SEMESTER-I

Basics of Biochemistry and Bioinorganic Chemistry

Paper code: MSAC-I
(3 Credit)

Unit 1: Basics of Biochemistry **(12 marks)**

Principles of biophysical chemistry Thermodynamics, Colligative properties, Stabilizing interactions: Van der Waals, Electrostatic, Hydrogen bonding, Hydrophobic interaction, etc. Composition, structure, function and metabolism of Carbohydrates, Lipids, Amino Acids and Nucleotides.

Unit 2: Organometallic Compounds **(13 marks)**

Metal carbonyls-synthesis, structure and bonding in mononuclear and polynuclear carbonyls with and without bridging, metal carbonyl hydrides and metal carbonyl clusters. LNCC and HNCC. Complexes with linear π donor ligands: olefins, acetylenes, dienes and allyl complexes. Hapto nomenclature, Complexes with cyclic donors-cyclopentadiene, enzene. Cyclometallation reaction. Catalysis by organometallic compounds-hydrogenation, hydroformylation and polymerisation reactions. (Wilkinson's catalyst, Ziegler-Natta catalyst & Synthetic gasoline should be included among various examples) and various others applications.

Unit 3: Metal-Organic Framework **(13 marks)**

Macrocycles and supramolecules non-covalent forces and interactions in supramolecules: crown ethers, cryptates, cryptands, carcerands, calixarenes, cyclodextrins, fullerenes, dendrimers, rotaxanes, cucurbiturils, self-assembly and preorganization, coordination driven self-assembly of supramolecular two and three dimensional architectures, host-guest chemistry, metal-organic frameworks and their applications.

Unit 4: Bioinorganic Chemistry **(12 marks)**

Principles of coordination chemistry related to bioinorganic chemistry, Essential and trace metal ions in biological systems, Porphyrin and related ligands, ATP as energy source, oxidative phosphorylation and phosphorylation of glucose. Transport and storage of dioxygen: Structure and function of hemoglobin, myoglobin, hemocyanin and hemerythrin. Synthetic oxygen carriers.

Reference books:

1. F. A. Cotton, G. Wilkinson, C. A, Murillo, and M. Bochmann Advanced Inorganic Chemistry, 6th Edition Wiley-Interscience: New York, 1999.
2. J.E. Huheey, Ellen A. Keiter and Richard L. Keiter "Inorganic Chemistry, Principles of structure and Reactivity", 4th Ed., Harper Collin College Publishers, 1993
3. J. W. Steed, J. L. Atwood, Supramolecular Chemistry, 2nd edition, John Wiley & Sons Ltd., (2009)
4. D. F. Shriver, P. W. Atkins, C. H. Langford, Inorganic Chemistry, 3rd Ed. ELBS, 1999.
5. B. Douglas, D. McDaniel, J. Alexander, Concepts and Models of Inorganic Chemistry, 3rd Ed., Wiley.
6. Berg, J.M., Tymoczko, J.L. and Stryer, L. (2010). Biochemistry. W.H. Freeman & Company. USA.
7. Brown, T.A. (2006). Gene Cloning and DNA analysis: In Introduction. Blackwell Publishing Professional. USA.
8. Haynie, D.T. (2007). Biological thermodynamics. Cambridge University. UK.

9. Mathews, C.K., Van Holde, K.E. and Ahern, K.G. (2000). Biochemistry. Oxford University Press Inc. New York.
10. Nelson, D. and Cox, M.M. (2013). Lehninger Principles of Biochemistry. BI publications Pvt. Ltd. Chennai, India.

Organic Chemistry-I and Biomacromolecules

Paper code: MSAC-II
(3 Credit)

Unit 1: Organic Reaction Mechanism **(12 marks)**

Methods of determining reaction mechanisms (kinetic and non-kinetic methods): The Hammond postulate, reactivity vs selectivity principle, the Curtin-Hammett principle, microscopic reversibility, kinetic vs thermodynamic control. Isotope effects. Carbon acids: pKa of weak acids, Effect of structure on acidity and basicity. Linear free energy relationships: Hammett and Taft parameters, Solvent effects (Grunwald-Winstein plots and Schleyer adaptation), nucleophilicity and nucleofugality. Other Experimental techniques to determine reaction mechanisms: cross - over experiments, isotope scrambling, radical clocks and traps, matrix isolation.

Unit 2: Pericyclic reactions **(13 marks)**

Study of Frontier Molecular Orbital theory, aromatic transtion state theory and the generalized Woodward – Hoffmann rule applied to cycloaddtions, electrocyclic reactions, sigmatropic rearrangements and chelotropic reactions– Stereochemistry and regiochemistry of cycloaddtions. Substituent and medium effects, secondary orbital interactions in [4+2] cycloadditionsIntramolecular Diels–Alder reactions. 1,3-dipolar cycloaddition reactions. Photochromism and thermochromism, Cope rearrangement, Claisen rearrangement, and ene-reaction.

Unit 3: Oxidising and reducing agents in organic synthesis **(13 marks)**

(a) Oxidation: metal-based oxidants (Cr, Mn, Os, Ag, Ru and Pb); non-metal-based oxidation: Swern oxidation, Moffat oxidation, hypervalent iodine based oxidants, CAN as oxidant.
(b) Reduction: metal hydrides (B-H, Al-H, Zn-H, Sn-H, Si-H based reagents); hydrogenation; dissolving metal reductions; samarium iodide.

Unit 4: Rarrangements **(12 marks)**

General mechanistic considerations - nature of migration - migratory aptitude - nucleophilic, electrophilic and free radical rearrangements - Wagner-Meerwein, McLafferty, Demyanov, Benzil-benzilic acid, Favorskii, Fritsch-Buttenberg-Wiechell, Neber, Hofmann, Curtius, Beckmann, Schmidt, Lossen, Wolff, Baeyer-Villiger, Dienone-phenol, Pinacol, Stevens, Wittig, Chapman, Wallach, Orton, Bamberger, Pummerer and von Richter rearrangements.

Refrence books:

1. March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure, 7th ed. 2013, Wiley
2. T H.Lowry and K.S.Richardson: Mechanism and Theory in Organic Chemistry, 3rd ed. 1997, Benjamin-Cummings Publishing Company.
3. F. A. Carey and R. J. Sundberg: Advanced Organic Chemistry (parts A and B), 5th Edition2008, Springer.

4. E. V. Anslyn and D. A. Dougherty: Modern Physical Organic Chemistry. University Science Books, 2006 edition.
5. F. A. Carroll: Perspectives on structure and mechanism in organic chemistry, Wiley, 2011 edition.
6. N. S. Issacs: Physical Organic Chemistry, Second Edition, 2nd Edition, 1995, Prentice Hall.
7. A. Pross: Theoretical and Physical Principles of Organic Chemistry, I Edition,1995, Wiley..
8. J. Clayden, N. Green, S. Warren and P. Wothers: Organic Chemistry, 2nd Edition. 2012, Oxford University Press,
9. I. Flemming: Frontier orbitals and organic chemical reactions, 1976 Edition, Wiley-Blackwell.
10. I. Flemming: Molecular orbitals and organic chemical reactions, student edition, 2009, Wiley.
11. J. McMurry, Organic Chemistry, Fifth Edition, 2000, Brooks/Cole .
12. R. Bruckner, Advanced organic chemistry: Reaction Mechanisms. Academic Press, 2001 Edition.

Statistical methods for Chemical and Biochemical Applications

Paper code: MSAC-III
(2 credit)

Unit 1: **(12 marks)**

Overview of Biostatistics: Difference between parametric and non-parametric statistics, Univariant and multivariant analysis, Confidence interval, Errors, Levels of significance, Hypothesis testing. Descriptive statistics: Measures of central tendency and dispersal, Histograms, Probability distributions (Binomial, Poisson and Normal), Sampling distribution, Kurtosis and Skewness.

Unit 2: **(13 marks)**

Experimental design and analysis: Sampling techniques, Sampling theory, Various steps in sampling, collection of data-types and methods. Inferential Statistics: Student's t-test, Paired t-test, Mann-Whitney U-test, Wilcoxon signed-rank, One-way and two-way analysis of variance (ANOVA), Critical difference (CD), Least Significant Difference (LSD), Kruskal–Wallis one-way ANOVA by ranks, Friedman two-way ANOVA by ranks, $\chi 2$ test. Standard errors of regression coefficients, Comparing two regression lines, Pearson Product-Moment Correlation Coefficient, Spearman Rank Correlation Coefficient, Power and sampling size in correlation and regression.

Reference books:

1. Gookin, D. (2007). MS Word 2007 for Dummies. Wiley, USA.
2. Johnson, S. (2009). Windows 7 on demand. Perspiration Inc. USA.
3. Norman, G. and Streiner, D. (2008). Biostatistics: The Bare Essentials. 3/e (with SPSS). Decker Inc. USA.
4. Sokal, R.R. and Rohlf, F.J. (1994). Biometry: The Principles and Practices of Statistics in Biological Research. W.H. Freeman publishers, USA.
5. Thurrott, P. and Rivera, R. (2009). Windows 7 Secrets. Wiley, USA.

Advanced Physical Chemistry

(Focused on Computer aided problem solvation) **Paper code: MSAC-IV**
(3 Credit)

Unit 1: Quantum Chemistry (13 marks)

Stern-Gerlach expt., ket, bra, operator algebra, representations & transformations, uncertainty relation, translation & momentum, position & momentum wave function; simple potential systems–free particle, wells, barriers; simple harmonic oscillator. Vibrational motion, Harmonic oscillator, Hermite equation and Hermite Polynomials, Recursion formula, Rodrigues formula, wave function and energy. Rigid rotator, Wave function in spherical polar coordinates, Planar rotator, phi equation, wave functions in real forms, Polar diagrams, Nonplanar rotator, Theta equation and solutions Lagendre equation and Lagendre polynomials, Spherical harmonics, Angular momentum operator L2 and Lz, Space quantization. H atom, the R equation. Computational solutions to problems.

Unit 2: Symmetry & Group Theory (12 marks)

Symmetry elements & operations; group, subgroup, class, point groups, group multiplication tables for cyclic and non-cyclic groups; matrix representations of symmetry operations and their characters, reducible representations, irreducible representations and great orthogonality theorem (no derivation), construction of character tables; application of group theory.

Unit 3: Kinetics (13 marks)

Brief review of collision theory & activated complex theory; ionic reaction, kinetic salt effect; steady state kinetics, kinetic & thermodynamic control of reactions; unimolecular reactions; chain reactions, fast reactions. Computational approach to understand the chemical kinetics of different ordered reactions.

Unit 4: Electrochemistry (12 marks)

Activity and Activity coefficient of electrolytes, ionic strength, Debye Huckel theory of strong electrolytes. Debye Huckel limiting law, Mean ionic activity coefficient. Application of Debye Huckel theory to conductance bahaviour, Relaxation and electrophoretic effect, Debye-Huckel-Onsager equation and its derivation. Debye Falkenhagen effect. Wein effect.

Reference books:

1. I. N. Levine , Quantum Chemistry, 6th Edn., Pearson Education, London, 2008
2. D. A. McQuarrie , Quantum Chemistry , 3rd Edn., Univ. Sci. Books, Mill Valley, California, 1983
3. J. P. Lowe, Quantum Chemistry 3rd Edn., Academic Press, New York, 2008
4. D. D. Fitts, Principles of Quantum Mechanics as Applied to Chemistry and Chemical Physics, CUP, Cambridge, New York, 2002
5. M. Taketani, The Formation and Logic of Quantum Mechanics, Vol. I-III, World Scientific, New Jersey,2001
6. G. Esposito, G. Marmo and G. Sudarshan, From Classical to Quantum Mechanics. An Introduction to the Formalism, Foundations and Applications, Cambridge, 2004
7. L. Piela, Ideas of Quantum Chemistry, Elsevier, Amsterdam, 2007
8. P. W. Atkins, Molecular Quantum Mechanics, OUP, Oxford, 1983
9. P.W. Atkins, Physical Chemistry, 8th Edn., Wiley, New York, 2006
10. J. Bockris and A.K.N. Reddy, Modern Electrochemistry, 2B, 2nd Edn., Wiley, New York, 1998
11. D .R. Crow, Principles and Applications of Electrochemistry, Chapman & Hall, 3rd Edn., New York, 1994

Analytical Lab Techniques

Paper code: MSAC-V
(2 Credit)

Unit 1: Spectroscopy **(13 marks)**
Principles and applications of UV-Vis, Vibrational and Raman spectroscopy. Fluorescence and NMR spectroscopy in understanding chemical and biological interactions.

Unit 2: Electron Microscopy and Mass spectroscopy **(12 marks)**
SEM, TEM, Tunnelling Electron Microscope. Instrumentation, Mass spectral fragmentation of organic compounds, McLafferty rearrangement, structure determination.

Unit 3: Thermal Methods: **(12 marks)**
Theory and application of TGA, DSC and DTA.

Unit 4: Separation Techniques and Data Analysis **(13 marks)**
HPLC, GC, gel electrophoresis for biological samples. Uncertainties, errors, mean, standard deviation, least square fit, testing the fit (C2 test, residual etc.). Signal to noise ratio.

Analytical Lab Techniques **(LAB)**

Paper code: MSAC-VI
(3 Credit)

Spectroscopy Laboratory Analysis:
Fourier Transform Infrared (FTIR), Attenuated Total Reflection Infra-Red Spectroscopy (ATR-FTIR), UV-visible Spectroscopy (UV-Vis), Far-Infra-Red and Near Infra-Red and Circular Dichroism (CD), Fluorescence spectroscopy. Analysis and interpretation of sample data of given chemicals or compounds using Origin/ ChemOffice softwares.

Chromatographic Laboratory Analysis:
Chromatographic separation techniques to isolate single organic compound from mixture of compounds.

Introduction to C and MATLAB for simulation applications for Physical/Chemical Problems

Paper code: MSAC-VII
(3 Credit)

Group-A : Computional Laboratory-I

Basic concepts of operating systems like MS DOS, MS WINDOW, UNIX, Algorithm & flow chart.

C Fundamentals: The C character set identifiers and keywords, data type & sizes, variable names, declaration, statements. Operators & Expressions: Arithmetic operators, relational and logical operators, type, conversion, increment and decrement operators, bit wise operators, assignment operators and expressions, precedence and order of evaluation. Input and Output: Standard input and output, formatted output -- printf, formatted input scanf.

Flow of Control: Statement and blocks, if - else, switch, loops - while, for do while, break and continue, go to and labels.

C Programming Laboratory: Problems should cover basic features of the Language.

Group-A : Computional Laboratory-II

Implementation of various Numerical problems using MATLAB/OCTAVE/C Programming and simulation applications in Physical/Inorganic and Organic Chemistry problems.

Determination of Stereo-chemical outcome of complex chemical reaction (Computer aided)

Paper code: MSAC-VIII
(2 Credit)

Analysis of Stereochemistry of single organic molecule and stereochemical outcome of complex chemical reaction using computer as analytical tool.

Use of ChemOffice (Chemdraw 14.0 suite and Chemdraw 3D ultra) in order to determine most stable conformation of certain chemical structure.

Research Methodology

Paper code: AC-IX
(2 credit)

One course from prescribed MOOC’s on Research methodology of minimum 8 weeks.

SEMESTER II

Quantum Chemistry

Paper code: MSAC-X
(3 Credit)

Unit 1: Fundamental Background **(13 marks)**

Postulates of quantum mechanics, Eigen values and Eigen functions, operators, hermitian and unitary operators, some important theorems. Schrodinger equation-particle in a box (1D, 3D) and its application, potential energy barrier and tunneling effect, one-dimensional harmonic oscillator and rigid rotor. Angular momentum, eigenvalues of angular momentum operator, Particle on a Ring, Hydrogen Atom.

Unit 2: Approximate Methods **(12 marks)**

Perturbation theory for non-degenerate and degenerate states and its applications. The variation theorem and its application.

Unit 3: Symmetry Point Groups **(12 marks)**

Determination of point group of a molecule, representations, the great orthogonality theorem, character table, construction of character tables for c2v and c3v groups, symmetry adapted atomic basis sets, construction of molecular orbitals. The direct product representation.

Unit 4: Atomic and Molecular Structure **(13 marks)**

many electron wave functions, Pauli exclusion principle, Helium atom, atomic term symbols. The self-consistent field method. Slater-type orbitals. Born-Oppenheimer approximation. Molecular orbital treatment for H2+.MO treatment of homo- and hetero nuclear diatomic molecules.Hückel mo treatment of simple and conjugated polyenes and alternate hydrocarbons.

Reference books:

1. Quantum Chemistry, I.N. Levine, 5th edition, Pearson Educ., Inc. New Delhi (2000).
2. Physical Chemistry: A Molecular Approach, D. A. McQuarrie, and J. D. Simon, Viva Books (2011).
3. Valence Theory, J.N. Murrell, S.F.A. Kettle and J. M. Tedder, 2nd edition, John Wiley (1965).
4. Introductory Quantum Chemistry, A.K. Chandra, 4th Edition, Tata Mcgraw Hill (1994).
5. Chemical Applications of Group Theory, F. A. Cotton, John Wiley & Sons (2008).
6. Molecular Symmetry and Group Theory, R. L. Carter, J. Wiley (1998).
7. Group Theory and Chemistry, D. M. Bishop, Dover Publications (1993).
8. Quantum Chemistry, J. P. Lowe, and Peterson, K., Academic Press (2005).

Statistical Mechanics

Paper code: AC-XI
(3 Credit)

Unit 1: **(13 marks)**

Mathematical Review of Classical Mechanics: Lagrangian Formulation, Hamiltonian Formulation, Poisson Brackets and Canonical Transformations Classical approach to Ensembles: Ensembles and Phase Space, Liouville's Theorem, Equilibrium Statistical Mechanics and it's ensembles Partition Function: Review of rotational, vibrational and translational partition

functions. Application of partition functions to specific heat of solids and chemical equilibrium. Real gases.

Unit 2: **(12 marks)**

Elementary Probability Theory Distributions and Averages, Cumulants and Fluctuations, The Central Limit Theorem Distributions & Fluctuations: Theory of Ensembles, Classical and Quantum, Equivalence of Ensembles, Fluctuations of Macroscopic Observable.

Unit 3: **(13 marks)**

Basic Thermodynamics: Review of Concepts, The Laws of Thermodynamics, Legendre Transforms, The Maxwell Relations, The Gibbs-Duhem Equation and Extensive Functions, Intensive Function.

Unit 4: **(12 marks)**

Bose-Einstein distribution: Einstein condensation. Thermodynamic properties of ideal BE gas. Fermi-Dirac distribution: Degenerate Fermi gas. Electron in metals. Magnetic susceptibility.

References:

1. Kerson Haung, Statistical Mechanics, Wiley, 2nd Ed. (2008).
2. R. K. Pathria and P. D. Beale, Statistical mechanics, Elsevier, 3rd Ed (2011).
3. D. A. Mcquarrie, Statistical Mechanics, University Science Books (2011).
4. D. Chandler, Introduction to Statistical Mechanics, Oxford University Press (1987).

Organic Chemistry-II

Paper code: AC-XII
(3 Credit)

Unit 1: Reagents in Organic Synthesis **(13 marks)**

Diborane - lithium aluminium hydride - sodium borohydride - selenium-di-oxide - osmium tetroxide - phenyl isothiocyanate - N-bromo succinamide (NBS) – lead tetraacetate - dicyclohexylcarbodiimide (DCC) - pyridinium cholorochromate (PCC) - Swern oxidation - p-toluenesulphonyl chloride - trifluoroacetic acid – lithium diisopropylamide (LDA) - 1,3-dithiane (reactive umpolung) - crown ethers - trimethyl silyl iodide - Gilman reagent - dichlorodicyanobenzoquinone (DDQ) – lithium dimethylcuprate - tri-n-butyltin hydride - di-tert-butoxy dicarbonate - dihydropyran - phase transfer catalysts - Wilkinson's catalysts - Peterson synthesis – and diethylaluminium cyanide- IBX and Swern oxidations.

Unit 2: Organic Spectroscopy **(12 marks)**

Advanced Techniques and Applications of NMR: ^{1}H and ^{13}C NMR principles, rules for carbon 13 calculations, principles of decoupling, gated and inverse gated decoupling techniques, NOE, relaxation processes, population transfer, selective polarization transfer, NMR shift reagents and their applications, basic two-dimensional sequence.

Unit 3: Heterocycles **(12 marks)**

Synthesis and reactivity of furan, thiophene, pyrrole, thiazole, pyridine, indole and their derivatives, quinoline, isoquinoline, pyrimidine, purine and flavone – Skraup synthesis - Fischer indole synthesis and Pachmann coumarin synthesis - alkaloids -sources and classification -

structural elucidation by chemical degradation – total synthesis of quinine, morphine, reserpine, papaverine and nicotine (Any two).

Unit 4: Photochemistry (13 marks)

Basic principles, Jablonski diagram, photochemistry of olefinic compounds, cis-trans isomeriation, Paterno-Buchi reaction, Norrish type I and II reactions, photoreduction of ketones, di-pi-methane, oxo di-pi methane and aza di-pi methane rearrangements,Barton reaction, Hofmann-Loefflar-Freytag reactions, photochemistry of arenes, SRN1 reaction, photooxidation, Photoreaction in solid state. Method of generation and detection of radicals (ESR), radical initiators, reactivity pattern of radicals, substitution and addition reactions involving radicals, synthetic applications: cyclisation of radicals including various ring expansion, ring contraction, remote functionalisation and radical fragmentation reaction.

Reference books:

1. J. March, Advanced Organic Chemistry, 5th edition, Wiley-Intersciences, New York (2003).
2. F.A.Carey and R.J. Sundberg, Advanced Organic Chemistry, Part A and Part B, 5th edition, Plenum Press, New York (2005).
3. T.H. Lowry and K.S. Richardson, Mechanism and Theory in Organic Chemistry, 2nd edition, Harper and Row Publishers (1981).
4. R.K. Mackie and D.M. Smith, Guide book to Organic Synthesis, 2nd edition, ELBS Publications, London (1998).
5. R.K. Mackie and D.M. Smith, Guide book to Organic Synthesis, 2nd edition, ELBS Publications, London (1998).
6. R.K. Mackie and D.M. Smith, Guide book to Organic Synthesis, 2nd edition, ELBS Publications, London (1998).
7. R.M. Achesen, Chemistry of Heterocyclic Compounds, Wiley Eastern (1973).
8. W. Carruthers, Some Modern Methods of Organic Synthesis, 3rd edition, Cambridge University Press (1993).
9. B.I. Smith, Organic Synthesis, Chapman and Hall, New York (1980).

Nanoscience and Technology

Paper code: AC-XIII
(3 credit)

Unit 1: Introduction and History (12 marks)

Background to nanotechnology: - scientific revolutions –atomic structure-atomic size – bottom up/top down nanotechnology-chemical reactivity-Incremental nanotechnology-Evolutionary nanotechnology-Radical nanotechnology-Emergence of nanotechnology-Challenging in nanotechnology-Misnomers and misconception of Nanotechnology.

Unit 2: Evolution and growth of Nanosystem and classification (13 marks)

Basic problems and limitations - opportunities of nano scale -evolution of band structures and Fermi surface. Nanoparticles through homogeneous and heterogeneous nucleation-Growth controlled by surface and diffusion process- Oswald ripening process - influence of reducing agents-solid state phase segregation- grain growth and sintering precipitation in solid solutionhume rothery rule. Carbon Nanotubes (CNT) - Metals (Au, Ag, Pd, Cu) - Metal oxides (TiO_2, CeO_2, ZnO, MgO) -Semiconductors (Si, Ge, CdS, ZnSe). Classifications of nanomaterials-zero dimensional-one dimensional-two dimensional-three dimensional nanostructures- Quantum dots-Quantum wire Quantum well-semiconductors and ceramics.

Unit 3: Special nanomaterials **(12 marks)**

Carbon fullerenes-fullerene derived crystals- carbon nanotubes. Micro and Mesoporous material Ordered mesoporous materials-Random mesoporous materials-crystalline microporous materials. Core/Shell structures-Metal oxide structures-Metal polymer structures-Intercalation compounds-nanograined materials. Nanomaterials in drug delivery.

Unit 4: Materials Structure and Properties **(13 marks)**

Space lattice and unit cells, crystal system, Symmetry operation, Structures of common metallic, Semiconductor ceramic and superconductor materials, Miller Indices, Packing fractions, Formation of dangling bonds-atom like behavior of nanomaterials-physicochemical properties. Optical properties of nanomaterials-semiconductor-metal nanoparticles-Electrical and electronic properties, Thermal properties-Ferro electric properties-mechanical and magnetic properties.

Reference books:

1. Introduction to Nanoscience and Nanotechnology, By Gabor L. Hornyak, H.F. Tibbals, Joydeep Dutta, John J. Moore
2. Nanostructures and Nanomaterials: Synthesis, Properties, and Applications, By Guozhong Cao, Ying Wang
3. Organic Nanomaterials: Synthesis, Characterization, and Device Applications, By Tomas Torres, Giovanni Bottari
4. Nanochemistry: A Chemical Approach to Nanomaterials, By Geoffrey A. Ozin, André C. Arsenault, Ludovico Cademartiri
5. Nanostructures and Nanomaterials: Synthesis, Properties, and Applications, By Guozhong Cao,Ying Wang

Computational Methods

Paper code-AC-XIV
(3 Credit)

Unit 1: **(13 marks)**

Linear and Non –Linear equations: Solution of Algebra and transcendental equations, Bisection, Falsi position and Newton-Rhapson methods-Basic principles-Formulae-algorithms.
Simultaneous equations: Solutions of simultaneous linear equations-Guass elimination and Gauss Seidel iterative methods-Basic principles-Formulae-Algorithms, Pivotal Condensation.

Unit 2: **(12 marks)**

Matrix and Determinants: Matrix Inversion, Eigen-values, Eigen-vector, Diagonalization of Real Symmetric Matrix by Jacobi's Method.

Unit 3: **(13 marks)**

Interpolations: Concept of linear interpolation-Finite differences-Newton’s and Lagrange’s interpolation formulae-principles and Algorithms Numerical differentiation and integration: Numerical differentiation-algorithm for evaluation of first order derivatives using formulae based on Taylor’s series, Numerical integration-Trapezoidal Rule, Simpson’s 1/3 Rule, Weddle's Rule, Gauss Quadrature Formulae-Algorithms. Error in numerical Integration. Curve Fit: least square, straight line and polynomial fits.

Unit 4: **(12 marks)**

Numerical Solution of differential Equations: Picards Method, Taylor's Series Method, Euler's Method, Modified Euler's Method, Runge-Kutta Method, Predictor-Corrector Method.

Reference books:

1. V. Rajaraman, Computer Oriented Numerical Methods, PHI, 1993.
2. E. Balaguruswamy, Numerical Methods, Tata McGraw Hill, 2017.
3. F.Acton, Numerical Methods that Work, Harper and Row, 1997.
4. S. D. Conte and C.D.Boor, Elementary Numerical Analysis, McGraw Hill, 2005.
5. S. S. Shastri, Introductory Methods of Numerical Analysis, PHI, 2012.

Natural Products and Medicinal Chemistry

Paper code: AC-XV
(3 Credit)

Unit 1: Terpenoids and Alkaloids (13 marks)

Introduction, isoprene rule, general methods of isolation, structure elucidation and synthesis of some representative members of mono and sesquiterpenes. Biogenesis and biosynthesis of mono-, sesqui- and di-terpenoids.

Definition and classification, general methods of isolation and structure elucidation, structure and synthesis of ephedrine, piperine, nicotine and papaverine. Biosynthesis of ephedrine and nicotine.

Unit 2: Proteins and Nucleic Acids (12 marks)

Classification - structure and synthesis of amino acids – peptides – Merrifield solid phase peptide synthesis - structure determination - peptide sequence and synthesis of - primary, secondary, tertiary and quaternary structures- Merrifield solid phase peptide synthesis - nucleic acids - structure and synthesis of DNA - structure and synthesis of RNA-WC Model.

Unit 3: Medicinal Chemistry 1 (12 marks)

Antibiotics – Penicillins, Cephalosporins, tetracyclins, newer generation of antibiotics.

Vitamins - Definition of vitamins and coenzymes, classification of vitamins, mechanism of function with synthesis of vitamin A, B1, B6 and folic acid, etc.

Drugs - Introduction and classification of drugs, brief discussion on drug targets. Sulphur drugs, anti tubercular drugs, anti diabetic drugs and newer generation of antacids.

Unit-4: Medicinal Chemistry 2 (13 marks)

Drug design and synthesis, Molecular and quantum mechanics; Drawing chemical structures, equations, and diagrams; 3D structures; Molecular modelling and Energy Minimization; Molecular properties, Conformational analysis, Docking Procedures, *De novo* design, Molecular Recognition, Receptor Based Molecular Modeling, QSAR studies, Antineoplastic agents, cardiovascular drugs, Local anti-infective drugs, Antimalarial, Anticholenergic and CNS-active drugs.

Computational methods in Chemistry

Paper code: **AC-XVI**
(3 credit)

Computational Lab Group A:
Simutation and structures and geometry optimisation with the commercial program "Materials Studio" (Forcite, Force Field: COMPASS).

Computational Lab Group B:
Computational studies on opto-electronic and charge transport properties in conjugated systems. Other computational application introducing "ChemCraft", "Gaussian", "SCM ADF" softwares.

Computational Lab Group C:
Plotting, analysis and interpretation of data from UV-Vis or Fluorescence spectrophotometry using Origin.

Advanced Organic Chemistry Lab

Paper code: AC-XVII
(3 credit)

I. Some important techniques in practical organic chemistry: Recrystallization, mixed melting point, drying of solvents and steam distillation.

II. Preparation of
i) Methyl orange ii) Coumarin iii) Pyrazolone iv)Azalactone

III. Preparation of
i) Benzanilide by Beckmann's rearrangement:
(a) Preparation of benzophenone oxime
(b) Beckmann's rearrangement to benzanilide
ii) Benzilic acid from benzoin:
(a) Benzil from benzoin
(b) Benzilic acid from benzyl
iii) Anthranilic acid from phthalic anhydride:
(a) Phthalimide from Phthalic anhydride
(b) Hoffmann's rearrangement to anthranilic acid
iv) m-Nitroaniline from Nitrobenzene:
(a) m-Dinitrobenzene from Nitrobenzene
(b) m-Nitroaniline from m-Dinitrobenzene

Scheme of evaluation

Marks: 50 Time: 6 Hrs
Single step preparation and Recrystallization – 10
Two step preparation and Recrystallization – 30
Viva, Record and Samples – 10

Recommended books:

1) Vogel's textbook of practical organic chemistry – Arthur Israel Vogel, B. S. Furniss
2) Practical Organic Chemistry - Frederick George Mann and Bernard Charles Saunders
3) Advanced Practical Organic Chemistry - N K Vishnoi
4) Laboratory Manual of Organic Chemistry - R. K. Bansal