concepts, Non – covalent interaction, Van der waals bonding, hydrogen bonding, Idea of spatial periodicity of lattice, Unit cells, Bravias lattice, Atomic packing factor of SCC, BCC and FCC, Band theory, Conductors Semiconductors and insulators.

Unit-4

Co-Ordination Chemistry: Transition elements, Warner's co-ordination theory, Structure of Co-ordination Compounds corresponding to Co-ordination number 2 to 6, Types of ligands, Isomerism & its types viz. Geometrical, Optical, Ionization, linkage & Co-ordination isomerism, Theories of bonding in Co-ordination compounds viz. crystal field theory and valance bond theory.

Unit-5

Reactivity of Organic Molecules & Types of Reactions: Inductive effect, Resonance, Hyper conjugation, Electromeric effect, Carbocation, carbanion & free radicals, Substitution reactions,Elimination reactions, Addition reactions, & their Mechanisms.

Unit-6

Polymers& Fuel Chemistry: Polymerization, Mechanism of Addition polymerization, Classification of plastics, Preparation properties & industrial applications of PTFE, PVC, Phenolic resin & Polyester resin, Conducting polymers & Biopolymers. Solid Fuel: Coal, Classification of coal, Coal analysis. Liquid fuel: Petroleum, classification of petroleum, Thermal cracking, Octane number, Cetane number, Aviation Fuel Bio-diesel. Gaseous fuels: Natural gas, water gas, bio gas.

Course Structure & Syllabus For Integrated M.Sc. Chemistry (Session 2018-2023)

Text/ Reference Books

- P. W. Atkins, Physical Chemistry, ELBS/Oxford, 7th Edition, 1995
- 2.G.W.Castellan, Physical Chemistry
- D. A. McQuarrie and J.D. Simon, Physical Chemistry - a molecular approach, Viva Books Pvt. Ltd. (1998)
- P. C. Rakshit, Physical Chemistry, Sarat Book House (7th Edition)
- 5.Cotton, F A, Wilkinson G. and Gauss, P L, Basic Inorganic Chemistry
- J. D. Lee, Concise Inorganic Chemistry, 4th Edition, ELBS, 1991
- 7.I.L. Finar,Organic Chemistry,Vol – I & II, Pearson Education
- 8. Morrison & Boyd, Organic Chemistry
- 9. P. Sykes, Mechanism in Organic Chemistry, Orient Longman
- 10. Joel R. Fried, Polymer Science and Technology, Pearson Education (2nd Edition)
- 11. S. Sarkar, Fuels and Combustion, Taylor & Francis (3rd Edition), 2009
- 12.Kuriacose & Raja Ram,Chemistry in Engineering and Technology, Vol.1 & 2 by, Tata McGraw Hill & Co

Engineering Chemistry Laboratory

Code: CY1185
Contact: 30
Credits: 2

List of experiments (Any 8 Experiments)

1. Determination of total hardness of water by complexometric titration method
2. Determination of carbonate and bicarbonate in water
3. Estimation of iron by permanganometry
4. Estimation of ferrous ion in Mohr salt
5. Dissolved oxygen by Winkler's method
6. Measurement of the coefficient of viscosity
7. Measurement of the surface tension
8. Kinetics of ester hydrolysis
9. pH metric titration

10. Conductometric titration
11. Determination of standard EMF of a Daniel Cell
12. Verification of Beer Lambert's law
13. Partition coefficient of iodine
14. Identification of organic Compounds using melting point
15. Solubility, functional group test

SEMESTER-IV

CHEMISTRY -SCY52102: PHYSICAL CHEMISTRY-II

(Credits: 4)

Theory: 60 Lectures

Unit 1 –Quantum Mechanics I (25 L)

Breakdown of classical ideas – Line Spectra, black body (or cavity) radiation, Planck's quantization, photoelectric effect, Elementary idea of Bohr Theory, Compton scattering for relativistic (preliminary idea only); wave properties of particles: de Broglie hypothesis and the concept of matter waves, Davisson-Germer experiment, nature of matter waves: group and phase velocities and the idea of a wave packet; Heisenberg uncertainty principle and its relation to the measurement process, Differentiation of small and large particles on the basis of Uncertainty Principle, necessity of more general theory.

Time-independent form of the Schrödinger equation; probabilistic interpretation of the wave function; conditions for acceptability of wave functions; elementary idea of operator, operator algebra, eigen value equation, expectation value; time dependent Schrödinger equation, concept of stationary states, study of a simple (model) system: Free particle, particle in a box problem: setting up of the Schrödinger equation, its solution, interpretation of the solutions (in the light of energies and wave functions) – normalization, orthogonality and probability eigenfunctions and eigenvalues, energy quantization (and its connention to the boundary conditions), evaluation of expectation values of x, x^2, p_x, p_x^2, their significance in the light of uncertainty principle, extension of the particle in one-dimensional box to two- and three- dimensional cases, idea of degenerate energy states and relationship of symmetry and degeneracy.

Unit2- Quantum Mechanics II (25 L)

Simple harmonic oscillator (SHO): setting up of the Schrödinger equation, connection with the uncertainty principle, classical turning points, expressions for energy and wave functions for the ground and the first excited states (quantitative treatment), series solutions of differential equation: Hermite equation, recursion relation, their characteristics features, the zero-point energy and its importance, limitations thereof and the idea of the anharmonic oscillator.

Central force problem: setting of the Schrödinger equation in Cartesian coordinates, Transformation of coordinate systems, transforming the Schrödinger equation to spherical polar coordinates, Rigid rotor and Hydrogen atom: separation of variables into radial (r) and angular (Θ and φ) parts, solution of the φ dependent equation and the idea of the magnetic quantum number (m_l), energy expression (no derivation required), idea of degeneracy, the principal (n) and the azimuthal (l) quantum numbers, hydrogen wave functions (up to n=3), the concept of an orbital, real orbitals (suitable linear combinations), radial density distributions, radial and angular nodes, shapes of s, p and d orbitals.

Unit 3- Colligative Properties (10 L)

ΔG, ΔS, ΔH and ΔV of mixing for binary solutions, vapour pressure of solution, ideal solutions, ideally dilute solutions and colligative properties, Raoult's law, thermodynamic derivation (using chemical potentials) of colligative properties of solution and their inter-relationships, abnormal colligative properties, van't Hoff factor; biomedical application: osmosis and dialysis.

Reference Books:

- Atkins, P. W. & Paula, J. de *Atkin's Physical Chemistry* 10th Ed., Oxford University Press (2014).
- Ball, D. W. *Physical Chemistry* Thomson Press, India (2007).
- Castellan, G. W. *Physical Chemistry* 4th Ed. Narosa (2004).
- Mortimer, R. G. *Physical Chemistry* 3rd Ed. Elsevier: NOIDA, UP (2009).
- Engel, T. & Reid, P. *Physical Chemistry* 3rd Ed. Pearson (2013).

CHEMISTRY -SCY52202: PHYSICAL Lab-II

(Credits: 3)

Practical: 45 Lectures

Physical Lab II

1. Determination of the equilibrium constant of the reaction KI + I_2 = KI_3 by partition method as a prerequisite to this, determine the partition coefficient of I_2 between CCl_4 and H_2O.
2. Determination of the rate constant of the first order acid catalysed hydrolysis of an ester

(preferably methyl acetate) titrimetrically **OR** Determination of the rate constant of decomposition of H_2O_2 by acidified KI solution using the clock reaction **OR** Determination of the rate constant(s) for the acid catalysed inversion of sucrose using the supplied catalysed solution(s) polarimetrically

3. Determination of the specific ratio of a given optically active compound and percent composition of its aqueous solution polarimetrically and determination of optical rotation of a mixture to determine the concentration of one component of the mixture.
4. Calorimetric experiment: Temperature sensor to measure the heat of reaction and related instrumentation.

Reference Books:

- Garland, C. W.; Nibler, J. W. & Shoemaker, D. P. *Experiments in Physical Chemistry 8th Ed.*; McGraw-Hill: New York (2003).
- Halpern, A. M. & McBane, G. C. *Experimental Physical Chemistry 3rd Ed.;* W.H.

Freeman & Co.: New York (2003).

Inorganic II

(Credit:4)

Unit-1: Precipitation and redox reaction (20L): Solubility product principle, common ion effect and their applications to the precipitation and separation of common metallic ions as hydroxides, sulfides, phosphates, carbonates, sulfates and halides.Ion-electron method of balancing equation of redox reaction.Elementary idea on standard redox potentials with sign conventions, Nernst equation (without derivation).Influence of complex formation, precipitation and change of pH on redox potentials; formal potential.Feasibility of a redox titration, redox potential at the equivalence point, redox indicators.Redox potential diagram (Latimer and Frost diagrams) of common elements and their applications.Disproportionation and comproportionation reactions (typical examples)Complementary/non-complementary redox reactions (examples)

Unit-2: Coordination Chemistry 1 (10 L): Werner's theory; IUPAC nomenclature of coordination complexes, classification and binding modes of ligands, chelate effect, Types of isomerism (elementary idea), Determination of configuration of cis- and trans- isomers by chemical methods. Labile and inert complexes, substitution reaction on square planer complexes, trans effect (example and applications).

Chemistry of s and p block elements (10 L):

(i) Structure, bonding and reactivity of B_2H_6; $(SN)_x$ with x = 2, 4; phosphazines; interhalogens. (ii) Structure of borates, silicates, polyphosphates, borazole, boron nitride, silicones, thionic acids. (iii) Reactivity of polyhalides, pseudo halides, fluorocarbons, freons and NOx with environmental effects. (iv) Chemistry of hydrazine, hydroxylamine, N_3^-, thio- and per-sulphates. Noble gases from air; oxides, fluorides and oxofluorides of xenon; chemical and photochemical reactions of ozone.

Unit-3: Theory of acid and bases (20 L):

Bronsted and Lowry's concept, solvent system concept, Lewis concept, Lux-Flood concept, relative strength of acids, hydracids and oxyacids, Pauling's rules, amphoterism, and super acids, HSAB principle, HOMO-LUMO and acid-base interaction, acid-baseequilibria in aqueous solution, pH, buffer solutions and buffer actions, acid-base neutralization curves, acid-base indicators, choice of indicators, Acid-base titrations. Physical properties of a solvent, types of solvents and their general characteristics, reactions in non-aqueous solvents.

Reference Books:

| | Lee, J.D. *Concise Inorganic Chemistry*, ELBS, 1991.
| | Douglas, B.E; Mc Daniel, D.H. & Alexander, J.J. *Concepts & Models of Inorganic Chemistry 3rd Ed.*, John Wiley Sons, N.Y. 1994.

Course Structure & Syllabus For Integrated M.Sc. Chemistry (Session 2018-2023)

| | Greenwood, N.N. &Earnshaw.*Chemistry of the Elements*, Butterworth-Heinemann. 1997.
| | Cotton, F.A. & Wilkinson, G. *Advanced Inorganic Chemistry*, Wiley, VCH, 1999.

ORGANIC II (60 Lectures)

Unit 1-Stereochemistry of Cyclic Systems (15L)

Conformational analysis and reactivity: 4, 5, 6-membered rings; substituted cyclohexane.

Unit 2– Organic Reaction: Reaction to carbon- heteroatom multiple bonds (20L)

Addition to C=O: Mechanism, reactivity, equilibrium and kinetic control. Reactions withalcohols, amines, thiols, HCN, bisulfite, Wittig reaction.

Carbonyl Reduction: hydride addition, Wolff-Kishner reduction, dissolving metal (Bouveault-Blanc reduction, Clemmensen Reduction), Cannizzaro reaction, Tischenko reaction, aldol condensation, benzoin condensation. Hydrolysis of nit riles and isonitriles.

Nucleophilic addition to α,β-unsaturated carbonyl system (general principles).

Radical coupling (pinacol, acyloin, McMurry), epoxides, phenols and quinones.

Unit 4- Addition Reaction (10L)

Addition reaction [reaction of carbon-carbon multiple bonds]:Addition to C=C:

Mechanism, reactivity, regioselectivity and stereoselectivity. Reactions: halogenations, hydrohalogenation, hydration, hydrogenation, epoxidation, hydroxylation, ozonolysis, addition to dienes, Diels-Alder reaction.

Radical addition*:*Dissolving metal reduction of alkynes and bezenoid aromatics (Birch).

Unit 5 – Aromatic Substitution (Nucleophilic and Electrophilic), Radical Substitution (15L) Nucleophilic aromatic substitution: Addition-elimination mechanism, S_N1 mechanism, benzyne mechanism.

Electrophilic aromatic substitution: Mechanisms, orientation and reactivity. Reactions:nitration, nitrosation, sulfonation, halogenation, Friedel-Crafts reactions, one carbon electrophiles (reactions: chloromethylation, Gatterman-Koch, Gatterman, Hoesch, Vilsmeier-Haack reaction, Reimer-Tiemann, Kolbe - Schmidt).

Reference Books:

- | | Ernest L. Eliel. *Stereochemistry of Organic Compounds*. Wiley VCH
- | | D. Nasipuri. *Stereochemistry of Organic Compounds. Principles and Applications*. New Age.
- | | Morrison, R. N. & Boyd, R. N. *Organic Chemistry*, Dorling Kindersley (India) Pvt.Ltd. (Pearson Education).
- | | Finar, I. L. *Organic Chemistry (Volume 1)*, Dorling Kindersley (India) Pvt. Ltd.(Pearson Education).
- | | Clayden, J.; Greeves, N.; Warren, S.; Wothers, P.; *Organic Chemistry,* Oxford University Press.
- | | Carrey, F. A. &Sundberg, R. J.*Advanced Organic Chemistry Part B: Reactions and Synthesis,* Springer.
- R.O.C. Norman, J.M. Coxon. *Principles of Organic Synthesis.* Blackie Academic & Professional

Course Structure & Syllabus For Integrated M.Sc. Chemistry (Session 2018-2023)

Organic Lab I
(Credits: 4)
Practical: 60 Lectures

Organic Qualitative: Detection of elements and functional groups, detection of some single compounds

Lassaigne's tests of special elements (N, S, X). Preliminary Tests: Br_2& $KMnO_4$ test. Tests of functional groups including their solubility / miscibility behavior: -NH_2 (aliphatic & aromatic); -NO_2 (aromatic); -$CONH_2$; -NHCOR, -OH (phenolic); -CO_2H; C=O; -CO_2R.
Derivative preparation and melting point determination.

Reference Books

1) Furniss, B. S.; Hannaford, A. J.; Smith, P. W. G.; Tatchell, A. R. *Vogel's Textbook of Practical Organic Chemistry*, *5th Ed.,*Longman Scientific and Technical (1989).
2) Mann, F.G. & Saunders, B.C. *Practical Organic Chemistry,*Pearson Education (2009)
3) Furniss, B.S.; Hannaford, A.J.; Smith, P.W.G.; Tatchell, A.R. *Practical Organic Chemistry, 5th Ed.,* Pearson (2012)

Elective: SCY 52108, Material Science (Discipline specific)
(Credit: 4)
Theory (60L)

Unit 1 –Basics of solid state chemistry (20L)

Forms of solids, preliminary idea of symmetry elements, Crystal structure of solids: Fundamental of lattices, unit cell, atomic coordinates, crystal system, crystal direction and planes, Bravais lattice type and its identification of lattice planes, laws of crystallography: law of constancy of interfacial angle and law of rational indices, Weiss and Miller indices, packing in solids and the radius ratio rule, and their implications; Crystal diffraction by X-rays, idea of a simple diffraction grating, Bragg's law and its applications for the determination of crystal structure for cubic systems, crystal structure of NaCl and KCl, single crystal and powder diffraction methods (preliminary ideas), Structure determination by X-ray diffraction, packing in solids andcorresponding efficiency. Imperfectness in structures and crystal defects, Born-Haber cycle, lattice energy, metallic structure, band theory, Semiconductor.

Unit 2 – Nano Science (20L)

Fundamentals of Nano science: definition, nano versus bulk, quantum confinement: nano-scale in 1D, 2D and 3D with examples, synthesis of nano materials: top-down and bottom-up approaches, size dependent properties; nanoclusters and nanowires, semiconductor nanoparticles, nanotubes, graphene applications of nano materials, including nano-biotechnology, nano-materials and Drug Delivery.

Unit 3 – Polymer Chemistry (20L)

Macromolecules, degree of polymerization, different average molar masses in a poly disperse system, determination of molar mass by osmometry and viscometry; Donnan equilibrium, transport across membranes. Microporous materials, microgels, bioconjugate polymers, gels, ointments and creams, biodegradable polymers.

Course Structure & Syllabus For Integrated M.Sc. Chemistry (Session 2018-2023)

Elective: SCY 52208, Material Science (Discipline specific)
(Credit: 2)
Practical (30L)

Material Science Lab I (30L)

List of experiments will be provided separately

SEMESTER-V
CHEMISTRY -SCY53101: PHYSICAL CHEMISTRY-III
(Credits: 4)
Theory: 60 L

Unit I - Chemical Equilibrium and Ionic Equilibrium (20L)

Thermodynamics and equilibrium, degree of advancement, vant Hoff's reaction isotherm (deduction from chemical potential), equilibrium constant and standard Gibbs free energy change; definition of K_p, K_c, K_x; vant't Hoff's reaction isobar and isochore from different standard states; shifting of equilibrium due to change of external parameters like temperature and pressure and influence of inert gas; Le Chatelier principle of dynamic equilibrium (thermodynamics approach) and its application to homogeneous chemical equilibria.

Ionic equilibrium: concept of pH, hydrolysis of salts, buffer solution, elementary idea of biological buffers, acid-base indicators; solubility equilibria and influence of common and indifferent ions there on.

Unit 2 - Phase rule (10L)

Definition of phase, number of component and degrees of freedom, Gibbs phase rule and its derivation, definition of phase diagram, phase equilibria for one component system, first order phase transition and Clapeyron equation , Clausius-Clapeyron equation: derivation and its use; liquid vapour equilibrium for two component systems; ideal solution at a fixed temperature and pressure, principle of fractional distillation, Duhem-Margules equation, Henry's law, Konowaloff's rule; positive and negative deviations from ideal behaviour, azeotropic solutions, liquid-liquid phase diagram using phenol-water system, solid-liquid phase diagram, simple eutectic diagram.

Unit 3- Statistical Thermodynamics (15L)

Concept of probability. Microscopic and microstates, thermodynamic probability, entropy and probability, the Boltzmann-Planck entropy formula, the Maxwell-Boltzmann distribution law for the distribution of molecular energies, partition function: molecular and molar, the transitional partition function, thermodynamic quantities from partition function, vibrational partition functions, Einstein's theory of heat capacity of solids, the characteristics temperature, its limitations and Debye's modification thereof.

Nernst heat theorem, approach to zero Kelvin, adiabatic demagnetization, Planck's formulation of third law and the concept of absolute entropies.

Unit 4 - Colloid and Surface science (15L)

Lyophobic and lyophilic sols, origin of charge and stability of lyophobic colloids, coagulation and Schultz-Hardy rule, zeta potential and Stern double layer (qualitative idea); Tyndall effect, electrokinetic phenomenon (qualitative idea only);

Special features of interfaces compared to bulk, surface dynamics: physical and chemical adsorption, Freundlich and Langmuir adsorption isotherm, multilayer and BET isotherm (without derivation) and applications, Gibbs adsorption isotherm and surface excess, effect of addition of substances on surface tension, surfactants and micelles and reverse micelles: applications, size and solubility; Microencapsulation for personal care; Nanoencapsulation. Heterogeneous catalysis (single reactant).

Reference Books:

- Atkins, P. W. & Paula, J. de *Atkin's Physical Chemistry* 10th Ed., Oxford University Press (2014).
- Ball, D. W. *Physical Chemistry* Thomson Press, India (2007).
- Castellan, G. W. *Physical Chemistry* 4th Ed. Narosa (2004).
- Mortimer, R. G. *Physical Chemistry* 3rd Ed. Elsevier: NOIDA, UP (2009).
- Engel, T. & Reid, P. *Physical Chemistry* 3rd Ed. Pearson (2013).

Organic III (60 Lectures)

Unit 1 – Substitution at sp^2 carbon, Carbonyl System (5L)

Mechanism: $B_{AC}2$, $A_{AC}2$, $A_{AC}l$, $A_{AL}1$.Systems: acids, esters, amides, anhydrides & acyl halides.

Unit 2- Rearrangements (20L)

1,2-shifts: Rearrangement to electron-deficient carbon: Wagner-Meerwein rearrangement, pinacol-pinacolon and related rearrangements, dienone-phenol; benzil-benzilic acid rearrangement. Rearrangement to electron-deficient oxygen: Baeyer-Villiger oxidation, hydroperoxide rearrangement cumenehydroperoxide-phenol rearrangement, Dakin reaction.

Aromatic rearrangements: migration from oxygen to ring carbon (Fries rearrangement, Claisen rearrangement); migration from nitrogen to ring carbon (Hofmann-Martius rearrangement, Fischer-Hepp rearrangement, N-azo to C-azo rearrangement, Bamberger rearrangement, Orton rearrangement, Benzidinerearrangement.Electron-deficient nitrogen (Beckmann rearrangement, Schmidtrearrangement, Hofmann rearrangement, Lossen rearrangement, Curtius rearrangement

Unit 3-Nitrogen compounds (10L)

Amines, nitrile, isonitrile, diazomethane, diazoacetic ester, aromatic nitro compounds, aromatic diazonium salts.

Unit 4- Pericyclic Reactions (10L)

Electrocyclic reactions: 4e and 6e neutral systems; cycloaddition reactions: [4 + 2] and [2 + 2] reactions, cheletropic addition of carbene; sigmatropic rearrangements: [1,3] and [1,5] H shifts, [3,3] Cope and Claisen rearrangements. FMO analysis and Woodward-Hoffmann selection rules.

Unit-5 Organometallic Chemistry (15L)

Preparation of Grignard and organo lithium reagents; addition ofGrignard and organo lithium to carbonyl compounds, substitution on -COX; conjugate addition by cuprates, Reforrnatsky reaction.

Reference Books:

- Morrison, R. N. & Boyd, R. N. *Organic Chemistry*, Dorling Kindersley (India) Pvt.Ltd. (Pearson Education).
- Finar, I. L. *Organic Chemistry (Volume 1)*, Dorling Kindersley (India) Pvt. Ltd.(Pearson Education).
- Clayden, J.; Greeves, N.; Warren, S.; Wothers, P.; *Organic Chemistry,* Oxford University Press.
- Carrey, F. A. &Sundberg, R. J.*Advanced Organic Chemistry Part B: Reactions and Synthesis,* Springer.
- R.O.C. Norman, J.M. Coxon. *Principles of Organic Synthesis.* Blackie Academic & Professional.

Organic Lab II (45 Lectures)

1. Organic preparations:

i. Acetylation of one of the following compounds: amines (aniline, o-, m-, p- toluidines and o-, m-, p-anisidine) and phenols (β -naphthol, vanillin, salicylic acid) by any one method:
   a. Using conventional method.
   b. Using green approach

ii. Benzolyation of one of the following amines (aniline, o-, m-, p- toluidines and o-, m-, p-anisidine) and one of the following phenols (β -naphthol, resorcinol, p- cresol) by Schotten-Baumann reaction.

iii. Oxidation of ethanol/ isopropanol (Iodoform reaction).

iv. Selective reduction of meta dinitrobenzene to m-nitroaniline.

v. Hydrolysis of amides and esters.

vi. Semicarbazone of any one of the following compounds: acetone, ethyl methyl ketone, cyclohexanone, benzaldehyde.

Reference Books

- Mann, F.G. & Saunders, B.C. *Practical Organic Chemistry,* Pearson Education(2009)
- Furniss, B.S.; Hannaford, A.J.; Smith, P.W.G.; Tatchell, A.R. *Practical OrganicChemistry, 5th Ed.,* Pearson (2012)

INORGANIC III (60L)

Unit-1: Coordination Chemistry 2 (25 L)

Structure and bonding: VB description and its limitations. Elementary Crystal Field Theory: splitting of d^n configurations in octahedral, square planar and tetrahedral fields, crystal field stabilization energy in weak and strong fields; pairing energy. Jahn-Teller distortion.Metal-ligand bonding (MO concept, elementary idea), sigma- and pibonding in octahedral complexes (qualitative pictorial approach) and their effects on the oxidation states of transitional metals.

Unit-2: Magnetism and spectra of coordination compounds (15 L):

Magnetism and Colour: Orbital and spin magnetic moments, spin only moments of d^nions and their correlation with effective magnetic moments, including orbitalcontribution; quenching of magnetic moment: super exchange and antiferromagnetic interactions (elementary idea with examples only); d-d transitions; L-S coupling; qualitative Orgel diagrams for $3d^1$-$3d^9$ ions and their spectroscopic ground states; selection rules for electronic spectral transitions; spectrochemical series of ligands; charge transfer spectra (elementary idea).

Unit-3: Chemistry of d and f block elements (20L):

General comparison of 3d, 4d and 5d elements in term of electronic configuration, elemental forms, metallic nature, atomization energy, oxidation states, redox properties, coordination chemistry, spectral and magnetic properties. f-block elements: electronic configuration, ionization energies, oxidation states, variation in atomic and ionic (3+) radii, magnetic and spectral properties of lanthanides, comparison between lanthanide and actinides, separation of lanthanides (by ion-exchange method).Chemistry of some representative compounds: $K_2Cr_2O_7$, $KMnO_4$, $K_4[Fe(CN)_6]$, $K_2[Ni(CN)_4]$, H_2PtCl_6, $Na_2[Fe(CN)_5NO]$.

Reference Book:

1 .Lee, J.D. *Concise Inorganic Chemistry*, ELBS, 1991.
2. Douglas, B.E; Mc Daniel, D.H. & Alexander, J.J. *Concepts & Models of*
3. Inorganic Chemistry 3rd Ed., John Wiley Sons, N.Y. 1994.
Greenwood, N.N. &Earnshaw. *Chemistry of the Elements*, Butterworth-
Heinemann. 1997.
Collman, J. P. *et al. Principles and Applications of Organotransition Metal*
Chemistry. Mill Valley, CA: University Science Books, 1987.
Crabtree, R. H. *The Organometallic Chemistry of the Transition Metals*.*j*New
York, NY: John Wiley, 2000.
Spessard, G. O. &Miessler, G.L. *Organometallic Chemistry*. Upper Saddle River,
NJ: Prentice-Hall, 1996.

Inorganic Lab II: (Credit: 2)

(A) Iodo / Iodimetric Titrations

(i) Estimation of Cu(II) and $K_2Cr_2O_7$ using sodium thiosulphate solution (Iodometrically).
(ii) Estimation of antimony in tartar-emetic iodimetrically

(B) Complexometric titrations using disodium salt of EDTA

(i) Estimation of Mg^{2+}, Zn^{2+}

(ii) Estimation of Ca^{2+} by substitution method

(C) Inorganic preparations

(i) Cuprous Chloride, Cu_2Cl_2

(ii) Manganese(III) phosphate, $MnPO_4.H_2O$

(iii) Aluminium potassium sulphate $KAl(SO_4)_2.12H_2O$ (Potash alum) or Chrome alum.

Reference Books:

- Vogel, A.I. *A Textbook of Quantitative Inorganic Analysis*, ELBS. 1978
- Marr, G. and Rockett, R.W. *Practical Inorganic Chemistry,* Van Nostrand Reinhold. 1972.

Biomolecules I (60Lectures)

Unit 1 – Chemistry of Bio-molecules: Structure and Function (30L)

Carbohydrates:

Monosaccharides: Aldoses upto 6 carbons, structure of D- glucose & D-fructose (configuration & conformation), anomeric effect, mutarotation. Important reactions and conversions including protection / deprotection protocol. Disaccharides and poly- saccharide: nature of glycosidic linkages.

Unit-2-Aminoacids and peptides:

Amino acids: Synthesis: (Strecker, Gabriel, acetamidomalonic ester, azlactone); isoelectric point, ninhydrin reaction. Peptides: peptide linkage, synthesis of peptides using N-protection & C-protection, solid phase synthesis; peptide sequence: C-terminal and N-terminal amino acid determination.

Problems based on chemical reactions and structure covering the above topics.

Proteins and Nucleic acids:

Primary, secondary, tertiary and quaternary structure of proteins and protein folding. Nucleic acids: Structure of nucleosides and nucleotides, RNA and DNA. Their role in protein synthesis.

Lipids:

Definition and classification.Fatty acids- properties of saturated and unsaturatedfatty acids.Esters of fatty acids-formation and hydrolysis; Essential fatty acids, Triacylglycerols.Reactions and characterization of fats hydrolysis, saponification value, iodine number, rancidity of fats, Reichert-Meissel number. Biological significance of fats.Characterization of fats, Phospholipids, Micelle bilayer, liposomes, Glycolipids, steroids and sterols.

Preliminary idea of Proteins and Nucleic acids as drug targets.

Unit 3 – Biochemistry: Bioenergetics (30L)

Bioenergetics and Metabolism: Principles of Bioenergetics: Bioenergetics and Thermodynamics, Phosphoryl group transfers and ATP generation, Biological Oxidation and Reduction reaction.

Carbohydrate metabolism: Intracellular metabolism of glucose - glycolysis, reaction and energetic of TCA cycle, (gluconeogenesis, glycogenesis, glycogenolysis, reactions and physiological significance of pentose phosphate pathway, regulation of glycolysis, TCA cycle, and glycogen metabolism).

Oxidative phosphorylation and electron transport chain: Structure of mitochondria, sequence of electron carriers, ATP synthesis, inhibitors of ETC, basic concept of oxidative phosphorylation, inhibitors and uncouplers of oxidative phosphorylation, photophosphorylation.

Lipid metabolism:
Metabolism (anabolism and catabolism) of triglyceride, Transport of fatty acid into
mitochondria, Beta-oxidation of fatty acids, reactions and energetic of beta oxidation, biosynthesis of saturated and unsaturated fatty acids, metabolism of ketone bodies, biosynthesis of phospholipids and cholesterol.

Amino acid metabolism:
General reactions of amino acid metabolism (oxidative
deamination, transamination, decarboxylation etc), glucogenic and ketogenic amino acids, urea cycle, biosynthesis and catabolism of amino acids (glycine, phenylalanine, glutamic acid), inborn errors of amino acid metabolism biosynthesis and catabolism of purines and pyrimidines (Adenine and cytosine)

Enzymes
Cofactors – Definition, examples of a) metal ions b) coenzymes c) prosthetic group
Definition, examples of holoenzymes, Apoenzyme.

Classification of enzymes, IUPAC system, Name & examples of each class Mechanism of enzyme activity—standard free energy change in a reaction-transition state, activation energy both in non-enzymatic and enzymatic reaction, reaction rate, rate

constant, rate limiting step, rate equation, binding energy, specificity of enzymes geometric and stereo specificity with example, lock & key hypothesis, induced fit hypothesis, proximity and orientation effect, strain and distortion theory, enzyme catalysis-i) acid- base catalysis, ii)metal ion catalysis iii) covalent catalysis – Examples .

Regulatory enzyme:
Allosteric enzyme, definition & example, allosteric modulators, feedback inhibition, kinetic properties of allosteric enzyme, K enzymes, M enzymes, sequential model & symmetry model, examples, regulation by covalent modification (likephosphorylation), example, regulation by proteolytic cleavage of protein, zymogens,example, **Isozymes**-Definition and basis of difference, example-lactate dehydrogenase.

Reference Books:

- Finar, I. L. *Organic Chemistry (Volume 2)*, Dorling Kindersley (India) Pvt. Ltd.(Pearson Education).
- Dugas, H. *Bioorganic Chemistry: A Chemical Approach to Enzyme Action.* 3rd ed. Springer-Verlag, New York.1996
- Berg, J.M., Tymoczko, J.L. &Stryer, L. (2006) *Biochemistr*y. 6th Ed. W.H. Freeman
- and Co.
- Nelson, D.L., Cox, M.M. &Lehninger, A.L. (2009) *Principles of Biochemistry. IV*
- *Edition.*W.H. Freeman and Co.
- Murray, R.K., Granner, D.K., Mayes, P.A. &Rodwell, V.W. (2009) *Harper's*
- *Illustrated Biochemistry.*XXVIII edition.Lange Medical Books/ McGraw-Hill.

Biomolecules Lab I (Credit:2)

1. To perform quantitative estimation of protein using Lowry's method. Determine

the concentration of the unknown sample using the standard curve plotted.

2. Study of the action of salivary amylase at optimum conditions

3. Effect of pH on the action of salivary amylase

4. Effect of temperature on the action of salivary amylase

5. Effect of inhibitor on the action of salivary amylase

6. Study of the activity of Trypsin using fresh tissue extracts.

7. To study the effect of temperature, organic solvents, on semi-permeablemembrane.

8. Isolation of Genomic DNA from E Coli

9. Qualitative analysis of the soil from different locations for pH and different water soluble cations and anions

10. Quantitative estimation of oxidisable organic matter in soil, carbonate and bicarbonates by volumetry and calcium and magnesium by EDTA titration.

11. Hardness of water by EDTA titration

12. Study of pH and conductivity of tap water and polluted water

13. Determination of Iodine number of an oil/ fat.

14. Isolation and characterization of DNA from onion/ cauliflower/peas.

Reference books:

- 1 Manual of Biochemistry Workshop, 2012, Department of Chemistry, Universityof Delhi.
- 2) Arthur, I. V. *Quantitative Organic Analysis,* Pearson.
- 3) D.A. Skoog, F.J. Holler & S. Crouch (ISBN 0-495-01201-7) *Principles of Instrumental Analysis*, Cengage Learning India Edition, 2007.
- 4) Willard, Merritt, Dean, Settle, *Instrumental Methods of Analysis*, 7th ed, IBH Book House, New Delhi.

SEMESTER-VI

CHEMISTRY -SCY53102: PHYSICAL CHEMISTRY-IV

(Credits: 4)

Theory: 60 L

Unit 1-Molecular Properties (10L)

Dielectric polarization. Mossotti- Clausius relation, polar molecule.Debye equation.Dipole moment and molecular structure. Intermolecular forces. Attraction and repulsion potentials: van der Waals forces, Keesom, Debye and London forces, their relative contribution; Lennard-Jones potential.

Unit 2- Spectroscopy I (20L)

Molecular & Electronic : Rotational spectroscopy of diatomic molecules: the rigid rotor model, selection rules, spectrum, characteristic features of spectral lines (spacing and intensity); determination of bond length, effect of isotopic substitution; vibrational spectroscopy of diatomic molecules: selection rules stemming out of the SHO model, spectra, anharmonicity and its consequence on energy levels, overtones, hot bands. Raman effect, characteristic features and conditions of Raman activity with suitable illustrations, rotational and vibrational Raman spectra, the rule of mutual exclusion with examples. Potential energy curve (diatomic molecules), Electronic transitions and Quantum theory, Theory of Electronic Spectra,

Intensities of Electronic transitions, The Franck Condon principle, vibratonal structure of electronic spectra, Franck-Condon factor, bond dissociation and principle of determination of dissociation energy (ground state). Molecular electronic absorption spectra, Molecular electronic emission spectra, Radiationless transitions, Jablonski diagram, non-radiative transitions, Kasha's rule, fluorescence and phosphorescence.

Unit 3: Spectroscopy II (20L)

NMR Spectra: Nuclear spin, NMR active nuclei, principle of nuclear magnetic resonance,equivalent and non equivalent carbons and protons, chemical shift δ), shielding / deshielding, upfield and downfield shifts. NMR peak area (integration for PMR), diamagnetic anisotropy, relative peak positions of different kinds of carbons and protons

IR Spectra: Modes of molecular vibrations, application of Hooke's law, characteristic stretchingfrequencies and factors effecting stretching frequencies.

Unit 4- Photochemistry (10L)

Brief history of Photochemistry, Laws of photochemistry: Grotthus-Draper law, Stark-Einstein law of photochemical equivalence and Lambert-Beer‘s law; quantum yield and its measurement for a photochemical process, Photosensitized reaction. Actinometry.

Reference books:

- Atkins, P. W. & Paula, J. de *Atkin’s Physical Chemistry* 10th Ed., Oxford University Press (2014).
- Ball, D. W. *Physical Chemistry* Thomson Press, India (2007).
- Castellan, G. W. *Physical Chemistry* 4th Ed. Narosa (2004).
- Mortimer, R. G. *Physical Chemistry* 3rd Ed. Elsevier: NOIDA, UP (2009).
- Engel, T. & Reid, P. *Physical Chemistry* 3rd Ed. Pearson (2013).

Inorganic IV

(Credit: 4)

Unit-1:Analytical Chemistry: Statistical Methods in Chemical Analysis and Environmental Analysis(15 L): Statistical methods in chemical analysis and environmental analysis Errors in chemical analysis: Accuracy and precision of measurements, determinate indeterminate, systematic and random errors in chemical analysis with examples, absolute and relative errors; source, effect and detection of systematic errors; distribution of random errors, normal error curve, standard deviations, standard deviation of calculated results- sum or difference, product or quotient, significant figures, rounding and expressing results of chemical computations. Principles for determination of BOD, COD, DO, TDS, in water samples. Detection and estimation of As, Hg, Cd, Pb, NH_4^+, and F^-, NO_3^-, NO_2^- in water sample. Detection, collection and principles of estimation of CO, NOx, SO_2, H_2S and SPM in air samples.

Course Structure & Syllabus For Integrated M.Sc. Chemistry (Session 2018-2023)

Unit-2:Analytical Chemistry: Analytical Separation (15 L): Ion exchange resins and their exchange capacities, principle and simple applications of ion exchange separation. Chromatographic separations: General description and classification of chromatographic methods, thin layer, paper and column chromatographic techniques and their simple applications, R_f-values and their significance, elution in column chromatography, migration rates of solutes, band broadening and column efficiency, column resolution.

Unit-3:Organometallic Chemistry (15 L):18-electron rule and its applications to carbonyls (including carbonyl hydrides and carbonylates), nitrosyls, cyanides, and nature of bonding involved therein. Simple examples of metal-metal bonded compounds and metal clusters. Metal-olefin complexes: zeises salt (preparation, structure and bonding), Ferrocene (preparation, structure and reactions). Hapticity(η) of organometallic ligands, examples of mono tri and penta-haptocyclopentadienyl complexes. Simple examples of fluxional molecules. Coordinative unsaturation: oxidative addition and insertion reactions. Homogeneous catalysis by organometallic compounds: hydrogenation, hydroformylation and polymerization of alkenes (Ziegler-Natta catalysis).

Unit-4: Bio-inorganic Chemistry(15 L): Elements of life: essential major, trace and ultra trace elements. Basic chemical reactions in the biological systems and the role of metal ions (specially Na^+, K^+, Mg^{2+}, Ca^{2+}, $Fe^{3+/2+}$, $Cu^{2+/+}$, and Zn^{2+}).Metal ion transport across biological membrane Na+-ion pump, ionophores. Biological functions of hemoglobin and myoglobin, cytochromes and ferredoxins, carbonate bicarbonate buffering system and carbonicanhydrase. Biological nitrogen fixation, Photosynthesis: Photosystem-I and Photosystem-II. Toxic metal ions and their effects, chelation therapy (examples only), Pt and Au complexes as drugs (examples only), metal dependent diseases.

Reference Books:

Christian, G.D. *Analytical Chemistry*, 6th Ed. John Wiley & Sons, New York, 2004.
| | Harris, D.C.: *Exploring Chemical Analysis*, 9th Ed. New York, W.H. Freeman, 2016.
| | Khopkar, S.M. *Basic Concepts of Analytical Chemistry*. New Age International Publisher, 2009.
| | Skoog, D.A. Holler F.J. &
| | Purcell, K.F &Kotz, J.C. *Inorganic Chemistry* W.B. Saunders Co, 1977.
| | Huheey, J.E., *Inorganic Chemistry*, Prentice Hall, 1993.
| | Lippard, S.J. & Berg, J.M. *Principles of Bioinorganic Chemistry* Panima Publishing Company 1994.
| | Cotton, F.A. & Wilkinson, G, *Advanced Inorganic Chemistry* Wiley-VCH, 1999
| | Basolo, F, and Pearson, R.C. *Mechanisms of Inorganic Chemistry*, John

Course Structure & Syllabus For Integrated M.Sc. Chemistry (Session 2018-2023)

Organic IV (60 Lectures)

Synthetic strategy: Retrosynthetic analysis- disconnections, synthons, donor and acceptorsynthons,functional group interconversion, C-C disconnections and synthesis [one group and two group (1,2 to 1,6-dioxygenated], reconnection (1,6-di carbonyl), natural reactivity and umpolung, protection-deprotection strategy [alcohol, amine, carbonyl, acid]

Heterocycles: Synthesis and reactions of heterocycles (monocyclic and bicyclic) with oneheteroatom.

NMR Spectra: Nuclear spin, NMR active nuclei, principle of nuclear magnetic resonance,equivalent and non equivalent carbons and protons, chemical shift δ), shielding / deshielding, upfield and downfield shifts. NMR peak area (integration for PMR), diamagnetic anisotropy, relative peak positions of different kinds of carbons and protons

IR Spectra: Modes of molecular vibrations, application of Hooke's law, characteristic stretchingfrequencies and factors effecting stretching frequencies.

UV Spectra: Electronic transition, relative positions of λ-max, Woodward's empirical rule.

Mass spectra: Elementary idea

Reference Books:

- Stuart Warren, Paul Wyatt. *Organic Synthesis: The Disconnection Approach*. 2nd Ed. Wiley-VCH, 2011
- John A. Joule, Keith Mills. *Heterocyclic Chemistry.* 5th Ed. Wiley-VCH, 2010
- Donald L. Pavia, Gary M. Lampman, George S. Kriz, James A. Vyvyan. *Introduction to Spectroscopy*. 5th Ed. Cengage Learning. 2015.

ELECTIVE -SCY53108: INSTRUMENTATION-I

(Credits: 4)

Theory: 60 L

Unit 1 - Basic electronics and Instrumentation. (12L)

Instrumentation and Basic electronics: Electronic components, transistors and multimeter; Basic concept of signal, noise and signal amplification; Elementary idea about the instruments used in Chemistry.

Unit 2 – Instrumental Methods of Analysis: Electrochemical and Spectral Methods, Instrumental Methods (48L)

Electrochemical and Spectral Methods:

Electrochemical methods: Conductometry, Potentiometry, pH-metry. Electrogravimetry, Coulometry. Spectrophotometry: Lambert-Beer law, Limits to Beer‘s law, Principle of spectrophotometric estimation of iron, manganese and phosphorous. Principles and instrumentations of atomic absorption and atomic emission spectrometry; estimation of sodium and potassium in water samples.

Instrumental Methods:

Flame Spectrometry, Introduction, Principles, Elementary theory and Instrumentation of Atomic Absorption and Atomic Emission Spectrometry; Determination of Ca and Mg in tap water (application), Radiochemical methods and Environmental analysis: Basic Instrumentation, Measurement of Radioactivity, Neutron activation analysis, Isotope dilution analysis, Radiometric titrations, Hazards of radiation and Safety measures.

Chemical Method of Analysis:

Gravimetric and tritimetric methods of analysis:

Requirements of gravimetry: properties of precipitates and precipitating regents, particle size and filterability of precipitates, colloidal and crystalline precipitates coprecipitation and post-precipitation drying and ignition of precipitates, principles of gravimetric estimation of chloride, phosphate, zinc, iron, aluminum and magnesium singly. Primary and secondary standard substances in acid-base, redox, complexometric (EDTA) and argentometric titrations. Principle and application of redox tritimetric estimation based on the use of the following reagents: $KMNO_4$, $K_2Cr_2O_7$, I_2, $Na_2S_2O_3.5H_2O$, $KH(IO_3)_2$ and $KBrO_3$. Principle of argentimetric estimation of chloride using adsorption indicators.

Principle of complexometric EDTA titration, metal ion indicators (examples), masking and demasking reactions, estimation of Cu-Zn, Fe-Al and Ca-Mg mixture by EDTA titration methods.

Dissolution, scheme of analysis and principles of estimation of the constituents ofthe following materials: dolomite, pyrolusite, chalchopyrites, Portland cement, basic slag, brass, steel and type metal.

Reference books:

| | D.A. Skoog, F.J. Holler & S. Crouch (ISBN 0-495-01201-7) *Principles of Instrumental Analysis*, Cengage Learning India Edition, 2007.

| | Willard, Merritt, Dean, Settle, *Instrumental Methods of Analysis*, 7th ed, IBH Book House, New Delhi.

ELECTIVE -SCY53208: INSTRUMENTATION LAB-I

(Credits: 2)

Practical: 30 L

Instrumentation Lab I (30 L)

1. Safety Practices in the Chemistry Laboratory
2. Determination of the isoelectric pH of a protein.
3. Titration curve of an amino acid.
4. Determination of the void volume of a gel filtration column.
5. Determination of a Mixture of Cobalt and Nickel (UV/Vis spec.)
6. Study of Electronic Transitions in Organic Molecules (i.e., acetone in water)
7. IR Absorption Spectra (Study of Aldehydes and Ketones)

8. Determination of Calcium, Iron, and Copper in Food by Atomic Absorption

9. Quantitative Analysis of Mixtures by Gas Chromatography (i.e., chloroform and

carbon tetrachloride)

10. Separation of Carbohydrates by HPLC

11. Determination of Caffeine in Beverages by HPLC

Reference books:

| | D.A. Skoog, F.J. Holler & S. Crouch (ISBN 0-495-01201-7) *Principles of Instrumental Analysis*, Cengage Learning India Edition, 2007.
| | Willard, Merritt, Dean, Settle, *Instrumental Methods of Analysis*, 7th ed, IBH Book House, New Delhi.

SEMESTER –VII

CHEMISTRY -SCY54101: PHYSICAL CHEMISTRY-V

(Credits: 4)

Theory: 60 L

Unit 1- Equilibrium Thermodynamics and Surface Phenomena: (22 L)

Recapitulation of 1st and 2nd law of thermodynamics, Mathematical theorems on Pfaffianequations, Caratheodory's theorem, entropy in the light of caratheodory's principle, Nernst heattheorem, the third law of thermodynamics, entropy determination. Excess function, fugacity,activity and activity coefficients, Concept of standard state. Thermodynamics of polymersolution: entropy, heat and free-energy of mixing.

Vapour pressure over curved surface, the Young-Laplace eqution, the Kelvin equation,Interfacial region, adsorption on solid, the adsorption isotherms (Langmuir, BET – withderivation). Surface active agents, micelles, reverse micelles, solubilisation, and micro-emulsion.

Unit 2- Statistical Mechanics: (14 L)

Probability, thermodynamic probability and entropy, Maxwell-Boltzman statistics, Partitionfunction: translational (for ideal gas - concept of thermal wavelength), rotational, vibrational andelectronic partition functions (diatomic molecule); molecular and molar partition function,Qualitative idea of Quantum statistics (Bose-Einstein, Fermi-Dirac statistics): Thermodynamicprobability and distribution formula (without derivation), comparison with classical statistics -distinguishability and indistinguishability of identical particles. Application: Theory of specificheat of solids – Einstein's and Debye's pictures.

Unit 3- Chemical Kinetics: (14 L)

Collision theory: Lines of centre model. Introduction of potential energy surface and contour,internal coordinates and reaction coordinates, reaction path – valley and saddle point; saddlepoint – activation energy, classical trajectory, and theory of absolute rate. Comparison ofcollision and absolute rate theory. Rate constant expression for chemical reaction based onEyring equation with one example, Physical rate processes – viscosity and

diffusion, Non-equilibrium formulation: Passage to statistical approach – energy redistribution in activatedcomplex, Lindemann collision, Hinshelwood suggestion, Rice-Ramsperger- Kassel (RRK)theory, Reaction in solution. Diffusion-controlled reactions.

Fast reaction - relaxation methods.Branching chain reactions and explosion. Oscillatoryreactions: Lotka-Volterra model and its applications.Rate equation for electrode process. Butler-Volmer equation, High Field approximation, Tafelequation, Low field approximation, kinetic derivation of Nernst equation, exchange currentdensity and polarizability of interfaces, concept of overvoltage.

Unit 4- Electrochemistry: (10 L)

Ion-solvent interaction: Born model and Born equation, enthalpy of ion-solvent interaction andits calculation Debye-Hückel theory of strong electrolytes, concept of ionic atmosphere. Debye-Hückel limiting law for single ionic activity coefficient and mean activity coefficient (withderivation), its relation to ionic strength. Bjerrum model for ion association: Formation of ionpairs, derivation of ion-association constant.

Reference books:

- Atkins, P. W. & Paula, J. de *Atkin's Physical Chemistry* 10th Ed., Oxford University Press (2014).
- Ball, D. W. *Physical Chemistry* Thomson Press, India (2007).
- Castellan, G. W. *Physical Chemistry* 4th Ed. Narosa (2004).
- Mortimer, R. G. *Physical Chemistry* 3rd Ed. Elsevier: NOIDA, UP (2009).
- Engel, T. & Reid, P. *Physical Chemistry* 3rd Ed. Pearson (2013).

Inorganic V

Unit 1:Nature of Chemical Bonding (24L): Preamble, LCAO and/or Huckel treatments of sigma- and pi-MOs (inorganic di- and polyatomic species and organic units like alkanes, alkenes, allyl system, dienes, polyenes.VBT of heteronuclear diatomic molecules, inadequacies of the simple VBT. Hybridization, participation of d orbitals in hybridization in polyatomic species.Molecular orbital theory (MOT), linear combination of atomic orbitals (LCAO), criteria for the formation of stable MOs. Sigma, Pi and Delta molecular orbitals, open and cyclic, sandwich molecules, boron compounds.Homonuclear and heteronuclear diatomic molecules and ions.MO theory of polyatomic molecules and ions. MO theory of π bonding and multi-centre bonding. MO concept of metal-ligand bonding (pictorial approach).Koopmans' theorem, Walsh diagram, isolobal analogy.

Unit-2 Coordination chemistry-stereochemistry, bonding, geometric and electronic structures (36L): Fundamentals, Thermodynamic aspects of crystal field splitting, kinetics aspects of crystal field splitting, crystal field activation energy, labile and inert complexes. Single ion magnetic behavior, metal centered transitions.

Limitations of CFT, Free ion terms arising from d^n configuration and their splitting in Oh and Td fields.Orgel diagram, Tanabe-Sugano diagram, ligand symmetry orbital, molecular orbital, spectral properties, Nephelauxetic effect, Racah parameter, vibronic coupling, band broadening, spin-orbit coupling, spin-forbidden transition, intensity stealing, magnetic properties, anomalous and subnormal magnetic moments, lowering of symmetry,

electronic, steric, Jahn-Teller and Renner-Teller effects on energy levels, conformation of chelator/congregator, structural equilibrium and implication. Charge transfer spectra – LMCT and MLCT transition in O_h and T_d complexes

Structural and stereoisomerism of coordination compounds, optically active coordination compounds and their resolution procedures, absolute configuration of enantiomers.

Reference books:

1 .Lee, J.D. *Concise Inorganic Chemistry*, ELBS, 1991.
2. Douglas, B.E; Mc Daniel, D.H. & Alexander, J.J. *Concepts & Models of*
3. Inorganic Chemistry 3rd Ed., John Wiley Sons, N.Y. 1994.
Greenwood, N.N. &Earnshaw. *Chemistry of the Elements*, Butterworth-
Heinemann. 1997.
Collman, J. P. *et al. Principles and Applications of Organotransition Metal*

ORGANIC V (Course Credit 4 and Lecture No. 60)
STEREOCHEMISTRY (20L)

Static Aspects: Symmetry properties, point group; configuration – acyclic and cyclic systems; conformation – cyclic systems (cyclohexene, cyclohexanone, substituted cyclopentanes and cyclopentanones, medium rings, decalin and hydrindane systems).Dynamic Aspects: cyclisation reactions, Baldwin‘s Rules; conformation and reactivity with reference to substitution, elimination, addition and rearrangement reactions.Curtin-Hammett Principle and examples of asymmetric reaction: Zimmerman Traxler model for Aldol reaction. Determination of configuration and conformation by ORD and CD and Cotton Effect

PERICYCLIC REACTION (24L)

Pericyclic reactions: Molecular orbitals for acyclic conjugated systems. Theory of pericyclic reactions – i) Frontier Molecular Orbital (FMO) approach ii) concept of aromaticity of transition states (Hückel / Möbius systems). The Woodward-Hoffmann selection rules and general rules.

General perturbation molecular orbital theory in cycloadditions: Symmetry principles in pericyclic reactions, orbital and state correlation diagram for electrocyclic and cycloaddition reactions. Reactivity,regioselectivity and periselectivity.Cycloaddition reactions: antarafacial and suprafacial additions, 4n and 4n+2 systems; 2,2 addition of ketenes, 1,3 dipolar cycloadditions and cheleotropic reactions. Ene reactions, group-transfer reactions and eliminations. Scope, reactivity and stereochemical features of electrocyclic reactions (4e, 6e and 8e neutral systems).Electrocyclic reactions of charged systems (cations and anions), Electrocyclic reactions: conrotatory and disrotatory motions, 4n, 4n+2 and allyl systems.Sigmatropic rearrangements: [1, j] shifts – [1, 5] and [1, 7] shifts in neutral systems and [1,4] shift in charged species: [i, j] shifts – [3, 3] shifts, Sommelet-Hauser, Cope, aza-Cope rearrangements, Fluxional tautomerism. Claisen rearrangements; [5, 5] shifts, [2, 3] shifts in ylids.

ORGANIC PHOTOCHEMISTRY (16L)

Introduction to organic photochemistry, Primary photochemical reactions of n,π*states, Photophysical process of n,π*states: Electronic energy transfer, primary photochemical process of α- cleavage, primary photochemical process of hydrogen abstraction, photochemical process of addition to π system, electron transfer reactions, Primary photochemical reactions of π,π*states, cis-trans isomerisations, di- π-methane rearrangements, Photochemical production and reactions of carbenesand nitrenes, Photochemical reaction of azo compounds, Photochemical oxygenations-Singlet Oxygen, Photochemistry of halogen containing compounds, Photoinduced electron transfer reactions, Applications of photochemistry.

Reference books:

- Ernest L. Eliel. *Stereochemistry of Organic Compounds*. Wiley VCH
- D. Nasipuri. *Stereochemistry of Organic Compounds. Principles and Applications*. New Age.
- Ian Fleming. *Pericyclic Reactions*. Oxford Publishers.
- J.M. Coxon, B. Halton. *Organic Photochemistry*. Cambridge University Press.

CHEMISTRY -SCY54201: PHYSICAL Laboratory-III

(Credits: 4)

Practical: 60 L

Physical Lab III (60 Lectures)

Phase Equilibria:

I. Determination of critical solution temperature and composition at CST of the phenol-water system and to study the effect of impurities of sodium chloride and succinic acid on it.

II. Phase equilibria: Construction of the phase diagram using cooling curves or ignition tube method: a. simple eutectic and b. congruently melting systems.

III. Distribution of acetic/ benzoic acid between water and chloroform or cyclohexane.

IV. Study the equilibrium of at least one of the following reactions by the distribution method:

(i) $I_2\,(aq) + I^-\,(aq) \rightarrow I_3^-\,(aq)$

(ii) $Cu^{2+}(aq) + nNH_3 \rightarrow Cu(NH_3)_n^{2+}$

Potentiometry:

V. Perform the following potentiometric titrations: i. Strong acid vs. strong base ii. Weak acid vs. strong base iii. Dibasic acid vs. strong base iv. Potassium dichromate vs. Mohr's salt

Reference Books:

| | Khosla, B. D.; Garg, V. C. & Gulati, A. *Senior Practical Physical Chemistry,* R. Chand & Co.: New Delhi (2011).

| | Garland, C. W.; Nibler, J. W. & Shoemaker, D. P. *Experiments in Physical Chemistry 8th Ed.*; McGraw-Hill: New York (2003).

| | Halpern, A. M. & McBane, G. C. *Experimental Physical Chemistry 3rd Ed.;* W.H. Freeman & Co.: New York (2003).

Organic Lab III (60 Lectures)

1. Purification of organic compounds by crystallization using the following solvents:

a. Water

b. Alcohol

c. Alcohol-Water

2. Chromatography

a. Separation of a mixture of two amino acids by ascending and horizontal paper chromatography.

b. Separation of a mixture of two sugars by ascending paper chromatography.

c. Separation of a mixture of o-and p-nitrophenol or o-and p-aminophenol by thin layer chromatography (TLC).

b. Separation of a mixture of two compounds by column chromatography.

Course Structure & Syllabus For Integrated M.Sc. Chemistry (Session 2018-2023)

Reference text:

- Mann, F.G. & Saunders, B.C. *Practical Organic Chemistry,* Pearson Education (2009)
- Furniss, B.S.; Hannaford, A.J.; Smith, P.W.G.; Tatchell, A.R. *Practical Organic Chemistry, 5th Ed.,* Pearson (2012)

SEMESTER-VIII

CHEMISTRY -SCY54102: PHYSICAL CHEMISTRY-VI

(Credits: 4)

Theory: 60 L

Unit 1- Quantum Mechanics: (22 L)

Introductory ideas of classical mechanics – Equation of motion: Newtonian mechanics,Lagrangian mechanics, Hamiltonian mechanics, Classical mechanical Poisson bracket.Identification of classical and quantum systems, Bohr's correspondence principle with examples;Double slit experiment. Uncertainty principle. Plausibility arguments leading to Schrödingerequation, Probability concept.Continuity equation. Elementary applications – different potentialproblems: free particle, confined particle in a box, step potential barrier problem: tunnelling andits applications.Linear operators in quantum mechanics.Eigen value equation. Hermitian operator, Heisenbergequation of motion, constant of motion, Ehrenfest's theorem. Commutator and relationship withPoisson bracket, non compatibility and uncertainty; Formal derivation of Heisenberg uncertaintyprinciple: commutability and compatibility.Simple harmonic oscillator (operator method).Approximate method: Elementary perturbation theory, Variation theorem, Simple applications.The Hydrogen atom Problem: Cartesian and polar coordinates. Centre of mass and relativecoordinates. General forms of solutions and orbital specifications.Spherical harmonics.Real andcomplex orbitals. Role of constants of motion.

Unit 2- Atomic Structure: (16 L)

Motion under central force: Conservation of angular momentum and its consequence. Motion ofangular momentum under magnetic field.Larmorprescision.Quantization rule and quantumnumbers. Zeeman effect. Stern-Gerlach experiment.Spin-orbit interaction, conservation of totalangular momentum J, Vector atom model. Anomalous Zeeman effect, Paschen-Beck effect.Multielectron system- Pauli exclusion principle. Term symbols for simple multi-electron system.Magnetic moment and Lande's g factor.

Unit 3- Molecular Spectroscopy and Molecular Interaction: (22 L)

Molecular spectroscopy: Introduction, elementary idea about spectroscopic instrumentation,spectral broadening. Electromagnetic spectrum and molecular processes associated with theregions. Rotational spectra of polyatomic molecules: classification of molecules into spherical,symmetric and asymmetric tops; linear triatomic molecules, Non-rigid rotor. Elementary idea of Stark effect. Anharmonic oscillator and dissociation.Elementary

idea of Born-Oppenheimerapproximation.Vibration rotation spectra for diatomic molecule, Rotational-vibrational coupling.Raman spectra: classical theory of Raman scattering, concept of polarizability ellipsoid.

Reference books:

- Atkins, P. W. & Paula, J. de *Atkin's Physical Chemistry* 10th Ed., Oxford University Press (2014).
- Ball, D. W. *Physical Chemistry* Thomson Press, India (2007).
- Castellan, G. W. *Physical Chemistry* 4th Ed. Narosa (2004).
- Mortimer, R. G. *Physical Chemistry* 3rd Ed. Elsevier: NOIDA, UP (2009).
- Engel, T. & Reid, P. *Physical Chemistry* 3rd Ed. Pearson (2013).

INORGANIC-VI

Unit-1: CHEMISTRY OF d-BLOCK AND f-BLOCK ELEMENTS (30 L)

d-BLOCK ELEMENTS:

Structure and bonding of higher boranes, Lipscomb's tropological diagrams and Wade's rules. Metal-metal bonded complexes of transition metals (structure and bonding): dirhenium complexes, molybdenum blue, tungsten blue, tungsten bronze, ruthenium red, Creutz-Taube complex, transition metal dioxygen and dinitrogen complexes (structure, bonding and reactivity), Vaska'scomplex.Alkali metal complexes with macrocyclic ligands, crown ether and cryptate complexes.Chlorophyll-Mg complex (active centre).

f-BLOCK ELEMENTS :

Lanthanide and actinide elements: terrestrial abundance and distribution, relativistic effect, variation of atomic and ionic radius, ionization energy, electronic configuration and oxidation states, magnetic properties, electronic spectra, aqueous and complex chemistry in different oxidation states, comparison with those of d-block elements; organometallic compounds, use of lanthanide compounds as NMR-shift reagent and others. Super heavy elements.Production, properties and uses of Ce, Gd, Pu and Pt- metals and their compounds.

Unit-2.ORGANOMETALLIC CHEMISTRY (14 L)

Preliminary idea and applications of 16 and 18 electrons rule for organometallic compounds. Reaction of organometallic complexes: substitution, oxidative addition, reductive elimination, insertion and elimination, electrophilic and nucleophilic reactions of coordinated ligands.

Stereochemical non-rigidity and fluxional behaviour of organometallic compounds, catalysis by organometallic compounds: Wilkinson's catalyst, Tolman's catalytic loops; synthesis gas, water gas shift reaction, synthesis of methanol, hydroformylation (oxo process), hydrogenation of unsaturated compounds, Masanto acetic acid process, Waker process, synthetic gasoline, Fischer-Tropsch process and mobil process; Polymerisation, oligomerisation and metathesis reactions of alkenes and alkynes; Zieglar-Natta catalysis.

Unit-3.INSTRUMENTAL METHODS OF ANALYTICAL CHEMISTRY (16 L)

Spectroscopic Techniques

Theory, Instrumentation and application of Atomic absorption Spectroscopy, Atomic fluorescence spectrometry, Atomic emission spectrometry, UV-Visible molecular absorption Spectrometry (principles, instrumentation, and application), Molecular luminescence spectroscopy (fluorescence, phosphorescence, chemiluminescence), concept of Inductively coupled plasma-atomic absorption spectrophotometer, ICPA-AAS (Instrumentation and application).

Separation Techniques and Chemical Sensors

Principles of Chromatography, Classification of Chromatography, Paper Chromatography, Techniques of Column Chromatography, Thin layer Chromatography , Gas Chromatography, High-performance Liquid Chromatography, Ion-exchange Chromatography. Principle of chemical sensors, types of chemical sensors based on the modes of transductions, types of chemical sensors based on the chemically sensitive materials (solid electrolyte, gas , semiconductor), Humidity sensors, Biosensors, Electrochemical sensors (Potentiometric sensors, Ion-selective electrodes, Membrane electrodes, Amperometric sensors, Clark and Enzyme electrodes).

Voltametry and Thermal Analysis

Polarography: Current –Voltage relationship , Theory of Polarographic waves (DC and sampled DC (tast) polarograms), Instrumentation, Ilkovic equation, Qualitative and Quantitative applications.

Thermal Analysis: Theory, methodology and application of Thermo Gravimetric Analysis (TGA), Differential Thermal Analysis (DTA), and Differential Scanning Calorimetry (DSC). Principles, techniques, and application of thermometric titration methods.

Reference books:

- Christian, G.D. *Analytical Chemistry*, 6th Ed. John Wiley & Sons, New York, 2004.
- Harris, D.C.: *Exploring Chemical Analysis*, 9th Ed. New York, W.H. Freeman, 2016.
- Khopkar, S.M. *Basic Concepts of Analytical Chemistry*. New Age International Publisher, 2009.
- Skoog, D.A. Holler F.J. &

- Purcell, K.F &Kotz, J.C. *Inorganic Chemistry* W.B. Saunders Co, 1977.
- Huheey, J.E., *Inorganic Chemistry*, Prentice Hall, 1993.
- Lippard, S.J. & Berg, J.M. *Principles of Bioinorganic Chemistry* Panima Publishing
- Company 1994.
- Cotton, F.A. & Wilkinson, G, *Advanced Inorganic Chemistry* Wiley-VCH, 1999
- Basolo, F, and Pearson, R.C. *Mechanisms of Inorganic Chemistry*, John

Organic-VI

ORGANIC II (Course Credit 4 and Lecture No. 60)

SYNTHETIC CHEMISTRY: STRATEGY AND METHODOLOGY (24 L) METHODOLOGY

The roles of boron, phosphorus, sulfur and silicon in organic synthesis.Stereoselective hydroboration, hydrogenation, epoxidation and hydroxylation.

STRATEGY Retrosynthetic analysis, disconnection, typical examples to illustrate thedisconnection approach to organic synthesis.

HETEROCYCLIC CHEMISTRY (20 L)

Systematic nomenclature (Hantzsch – Widman system) for monocycle and fused heterocycles.General approach to heterocyclic synthesis – cyclisation and cycloadditionroutes.Heterocycles in organic synthesis – masked functionalities, umpolung, Stork annulation reaction and applications (synthesis of testosterone, estrone, progesterone, ranitidine, lansoprazole and/or recently discovered molecules etc. Rearrangement and ring transformation involving 5- and 6-membered heterocycles with one heteroatom.

CHEMISTRY OF NATURAL PRODUCTS (16 L)

Structural types; structure elucidation, reactions and synthesis of representative examples of (i) Alkaloids (ii) Terpenoids. Stereochemistry, reactions and synthesis of terpenoids and carotenoids: zingiberine, santonin, abietic acid, β-carotene. Stereochemistry, reactions and synthesis of alkaloids: quinine, morphine, camptothecin and recently discovered bioactive natural products.

Reference Books:

- Stuart Warren, Paul Wyatt. *Organic Synthesis: The Disconnection Approach*. 2nd Ed. Wiley-VCH, 2011
- John A. Joule, Keith Mills. *Heterocyclic Chemistry.* 5th Ed. Wiley-VCH, 2010
- Donald L. Pavia, Gary M. Lampman, George S. Kriz, James A. Vyvyan. *Introduction to Spectroscopy*. 5th Ed. Cengage Learning. 2015.
- Classics in Total Synthesis: Targets, Strategies, Methods- K.C. Nicolau, E.J. Sorensen. Wiley VCH

Course Structure & Syllabus For Integrated M.Sc. Chemistry (Session 2018-2023)

INORGANIC LAB I (Course Credit 4 and Lecture No. 60)

Part-I

Qualitative analysis of mixture of compounds containing two rare elements and insoluble samples

Rare elements: Ti, V, Mo, W, Zr, Ce, U

Insoluble Samples: $PbSO_4$, $BaSO_4$, $SrSO_4$, Fe_2O_3, CaF_2, Cr_2O_3, Al_2O_3, SiO_2, SnO_2, TiO_2, ZrO_2, CeO_2

Part II (any three)

1. Determination of the amount of calcium in milk powder by EDTA complexometry
2. Potassium trioxaltoferrate III: Sythesis, analysis and photochemistry.
3. Analysis of kidney stones by permanganometric titration
4. Preparation of $[Ni(NH3)_6]^{2+}$ and its analysis by different methods
5. Estimation of iodine in iodized common salt using iodometry
6. Estimation of phosphoric acid in cola drinks by molybdenum blue method
7. Paper and column chromatography of plant pigments

ANALYTIC LAB I (Course Credit 4 and Lecture No. 60)

1. Environmental Analysis: Sampling and analysis of air/water/soil. Analysis of drug samples.
2. Physico-chemical experiments.
3. Quantitative estimation of alloys, ores and minerals.

SEMESTER-IX

CHEMISTRY -SCY55101: Group Theory and Spectroscopy -I

(Credits: 4)

Theory: 60 L

Unit 1- Symmetry and Group Theory in Chemistry: (24 L)

Introduction, symmetry elements and group theory, group theory and quantum mechanics(elementary ideas), elementary ideas of representation theory, irreducible representations of pointgroup, definitions of classes and character, statement of grand orthogonality theorem,orthogonality theorem for characters, character tables, concept of character projection operator.

Selection rules in molecular spectroscopy, Vibration of polyatomic molecules – Normal modes,their symmetry properties, IR and Raman activity. Electronic spectroscopy, crystal field theory.

SALC – Hückel theory, Hybridization, Vibronic coupling,

Unit 2- Spectroscopy I : Absorption Spectroscopy (16 L)

Qualitative treatment of Born-Oppenheimer separation, Frank-Condon principle, selection rules,characteristics of π-π*, n-π* transitions, d-d transitions and their intensities.Apparent violation ofselection rule (vibrational and spin-orbit couplings).

Unit 3- Photochemistry and Photophysics (20 L)

Potential energy curves, mirror-image symmetry, deactivation – internal conversion andintersystem crossing, radiation less deactivation, fluorescence and phosphorescence.Quenchingof fluorescence, Life-time variation in presence of quencher.

Excimers and exciplexes. Intermolecular energy transfer (FRET). Energy transfer andconformation distributions of biopolymers, protein fluorescence.

Excited state proton transfer.Einstein theory – A, B coefficients, Principles of LASER and characteristic features, Laserspectroscopy.

Reference Books:

- Atkins, P. W. & Paula, J. de *Atkin's Physical Chemistry* 10th Ed., Oxford University Press (2014).
- Ball, D. W. *Physical Chemistry* Thomson Press, India (2007).
- Castellan, G. W. *Physical Chemistry* 4th Ed. Narosa (2004).
- Mortimer, R. G. *Physical Chemistry* 3rd Ed. Elsevier: NOIDA, UP (2009).
- Engel, T. & Reid, P. *Physical Chemistry* 3rd Ed. Pearson (2013).

Polymers and Molecules of Life(Course Credit 4 and Lecture No. 60)

Unit-1. Polymer Chemistry: (20 L)

Classification of polymers, kinetics of two dimensional polymerization, condensation and addition polymerizations; initiation, propagation and termination; chain transfer, co-polymerization; molecular weight of polymers; determination of molecular weights.Some specific methods for molecular weight determination of biopolymers – gel filtration, SDS – PAGE for proteins, Agarose gel method for nucleic acids. Thermodynamics of polymer solution: Polymer conformation.

Unit-2.Molecules of Life: (20 L)

Introduction: The molecules of life – nucleic acids, proteins and enzymes, carbohydrates, lipids. Mechanism in biological chemistry: (i) Mechanism of enzyme action, examples of enzyme mechanisms for chymotrypsin, ribonuclease, lysozyme and carboxypeptidase A (ii) Enzyme catalyzed reactions – examples of nucleophilic displacement on a phosphorus atom, coupling of ATP cleavage to endergonic processes, proton transfer reactions to and from carbon (iii) Mechanism of reactions catalyzed by cofactors including coenzyme A, NAD^+, NADH, FAD and thiamine

pyrophosphate; Chemical synthesis of peptides and proteins; Use of enzymes in organic synthesis; Structural analysis of proteins; Protein folding; Biotechnological applications of enzymes: Enzyme purification, immobilization of enzymes, enzyme therapy, enzyme and recombinant DNA technology.

Unit-3.Biophysical Chemistry: (20 L)

Structure of Bio-molecules: Protein structure – building blocks, peptide bond, levels of structure; Bio-molecular complexes: protein-ligand, enzyme-substrate. Techniques for study of bio-molecular structure and function- optical techniques: CD, ORD: Cotton effect, Faraday effect. Fluorescence anisotropy for bio-molecular structure determination.

Reference Books:

- Dugas, H. *Bioorganic Chemistry: A Chemical Approach to Enzyme Action.* 3rd ed. Springer-Verlag, New York.1996
- Berg, J.M., Tymoczko, J.L. &Stryer, L. (2006) *Biochemistr*y. 6th Ed. W.H. Freeman
- and Co.
- Nelson, D.L., Cox, M.M. &Lehninger, A.L. (2009) *Principles of Biochemistry. IV*
- *Edition.*W.H. Freeman and Co.
- Murray, R.K., Granner, D.K., Mayes, P.A. &Rodwell, V.W. (2009) *Harper's Illustrated Biochemistry.*XXVIII edition.Lange Medical Books/ McGraw-Hill

CHEMISTRY -SCY55105: Spectroscopy -II

(Credits: 4)

Theory: 60 L

Unit 1- Magnetic Resonance Spectroscopy(24 L): NMR, ESR: Basics and Application, PhotoelectronSpectroscopy:
Magnetic resonance spectroscopy – introduction, basis features of spectroscopy, relaxationprocesses: spin-spin and spin-lattice.
NMR: chemical shift and spin-spin coupling; chemical shielding – elementary idea ofdiamagnetic and paramagnetic shielding.
ESR: ESR spectrometer, line width, hyper-fine splitting, ESR of triplet state,applications. **PES:** - photoexcitation and photoionization; **XPS** - principle andapplications.

Unit 2- Mass Spectrometry, Mossbauer, FTIR, FTNMR, 2D NMR. (24 L)

Mass spectrometry: Fragmentation processes and structural analysis; ESI, GC/MS, LC/MS andMS/MS techniques. Interpretation of spectroscopic (NMR, IR and mass) data, as applied toorganic, inorganic and biological systems.

Principles of Mossbauer spectroscopy: experiments, center shift, quadroupleinteraction, magnetic interaction.

Fourier transformations, time domain versus frequency domain. Principles of FT NMR,instrumentation, the rotating frame of reference, simple 1D experiments. FT IR – principles andinstrumentation.

Introduction to 2D NMR: NOESY, COSY, HETCOR, HOMCOR, INADEQUATE, INDOR,INEPT for simple compounds and problems. Applications of multinuclear NMR in inorganiccompounds – Examples from 1 H, 11 B, 13 C, 19 F, and 31 P NMR of paramagnetic molecules Lanthanide shift.

Unit 3- Basic Electronics and Instrumentation: (12 L)

Characteristics and use of diodes, capacitors, inductors, transformers, FET, MOSFET, rectifier,power supply, clipper, oscillator and timer circuits, linear small signal amplifiers and theircharacteristics, integrated circuits, operational amplifier and its applications includingapplications in analytical and nuclear instruments, logic gates and elementary digital circuit.

Reference Books:

- Atkins, P. W. & Paula, J. de *Atkin's Physical Chemistry* 10th Ed., Oxford University Press (2014).
- Ball, D. W. *Physical Chemistry* Thomson Press, India (2007).
- Castellan, G. W. *Physical Chemistry* 4th Ed. Narosa (2004).
- Mortimer, R. G. *Physical Chemistry* 3rd Ed. Elsevier: NOIDA, UP (2009).
- Engel, T. & Reid, P. *Physical Chemistry* 3rd Ed. Pearson (2013).

PRACTICAL-V

Computational Chemistry Lab-I

Part-1

Computer programming based on FORTRAN 90 and Numerical methods akin to chemistry related problems

Exposure to available standard application packages like: Chemdraw, generation of graphs, data sheets creation, and tables using Excel Programme.

Part -2

i) Data analysis, error analysis, least squares method. Plot of Born Maeyer to determine for 1:1 type molecule to determine internuclear separation.Characterization of metal ligand bonding using IR spectroscopy.

ii) Computer Applications : (1) Electronic structure, vibrational characteristics and charge distributions in first row transition metal complexes. (2) Visualizing frontier MO's.

iii) Least square fitting of experimental data.

SEMESTER-X

CHEMISTRY -SCY55102: Supramolecular Chemistry and Nanoscience

(Credits: 4)

Theory: 60 L

Course Structure & Syllabus For Integrated M.Sc. Chemistry (Session 2018-2023)

Unit 1- Molecular Recognition and Supramolecular Chemistry (20 L)

Introduction, Origins and Concept of Supramolecule.Molecular recognition.Host-guestcomplex.supramolecular orbitals, non-covalent forces: soft interactions, Supramolecularreactivity and catalysis. Self-assembly and self-organisation, Liquid crystals and supramolecular polymers, polymer-surfactant interaction. New molecular receptors: crown ethers, siderophores,cyclophanes, cyclodextrin and their application in specific recognition processes.

Supramolecular reactivity and catalysis, switching devices, self-assembly of supramolecularaggregates, crystal engineering.

[Drug design and synthesis, Molecular and Quantum mechanics, Drawing chemical structures,equation and diagrams, 3D structures, Molecular modeling and energy minimization, Molecularproperties, Conformational analysis, docking procedures, De Novo design, Molecularrecognition, Receptor based molecular modeling, QSAR studies, Antineoplastic agent,Cardiovascular drugs, Local anti-infectaive drugs, Antimalarial, antibiotics, anticolenergic andCNS active drugs.] as practical in computer application

Unit 2- Solid State Chemistry and Crystallography: (20L)

Bonding in metal crystals: free electron theory, electrical conductivity, band theory, band gap,metal and semi-conductors – intrinsic and extrinsic semiconductors;semiconductor/metaltransition, p-n junctions, superconductivity, Bardeen, Cooper and Schriefer (BCS) theory. Dia-, para- and ferromagnetism.Defects in solids.The geometry of crystalline state; Reciprocal lattice. Nature and generation of X-rays,Production of monochromatic X-rays, Scattering of X-rays, Diffraction of X-rays by crystals,Bragg's law, 1, 2 and 3 dimensional Laue equations, atomic scattering factor, structure factor,systematic absences, Determination of space groups and crystal structures.

Unit 2- Chemical Sensor: (10 L)

CHEMICAL SENSORS AND BIOSENSORS

BIOSENSORS: Introduction–amperometric enzyme electrodes-characteristics- enzymeactivitydeterminations – biosensors fro enzyme immunoassay – Potentiometric enzyme electrodes –electrode characteristics and performance –pH glass and ion-selective electrodes – solid-state pHand redox electrodes –gas electrodes.

IMMUNO BIOSENSORS: Potentiometric immunobiosensors–immobilizationtechniques–analytical applications. Principle and measurements of enzyme thermistor devices.Transducer – experimental techniques – types of biological element: immobilized enzymes –immobilized cells – determination of enzyme activities in solution

CHEMICALLY MEDIATED FIBEROPTIC BIOSENSORS: Introduction–sensingchemistryand materials –sensing techniques –transducer types. Transducer-based fiber optic biosensors –Optical biosensors based on competitive binding

REDOX HYDRO-GEL BASED ELECTROCHEMICAL BIOSENSORS:

Electronconducting redox polymer in biosensors –enzyme electrodes – specific sensor examples.Hybridization at oligonucleotide sensitive electrodes: function of oligonucleotide sensitiveelectrodes – hybridization efficiency and sensitivity – probe oligonucleotide structure anddynamics – hybridization conditions – hybridization kinetics.

FLUOROPHORE AND CHROMOPHORES BASED FIBEROPTIC BIOSENSORS:

Enzyme based nonmediatedfiberoptic biosensors – chromophores and flurophore detection.Bioluminescence and chemiluminescence based fiberoptic sensors – bioluminescence andchemiluminecent reactions – analytical potential of luminescent reactions – applications

DETERMINATION OF METAL IONS BY FLUORESCENCE ANISOTROPY: Theoryofanisotropy based determination of metal ions – fluorescent aryl sulfonamides for zincdetermination- removal of zinc from carbonic anhydrase – determination of zinc using reagentapproach – determination of copper and other ions by using reagent less approach.

Unit 4- Nano Science and Materials : (10 L)

Nano-world- definitions and properties, typical synthetic strategies for nanomaterials,characterization and applications catalyst, nanoencapsulation, nanobiology and Drug delivery.

CHEMISTRY -SCY55104: Advanced Special -I

(Credits: 4)

Theory: 60 L

Advanced Special I:

(Physical):

Unit 1- Quantum Mechanics (Advanced) : (22L)

Vector space, matrix representation of operators, Hermitian operators and matrices, Virialtheorem, parity, time reversal symmetry; angular momentum operator – commutation relation,set-up and set-down operators, angular momentum operators in polar coordinates, angularmomentum eigenfunctions: solutions from corresponding eigenvalue equation.

Many electron Hamiltonian, its communication with composite L 2 and L z ; spin operator andPauli spin matrices; many electron atom and construction of wavefunction representingspectroscopic state; projection operators and their properties – projection operator technique andangular momentum. Perterbation theory (PT) – Rayleigh-Schrödinger PT for non-degeneratestates theorem, some simple applications: expression for polarizability, ground state of heliumatom; degenerate state PT – Stark effect, lifting of degeneracy by application of a magnetic field(e.g. , the 1 P 1 state of helium atom) variation method – Euler variation, principle and Rayleigh-Ritz variation theorem, applications.

Quantum chemistry: Born-Oppenheimer approximation, theories of valence, the MO and VBmethods for H 2 molecule – their relative merits, dissociation curve, excited state, configurationinteraction.

Many electron systems – its charectaristics, independent particle model (IPM), Hartree andHartree-Fock methods for closed shell (elementary ideas).

Unit 2- Quantum Mechanics and Spectroscopy (20L)

Time dependent perturbation theory – semiclassical treatment of interaction of matter withradiation, first and second order effects, Fermi golden rule, selection rule, selection rule forvibrational spectra, anharmonicity correction by perturbation – appearance of overtones;selection rule for rotational spectra, nucleur spin and rotational energy levels, stark effectrevisited.

Raman scattering: selection rule for rotational and vibrational raman spectroscopy.Quantummechanical theory of magnetic resonance; Bloch equations and their solutions; theories ofshielding – diamagnetic and paramagnetic shielding.

Unit 3- Dielectric behavior and Spectroscopy (18L)

Dielectric behavior and solvent effects: Limitation of Mossotti-Clausius, Debye equation,deviation from Debye's theory; Onsager reaction field; dielectric relaxation, frequencydependent dielectric property, relaxation time, Debye semicircle; Solvent effect on the emissionand absorption spectra - non-specific and specific interactions (H-bonding and charge transfer).Characteristics of CT interaction; Lippert equation; time resolved spectroscopy and the dielectricrelaxation effect.

CHEMISTRY -SCY55106: Advanced Special -II

(Credits: 4)

Theory: 60 L

Advanced Special II:

(Physical):

Unit 1- Statistical Mechanics: (18 L)

Introduction: Concept of ensemble and ergodic hypothesis, phase space; microcanonicalensemble, temperature; canonical ensemble distribution, probability distribution function, itsrelation with different thermodynamic state functions; Gibbs paradox and Sackur-Tetrodeequation; Chemical equilibrium and equilibrium constant in terms of partition functions,equipartition theorem and its validity; chemical potential and chemical equilibrium – Sahaionization formula; system of interacting molecules – imperfect gas. Grand canonical ensemble –nature of quantum particles; Bose-Einstein and Fermi-Dirac distributions; black body radiationand photon gas, Bose-Einstein condensation.

Unit 2- Non-equilibrium Thermodynamics: (12 L)

Thermodynamics of irreversible processes: (15 lectures) Limitations of classical (equilibrium)thermodynamics, entropy production in some simple irreversible processes, the concept of forcesand fluxes, linear phenomenological relations; Onsager reciprocity relation – derivation fromfluctuation theory; Curie-Prigogine principle – statement and proof using one scaler and onevector force, illustrations; Saxen's relations in connection with electrokinetic phenomena andtheir proof using Onsager reciprocity relations, stationary states: variation of entropy productionwith time, Prigogine's criterion for establishment of stationary state, applicability of LeChateliar's principle on stationary states

Unit 3 - Reaction Dynamics: (10L)

Reaction dynamics: Introduction, molecular dynamics – intermolecular collision and itsconsequence; role of intermolecular potential, reaction cross-section, energy threshold, reactionprobability; angular distribution in relative collision; scattering in velocity space; electronicenergy transfer; experimental methods in connection with molecular dynamics;chemiluminescence; chemical laser; crossed molecular beam; photofragmentation spectroscopy.

Unit 4 - Advanced Electrochemistry: (20L)

Limitation of Debye-Hückel limiting law and its extension; Pitzer ion-interactionapproach.Debye-Hückel- Onsagar (DHO) theory of electrical conduction of electrolytes,electrophoretic and relaxation effects, Wien effect, Debye-Falkenhagen effect, application ofDHO theory.Limitation of

DHO equation and Shedlovsky approach.Double layer studies: nature of the double layer across electrode-solution interface, polarizableand non-polarizable electrodes, electrocapilarity (EC) – nature of EC curves, itsthermodynamics, Lipmann equation, Helmholtz, Guoy-Chapman and Stern double layer models.Electron transfer reactions; fuel cells.

Advanced Special Lab I

Credit: 4

Practical: 60L

Physical:

1. Calculation the thermodynamic parameters of micellization of a surfactant from conductivitymeasurements
2. Thermodynamics of Denaturation of Bovine Serum Albumin
3. Electronic structure calculation of IR and Raman frequencies
4. Spectrophotometric determination of the acid dissociation constant of methylRed.
5. Fluorescence quantum yield determination of an unknown molecule
6. Determination of polarizability from refractive index measurements

ADVANCED INORGANIC SPECIAL I

Magnetochemistry (18 L)

Definition of magnetic properties, types of magnetic bodies, Curie equation, Curie's law and Curie-Weiss law. Anisotropy in magnetic susceptibility, diamagnetism in atoms and polyatomic system, Pascal's constants, two sources of paramagnetism, spin and orbital effects, spin-orbit coupling, Lande interval rule, energies of *J* levels, first order and second order Zeeman effects, temperature independent paramagnetism, simplification and application of van Vleck susceptibility equation, quenching of orbital moment, magnetic properties of transition metal complexes, low spin, high-spin crossover, magnetic behavior of lanthanides and actinides, magnetic exchange interactions. Experimental arrangements for determination of magnetic susceptibility: Gouy method, Faraday method, Evans method, SQUID.

Spectroscopic Application in Inorganic Systems (20 L)

Electronic spectroscopy: Orgel diagrams, correlation between weak field and strong field terms. Tanabe-Sugano diagram, bonding parameters and structural evidences from electronic spectra of d-metal complexes, f-f transition, lanthanide and actinide spectra. Applications of IR, Raman, ESR and Mossbauer spectroscopy to inorganic and bioinorganic systems, NMR spectra: ^{11}B, ^{13}C, ^{19}F, ^{27}Al, ^{31}P NMR spectroscopy with typical examples, ^{1}HNMR spectra of coordination compounds of paramagnetic metal ions, dipolar and contact shifts, magnetic susceptibility and resonance

shift. NQR spectroscopy: Principle, nuclear quadruple coupling constants, structural information from NQR spectra. Applications of CD and MCD; stereoselective and stereospecific effects.

Nuclear Chemistry and Radiochemical Analysis (22 L)

Nuclear models – Nuclear forces, liquid drop model, Fermigas model, Shell model. Magic numbers.Nuclear spin and nuclear isomerism.Nuclear reactor and particle accelerators.Interaction of radiation with matter. Detection and measurement of radiation – proportional counter, scintilater and detector. Radiation dosimetry.Chemical effects of nucleartransmutation (elementary idea), radiolysis of water.Application of radioactivity in geochemistry and cosmochemistry, methods of age determination, radioactive analysis. Tracer techniques: study of chemical reactions, isotopic exchange reactions, kinetic isotope effect. Radiation chemistry, carrier free tracers.Radiation hazards.

ADVANCED INORGANIC SPECIAL II

Inorganic Reaction Mechanism (16L)

Mechanism of substitution reactions: Solvent exchange, aquation, anation, base hydrolysis, acid catalysedaquation, pseudo-substitution. Four board classes of mechanism of substitution – _D‘, _A‘, _Ia‘ and _Id‘ Mechanism of isomerisation reaction–linkage isomerism, cis-trans isomerism, intramolecular and intermolecular racemisation, Ray– Dutta and Bailar twist mechanisms. Mechanism of electron transfer reactions: General characteristics and classification of redox reactions, selfexchange reactions. Outer sphere and inner sphere reactions, applications of Marcus expression (simple form), redox catalysed substitution reactions.

Photo inorganic Chemistry (14L)

Excitation modes in transition metal complexes, fate of photo excited species; photochemical processes: Photosubstitution and photoelectron transfer reactions in Co, Cr and Rh-complexes.

Bioinorganic Chemistry (15L)

Uniqueness of metal ion as bioelements. Interaction of metal ions with biomolecules, Metal ion in metabolic energy transfer and ATP hydrolysis; Genetic information transfer; replication, transcription and translation processes. Metalloproteins and metalloenzymes Oxygen uptake proteins:- hemoglobin and myoglobin; Electron transport proteins: – cytochromes (specially cytochrome C), ferridoxins; metalloenzymes: – catalase, peroxidase, urease, superoxide dismutase (SOD), cytochrome P 450, cytochrome C oxidase, carbonic anhydrase, carboxypeptidase; molybdoenzymes; respiratory electron transport chain and photosynthetic electron transport chain, Toxic metal ions and their effects, chelation therapy, Pt and Au complexes as drugs, metal dependent diseases.

Chemistry of Complex Equilibria (15L)

Characteisation of stability of mononuclear, polynuclear and mixed –ligand complexes in solution, determination of composition and stability constants of complexes by pH metric, spectrophotometric and polarographic methods, DTA, TGA.Conditional stability constants and their importance in complexometric (EDTA) titrations and solvent extraction of metal ions.Statistical and non-statistical factors influencing stability of complexes in solution, stability and reactivity of mixed ligand complexes.SoluilityEquilibria – quantitativeness of precipitation (of metal hydroxides, sulphides and chelates).

INORGANIC SPECIAL LAB

Inorganic Special Practical-I

(a) Quantitative estimation of inorganic ions by colorimetry/ion-exchange method

i) Separation and estimation of the following binary mixtures: Mg^{2+} - Zn^{2+}; Zn^{2+} - Cd^{2+}

ii) Colorimetric determination of 1) Fe^{3+} as sulphosalicylate complex 2) Fe^{2+} as phenanthroline complex 3)Manganese as MnO_4^- 4) Chromium as $Cr_2O_7^{2-}$ (any two).

(iii) Quantitative analysis of complex inorganic materials *viz.* ores, minerals and alloys etc. by conventional method. (any one)

(b) Physicochemical Experiments:

i) Determination of composition of complexes by continuous variation/ Mole-Ratio / Slope ratio method of the following systems: Fe (III) – sulphosalicylate complex; Fe (II) - phenanthroline complex
ii) A conductance study of the kinetics on inorganic reaction.
iii) A colorimetric study of the kinetics on inorganic reaction.

Inorganic Special Practical-II

Synthesis and characterization of Inorganic Compound:

Preparation of transition metal complexes and their characterization

ADVANCED ORGANIC SPECIAL I

ADVANCED ORGANIC SYNTHESIS

i) Newer Synthetic Methodologies : Application of Catalysts and Reagents in Organic Synthesis (35L)

Conventional and newer carbon-carbon bond forming reactions and functional group transformations focussing onchemoselectivity, regioselectivity and various aspects of stereoselectivity. Formation of carbon-carbon bonds using carbanions: Methods for the formation of organolithium and organomagnesium compounds (e.g. alkylation, transmetallation, transition-metal-catalysed cross-coupling and reactions with other electrophiles). Application of phosphorous, sulphur, boron and silicon in organic synthesis. Regio- and stereocontrolledenolate formation, applications of dianions in synthesis. Formation of carbon-carbon bonds using radicals. Transition metal catalysed reactions. Pericyclic reactions: Diels-Alder-, 1,3-dipolar- and

related cycloadditions; concerted electrocyclic ring opening and closure reactions (stereochemistry); sigmatropic rearrangements. Application of photochemistry, sono-chemistry and mechano-chemistry in organic synthesis.

Transition metal complexes in organic synthesis ; only Pd, Ni, Co, Fe (Metal mediated C-C and C-X bond formation reactions: Suzuki, Heck, Sonogashira, Stille, Fukuyama, Kumada, Hiyama, Negishi, Buchwald-Hartwig, Noyori, Reppe, Oxo process , C=C formation reactions: Wittig, Horner-Wordworth-Emmons, Shapiro, Bamford-Stevens, McMurry, Julia-Lythgoe and Peterson olefination reactions, Titanium-carbene mediated olefination: Tebbe, Petasis and Nysted reagent. Multi-component reactions: Ugi, Passerini, Biginelli and Mannich reactions [4L] 4. Ring formation reactions: Pausan-Khand, Bergman and Nazerov cyclization. Click chemistry: criterion for click reaction, Sharpless azides cycloadditions. Metathesis: Grubbs 1st and 2nd generation catalyst, Olefin cross coupling (OCM), ring closing (RCM) and ring opening (ROM) metathesis, applications. Other important reactions: Baylis Hilman, Eschenmoser-Tanabe fragmentation, Mitsunobu reaction.

Use of the following reagents in organic syntheses and functional group transformations, Complex metal hydrides, Gilman's reagent, Lithium dimethylcuprate, Lithium disopropylamide, 1,3-Dithiane, Trimethylsilyl iodide, Trimethylsilylchloride, Tri-n-butyltin hydride, Woodward and Prevost hydroxylation, Osmium tetroxide, DDQ, DCC, EDC.HCl, Thalium nitrate, Selenium dioxide, Phase transfer catalysts, Crown ethers and Merrifield resin, Peterson's synthesis, Wilkinson's catalyst, Baker yeast, solid immobilized reactions, protecting groups.

ii) Asymmetric Synthesis (25L)

Chiral induction – Diastereoselective synthesis Stereoselectivity and stereospecificity – Nucleophilic addition to a-chiral carbonyl compounds – 1,2-induction and 1,3-induction – Cram's rule and beyond – chelation control and non-chelation control directed functionalization – direct biomimetic polyene cyclization (Johnson) Chiral auxiliary - Diastereoselective synthesis Basic requirements of chiral auxiliary – 'chiral pool' sources – polular and generally adaptable chiral auxiliaries (Oppolzer, Evans, Enders, Davies, 8-phenylmenthol, BINOL etc.) – kinetic resolution by chiral auxiliary – boronic ester mediated homologation – disadventages of 'auxiliary' approach Asymmetric aldol condensation and alkylation Equilibrium-controlled condensation reaction has its own disadvantage – transition state – enolate of lithium, boron, zinc etc. – configuration of enolate and stereochemistry of aldehyde addition – product assignment and extent of stereocontrol – transition state model – 'double stereo differentiation' concept – Masamune's sugar synthesis – macrolide antibiotics as target – alkylation of chiral nucleophiles – Meyer's oxazoline based enolate - 'memory of chirality' – Evan's oxazolidinone derived enolates – polyanions in peptide backbone (Seebach) Chirality modified reagents Reducing agents like boron/aluminium hydrides – allylation and crotylation – oxazaboralidines – TADDOL – chiral lithium amides – chiral Lewis acids in enolate reaction, cycloadditions and sigmatropic rearrangements – enantioselectivedeprotonation and protonation – 'chiral cavity' for enantioselection Asymmetric catalysis Metal mediated catalysis – asymmetric hydrogenation; early advances DIPAMP, DIOP and Noyori's BINAP – Sharplessepoxidation,

dihydroxylation, aminohydroxylation of alkenes – metal biocatalysis – organocatalysis – Proline mediated aldol reaction and further expansion in the field of organocatalysis, 'non-linear effects' – 'ligand accelerated catalysis' and 'chiral amplification'.

Reference Books:

- Designing of organic synthesis – S. Warren (Wiley)
- Some modern methods of organic synthesis – W. Carruthers (Cambridge)
- Organic chemistry – J. Clayden, N. Greeves, S. Warren and P. Wothers (Oxford Press)
- Organic synthesis – Michael B. Smith
- Advanced organic chemistry, Part B – F. A Carey and R. J. Sundberg, 5th edition (2007)
- Guidebook to organic synthesis-R K Meckie, D M Smith and R A Atken
- Organic synthesis- Robert E Ireland
- Strategic Applications of named reactions in organic synthesis-Laszlo Kurti and Barbara Czako

ADVANCED ORGANIC SPECIAL II

Advanced Organic Spectroscopy (25L)

1H NMR Spectroscopy: Chemical shift, factors influencing chemical shift, deshielding, chemical shift values and correlation for protons bonded to carbons (aliphatic, olefinic, aldehydic, aromatic) and other nuclei (alcohols, phenols, enols, acids, amides and mercaptans), chemical exchange, effect of deuteration, spin-spin coupling, (n+1) rule, complex spin-spin interaction between two, three, four and five nuclei (first order spectra), factors effecting coupling constant "J", classification of spin system like AB, AX, AX_2, ABX, AMX, ABC, A_2B_2. Spin decoupling, Factors affecting coupling constant, simplification of complex spectra, nuclear magnetic double resonance, spin decoupling, contact shift reagents, solvent effects, nuclear overhauser effect (NOE).

Resonance of other nuclei: ^{31}P, ^{19}F, ^{15}N

^{13}C NMR spectroscopy: Types of 13C NMR Spectra: un-decoupled, Proton decoupled, Off resonance, APT, INEPT, DEPT, chemical shift, calculations of chemical shifts of aliphatic, olefinic, alkyne, aromatic, hetero aromatic and carbonyl carbons, factors affecting chemical shifts, Homo nuclear (13C-13C) and Hetero nuclear (13C-1H)coupling constants.

2D NMR Techniques: General idea about two dimensional NMR spectroscopy, Correlation spectroscopy (COSY)- Homo COSY (1H-1H), TOCSY, Hetero COSY (HMQC, HMBC), Homo and Hetero nuclear 2D resolved spectroscopy, NOESY and 2D-INADEQUATE experiments and their applications.

Mass Spectrometry: Instrumentation, various methods of ionization (field ionization, field desorption, SIMS, FAB, MALDI, Californium plasma), different detectors (magnetic analyzer, ion cyclotron analyzer, Quadrupoule mass filter, time of flight (TOF). Rules of fragmentation of different functional groups, factors controlling fragmentation

Problems based on joint application of UV, IR, PMR, CMR, and Mass. (10 L) (Including reaction sequences)

Bio-organic and Medicinal Chemistry (**25L**)

Chemical biology: definition, history. Peptide and Protein: amino acids, peptides, primary, secondary, tertiary, and quaternary structure of proteins, protein folding. Protein Synthesis: biosynthesis, chemical synthesis, solid phase peptide synthesis, strategy of combinatorial synthesis, combinatorial solid phase synthesis of antibiotics. Use of Enzymes in Organic Synthesis. Lipids: fatty acids, bilayer, lipidation of proteins and peptides, farnesylation of the Ras protein. Insertion of lipidated peptides into model membrane: biological membranes, transport across membranes, model membrane, biophysical properties of lipidated peptides in model membranes, basic concepts of fluorescence and fluorescence markers, synthesis of vesicles containing fluorescence quencher and lipidated peptides. Nucleic acids: base pairing, double helices, DNA replication, genetic information storage, transmission and gene expression, chemical synthesis of oligonucleotides, hybridization with synthetic oligonucleotides. Peptide nuclic acids (PNAs), synthesis of PNAs, doubly labeled PNAs as probes for the detection of point mutations. Use of small molecules to link a protein target to a cellular phenotype and as probes for biological processes.

Introduction to drugs, their action and discovery, Relation of Drug structure and its chemical and biological properties, Structure, activity and quantitative relationship, Drug targets, Antimicrobial drugs, Antibactaerials drugs, Discovery and development of Penicillins, Cephalosporins, Sulphones and sulphonamides, Tetracyclins, Macrolides, Polypeptides, Chloromycetin Antifungals: Fungal Diseases and Anti-fungal agents Antivirals: Viral diseases and Anti-viral drugs Anti-protozoals: Anti-malarials, Anti-amoebic. Anti-Cancer Chemotherapy.

Advanced Natural Product Synthesis (10L)

Total Synthesis of selected natural products:

Strychnine, Penicillin V, Reserpine, Vitamin B12, Progesterone (for example)

REFERENCE BOOKS:

- Introduction to Spectroscopy – D. L. Pavia, G.M. Lampman, G. S. Kriz, 3rd Ed. (Harcourt college publishers).

- Spectrometric identification of organic compounds R. M. Silverstein, F. X. Webster, 6th Ed.John Wiley and Sons.
- Spectroscopic methods in organic chemistry - D. H. Williams and I Flemming McGraw Hill
- Biochemistry- Donald Voet, Judith G. Voet. Wiley.
- An Introduction to Medicinal Chemistry – Graham L. Patrick.
- The Organic Chemistry of Drug Design and Drug Action- Richard Bruce Silverman.
- Classics in Total Synthesis: Targets, Strategies, Methods- K.C. Nicolau, E.J. Sorensen. Wiley VCH

ORGANIC SPECIAL LAB

Organic Special Practical-I

Preparation of organic compounds by typical organic reactions, purification and characterization of the product [by re-crystallization, column chromatography, TLC, PC, determination of R_f value as required, m.p/b.p.]. Characterization of organic compounds by spectroscopic means.

Organic Special Practical-II

Multistep Organic Preparation.Extraction and Purification of Natural Products and Biomolecules

REFERENCE BOOKS:

1) Furniss, B. S.; Hannaford, A. J.; Smith, P. W. G.; Tatchell, A. R. *Vogel's Textbook of Practical Organic Chemistry*, *5th Ed.,*Longman Scientific and Technical (1989).

2) Mann, F.G. & Saunders, B.C. *Practical Organic Chemistry,*Pearson Education (2009)

3) Furniss, B.S.; Hannaford, A.J.; Smith, P.W.G.; Tatchell, A.R. *Practical Organic Chemistry, 5th Ed.,* Pearson (2012)

Course Structure & Syllabus For Integrated M.Sc. Chemistry (Session 2018-2023)