

SCHOOL OF CHEMICAL SCIENCES

List of Compulsory Courses

Year/Semester	Course No.	Credits	Course Name
1/Semester I	C101	3	Chemistry I
	C141	2	Chemistry Lab I
1/Semester II	C102	3	Chemistry II
	C142	2	Chemistry Lab II
2/Semester III	C201	4	Basic Inorganic Chemistry
	C202	4	Chemical Thermodynamics
	C203	4	Reaction Mechanisms in Organic Chemistry
	C241	2	Chemistry Lab III
	C242	2	Electronics Lab
2/Semester IV	C204	4	Reagents in Organic Syntheses
	C205	4	Main Group and Organometallic Chemistry
	C206	4	Quantum Chemistry I
	C243	2	Physical Chemistry Lab I
	C244	2	Biomolecular Chemistry Lab
3/Semester V	C301	4	Physical Organic Chemistry
	C302	4	Molecular Spectroscopy and Group Theory
	C303	4	Statistical Mechanics
	C341	4	Organic Chemistry Lab I
	C342	4	Inorganic Chemistry Lab I
3/Semester VI	C304	4	Coordination Chemistry
	C305	4	Chemical Binding
	C306	4	Physical Methods in Chemistry I
	C343	4	Physical Chemistry Lab II
	C344	4	Organic Chemistry Lab II
4/Semester VII	C401	4	Physical Methods in Chemistry II
	C403	4	Chemistry of Heterocycles and Natural Products
	C498	12	Chemistry Project
4/Semester VIII	C402	4	Chemical Rate Processes
	C499	12	Chemistry Project
5/Semester IX	C598	16	Chemistry Project
5/Semester X	C599	20	Chemistry Dissertation

List of Elective Courses

Year/Semester	Course No.	Credits	Course Name
3rd or 4th year students of other streams	C351	4	Photochemistry
	C352	4	Pharmaceutical Chemistry
	C353	4	Classics in Molecules
4th or 5th year	C551	4	Molecular Modeling
	C552	4	Solid State Chemistry
	C554	4	Crystallography
	C555	4	Principles of Drug Action
	C556	4	Advanced Bio-inorganic Chemistry
	C557	4	Nuclear Magnetic Resonance
	C558	4	Advanced Functional Materials
	C559	4	Supramolecular Chemistry
	C560	4	Chemistry of Nanomaterials
	C561	4	Advanced Bio-organic Chemistry
	C562	4	Polymer Chemistry
	C563	4	Molecular Reaction Dynamics
	C564	4	Theory of Molecular Spectroscopy
	C565	4	Advanced Organic Chemistry
	C566	4	Catalysis: Reaction Mechanisms and Applications
	C567	4	Advanced Main Group Chemistry
	C568	4	Advanced Fluorescence Spectroscopy
C569	4	Biomacromolecules	
C570	4	Advanced Heterocyclic Chemistry	

1 Compulsory Theory Courses

C101: Chemistry I

1. **Thermodynamics and Chemical Equilibrium:** Laws of thermodynamics; Thermochemistry; Joule-Thompson Effect; entropy, Helmholtz and Gibbs free energies, Maxwell Relations, partial molar quantities, chemical potential, Gibbs-Duhem equation. [5]
Equilibrium constant and its relation with free energy changes, variation of chemical equilibrium constant with temperature and pressure, vant Hoff equation, applications of Gibbs-Helmholtz equation. [5]
2. **Elementary Chemical Kinetics:** Rate laws for first, second and third order reactions, reversible, parallel and consecutive reactions, steady state approximation, enzyme kinetics (Michaelis-Menten equation). [4]
3. **Rate Theories and Dynamics:** Temperature dependence of the rates of chemical reactions, Collision theory, qualitative concepts of transition state theory, Introduction to reaction dynamics. [5]
4. **Atomic and Molecular Structure:** Introduction to quantum mechanics: Particle in a box, Atomic structure: H atom, concept of atomic orbitals and wave functions, many electron atoms, Spin and Pauli principle. Molecules: Bonding in homo and heteronuclear diatomic molecules. [5]
5. **Spectroscopy:** Interaction of light with matter, Electronic spectroscopy, Beer-Lamberts law, Fluorescence, Phosphorescence, Rotation and vibrational spectroscopy, Introduction to nuclear magnetic resonance, Application of spectroscopy to biomolecules. [6]

Recommended Books:

1. Physical Chemistry, I. Levine, Tata McGraw Hill, 5th Edn., 2007.
2. Physical Chemistry : A Molecular Approach, D. A. McQuarrie and J. D. Simon, University Science Books, 1997.
3. Physical Chemistry, G. M. Barrow, McGraw Hill, 5th Edn., 2007
4. Chemical Kinetics, K.J. Laidler, 3rd Edn., Harper and Row, 1987.

C102: Chemistry II

1. Structure of simple inorganic molecules; VSEPR theory; Coordination complexes; Brief description of VBT, CFT and MO theory; Distortion in Octahedral complexes. [6]
2. Organometallic chemistry; metal carbonyls; metal nitrosyls; 18 electron rule; Ferrocene and its basic reactions; Catalysis of organometallic complexes; Hydrogenation and other industrially important reactions. [6]
3. Chemistry of biological systems; Hemoglobin, Myoglobin and Heme containing systems. [2]
4. Structure of organic molecules (Lewis structures, Acid-Base, HSAB principles, Hybridization, Resonance, Hyper-conjugation, Aromaticity, Functional groups, Nomenclature, Isomerism). [8]
5. Conformational analysis of acyclic and cyclic systems; Molecular chirality; Cahn-Ingold-Prelog R-S Notational system; Optical activity; Chiral Induction; Importance of chirality in chemical biology. [8]

Recommended Books:

1. S. H. Pine, Organic Chemistry, 5th Ed. Tata McGraw Hill Book Co., 2007.
2. T. W. G. Solomons, C. B. Fryhle, Organic Chemistry, 8th Ed. Wiley, 2007.
3. T. W. G. Solomons, C. B. Fryhle, R. G. Johnson, Study Guide and Solutions Manual to Accompany: Organic Chemistry, 8th Ed. John Wiley & Sons, 2005.
4. J. Karty, The Nuts and Bolts of Organic Chemistry: A Student's Guide to Success, Pearson, 2008.
5. R. J. Morrison and R. N. Boyd, Organic Chemistry, 6th Ed. Prentice Hall, 2007.
6. J. E. Huheey, E. A. Keiter, R. L. Keiter, O. K. Medhi, Inorganic Chemistry: Principles of Structure and Reactivity, 4th Ed. Pearson, 2007.
7. P. Atkins, T. Overton, J. Rourke, M. Weller, F. Armstrong, Shriver & Atkins Inorganic Chemistry, 4th Ed. Oxford, 2009.
8. B. D. Gupta, A. J. Elias, Basic Organometallic Chemistry: Concepts, Syntheses and Applications, Universities Press, 2010

References

1. Physical Chemistry, R. S. Berry, S. A. Rice and J. Ross, Oxford Univ. Press, 2nd Edn., 2000.
2. Physical Chemistry, R. J. Silby and R. A. Alberty, Wiley, New York, 3rd Edn., 2000.

C201: Basic Inorganic Chemistry

1. **Basic Solid State Chemistry:** The Ionic bond, Lattice Energy, Size effects, Covalent character in predominantly in Ionic bonds, Structures of complex solids, imperfections in Crystals, Conductivity in Ionic solids, Solids held together by Covalent bonding. [6]
2. **Molecular structure and Chemical Forces:** Molecular symmetry, point groups and introduction to Character Tables; Types of Chemical forces covalent bonding, Hydrogen bonding, Effects of Chemical forces. [4]
3. **Basic Main Group Chemistry:** First and Second Row Anomalies, Use of p-orbitals in pi bonding, Use (or not) of d- orbitals by nonmetals, reactivity of d-orbital participation, periodic anomalies of the nonmetals and post-transition metals, Chains catenation, Rings, Cages, Boron cage compounds. [8]
4. **Coordination Chemistry: Structure, Isomerism, stability, Reactions, Kinetics and Mechanisms:** Coordination Number 1 - 8, Higher coordination number, Types of Isomerism, Thermodynamic stability, Chelate Effect, Substitution reactions in Square Planar complexes, Thermodynamic and Kinetic stability, Kinetics of Octahedral substitution and Mechanisms of redox reactions. [7]
5. **Oxidation and Reduction:** Reduction potentials; Redox half reactions; Trends in standard potentials, Electrochemical series, the Nernst equation, Redox stability in water; Representation of electrode potential data diagrammatically. Latimer-Frost Diagrams, Chemical extraction of the elements through oxidation, reduction and electrochemical extraction. [7]
6. **Introduction to f-block Elements:** Special features of f-block elements, lanthanide contraction, coordination number, structures, and simple reactions. [3]
7. **Nuclear Chemistry:** Nuclear reactions and their characteristics, radioactivity, detecting and measuring radioactivity, radioactive decay rates, nuclear stability, energy changes during nuclear reactions, nuclear fission and fusion, nuclear transmutation, biological effects of radiation; Some applications of Nuclear Chemistry: Dating with radioisotopes, medical uses therapeutic and imaging procedures. [7]

Recommendend Books:

1. Inorganic Chemistry- Principles of Structure and Reactivity, J.E. Huheey, E. A. Keiter, R.L. Keiter and O. K. Medhi, Pearson Education, 2007.
2. Concise Inorganic Chemistry, J. D. Lee, 4th Edn., ELBS, 1991.
3. Advanced Inorganic Chemistry, F. A. Cotton, C. A. Murillo, and M. Bochmann, Wiley Interscience, 2001.
4. Inorganic Chemistry, D. F. Shriver and P. W. Atkins, Oxford University, 1999.
5. Molecular Symmetry and Group Theory: A Programmed Introduction to Chemical Applications, A. Vincent, John Wiley, 2001.

References:

1. Chemistry of the Elements, N. N. Greenwood and A. Earnshaw, 2nd Edition, Elsevier, 2005.
2. Chemistry, J. McMurry, R. C. Fay, 4th Edition, Pearson Education, 2005.
3. Group Theory and Chemistry, D. M. Bishop, Dover Publications, New York, 1973.
4. Chemical Applications of Group Theory, F. A. Cotton, John Wiley and Sons, 2003.

C202: Chemical Thermodynamics

1. **Recap:** Review of thermodynamics and chemical equilibrium. Phase equilibrium: Multicomponent systems, Ideal solution, Vapor-liquid equilibrium, Raoult's law, Henry's law, colligative properties. [8]
2. **Surfaces:** Thermodynamics of surfaces and interfaces, surface tension, vapour pressure; surface films on liquids, Gibbs adsorption equation; adsorption of gases on solids: Freundlich, Langmuir and BET adsorption isotherms; determination of surface areas; colloids. [7]
3. **Electrochemistry :** Arrhenius theory of electrolytic dissociation, Conductance of electrolytes in solutions, Debye-Huckel theory of electrolytes; ionic strength principle, activities of ions and activity coefficients, Debye-Huckel-Onsager theory of electrolytic conductance, ion association in electrolytic solution. [10]
Electrochemical cells and Electromotive Force(EMF), thermodynamics of cell reactions, Applications of EMF measurements: equilibrium constant, thermodynamic parameters, potentiometric titrations; basic principles of ion-selective membrane electrodes, batteries, Bioelectrochemistry. [7]
4. **Nonequilibrium Thermodynamics :** Conservation equations, linear transport processes, Onsager reciprocity relations, continuity and diffusion equations, steady states. [8]

Recommendend Books:

1. Physical Chemistry, I. Levine, Tata McGraw Hill, 5th Edn., 2007.
2. Physical Chemistry of Surfaces, A. W. Adamson and A. P. Gast, John Wiley and Sons, Inc., 1997.
3. Modern Electrochemistry, J.O.M. Bockris and A. K. N. Reddy, Springer, 2006.
4. Physical Chemistry, R. S. Berry, S. A. Rice and J. Ross, Oxford Univ. Press, 2nd Edn., 2000.
5. Thermodynamics of Irreversible Processes, R. Haase, Dover Publications, 1990.

C203: Reaction Mechanisms in Organic Chemistry

1. **Structural Effects on Stability and Reactivity:** Thermodynamic Stability; Chemical Kinetics; Thermodynamic Stability vs Reaction Rates; Electronic Substituent Effects on Reaction Intermediates; Kinetic Isotope Effects; Linear Free-Energy Relationships for Substituent Effects; Catalysis; Solvent Effects; Highly Strained Molecules. [5]
2. **Nucleophilic Substitution Reaction:** Nucleophiles, Electrophiles and Leaving Groups; Mechanisms for Nucleophilic Substitution; Kinetic and Stereochemical Analysis; Substituent Effects on Reactivity; S_N2 Reaction vs S_N1 Reaction; Neighboring Group Participation; S_Ni Reactions; Preparatively Useful S_N2 Reactions; Carbocationic Rearrangements. [9]
3. **Addition Reactions:** The Concept of cis- and trans-Addition; Electrophilic Addition of Alkenes; Selected examples-Hydrohalogenation, Halogenations, Hydration, Epoxidation, Dihydroxylation, Sulfenylation, Halolactonization, Metal ions, Hydroboration, Cyclopropanation; Electrophilic Addition of Alkynes and Allenes; Vocabulary of Chemoselectivity, Diastereoselectivity, Enantioselectivity, Stereospecificity, Stereoconvergence; Asymmetric Catalysis-Sharpless Oxidations of Allylic alcohols and Dihydroxylation; Noyori Hydrogenation. [9]
4. **Elimination Reactions:** Concepts of Elimination Reactions; Mechanism of E2, E1 and E1cb Reactions; Regioselectivity and Stereoselectivity of Elimination Reactions; the Competition between Elimination and Nucleophilic Substitution Reactions-Substrate Effects, Base Effects, Stereoelectronic Effect; Heck Reaction, Carbene, Nitrene. [9]
5. **Aromatic Substitution:** Aromaticity; Annulenes; Electrophilic Aromatic Substitution Reactions; Substituent Effects on Reactivity; Nucleophilic Aromatic Substitution; Ortho Metallation; Cross Coupling Reactions. [7]

Recommendend Books:

1. F. A. Carey, R. J. Sundberg "Advanced Organic Chemistry Part A and B: Structure and Mechanisms" 5th Edition, Springer, 2007.
2. R. Bruckner "Organic Mechanisms: Reactions, Stereochemistry and Synthesis" Springer, 2010.
3. J. Clayden, N. Greeves, S. Warren, P. Wothers "Organic Chemistry" Oxford University Press, 2001.
4. M. B. Smith, J. March "March's Advanced Organic Chemistry" 6th Edition, Wiley-VCH, 2007.
5. E. V. Anslyn, D. A. Dougherty "Modern Physical Organic Chemistry" California University Science Books, 2006.

C204: Reagents in Organic Syntheses

1. **Chemistry of Carbonyl Groups:** Nucleophilic Addition to Carbonyl Groups; Nucleophilic Substitution at Carbonyl groups and with Complete Removal of Carbonyl Oxygen; Carbanions and Enolisation; Building Organic Molecules from Carbonyl Compounds (Including Well-known Name Reactions); Nitrogen, Phosphorus and Sulfur Ylides; Micheal Addition. [20]
2. **Oxidation Reactions:** Transition Metal-based Oxidation Reagents; DMSO-based Oxidation Reactions; Other Oxidation Reagents; Oxidation of Functional Groups; Oxidative Cleavage of C=C bonds and Glycols; Ozonolysis; Barton Reaction; Oxidations at Unfunctionalized CH Bonds. [7]
3. **Reduction Reactions:** Reduction of Carbonyl Groups: Conformational Effects; Stereochemistry of Hydride Reduction Reactions-Aluminum Hydride and Borohydride Reducing Agents; Hydride Reductions of Functional Groups; Dissolving Metal Reductions; Other Reduction Methods; Corey-Bakshi-Shibaki Reduction. [8]
4. **Retrosynthesis:** Principles and Applications; Target-Oriented and Diversity-Oriented Organic Synthesis; Selected Examples. [7]

Recommendend Books:

1. F. A. Carey, R. J. Sundberg "Advanced Organic Chemistry Part B: Structure and Mechanisms" 5th Edition, Springer, 2007.
2. R. Bruckner "Organic Mechanisms: Reactions, Stereochemistry and Synthesis" Springer, 2010.
3. J. Clayden, N. Greeves, S. Warren, P. Wothers "Organic Chemistry" Oxford University Press, 2001.
4. M. B. Smith, J. March "March's Advanced Organic Chemistry" 6th Edition, Wiley-VCH, 2007.
5. E. J. Corey, X.-M. Cheng "The Logic of Chemical Synthesis" Wiley-Interscience, 1995.
6. T. Hudlicky, J. W. Reed "The Way of Synthesis: Evolution of Design and Methods for Natural Products" Wiley-VCH, 2007.

C205: Main-Group and Organometallic Chemistry

1. Basic Characterization techniques of main-group and organometallic compounds(NMR, Mass, IR). [5]
2. **Representative chemistry of main group elements :** [14]
 - (a) Organometallic chemistry of lithium and magnesium: synthesis, structures and reactivity
 - (b) Chemistry of boron: Boranes, bonding in boranes, topology of boranes, synthesis and reactivity, Carboranes and metallacarboranes. New Lewis acids based on boron; polymer-supported Lewis acids.
 - (c) Chemistry of Aluminum: Aluminum alkyls. Use of aluminum alkyls in polymerization of olefins.
 - (d) C₆₀ and carbon nanotubes: discovery, preparation and selected reactions.
 - (e) Chemistry of Silicon: Organosilicon compounds, Silicates and aluminosilicates.
3. **Unusual compounds of main group elements:** [6]
 - (a) Chemistry of multiple bonding: Multiple bonding in heavier main-group elements. Unusual compound of main group elements: Si=Si, Si≡Si, P=P double bond, Bi=Bi double bond. Synthesis, Structure and reactivity. Controversies.
 - (b) Chemistry of low valent compounds: Synthesis, Structure and bonding models and reactivity examples of Al(I), Si(II) low valent compounds.
 - (c) Low oxidation state main group metal hydrides: synthesis and reactivity studies.
 - (d) Inorganic rings and polymers. Cyclo and heterocyclophosphazenes and the polymers derived from them. Polysilanes. Borazine and boron nitride.
 - (e) Chemistry of halogens and noble gases-recent trends. CFCs and ozone layer.
4. **Organometallic Chemistry :** [17]
 - (a) σ - bonded ligands : Metal alkyls, aryls and hydrides. Stability, preparation and reactivity. Metal- carbonyls / Metal- phosphines / metal- nitrosyls / metal isocyanide: structures, reactivity and bonding. Metal- carbenes, metal-carbynes, Fischer carbenes, Schrock carbenes , N-heterocyclic carbenes, olefin metathesis.
 - (b) π - bonded ligands: Metal-olefins, metal alkynes, metal-dienes, Metal-Cp Metal-Cp* complexes. Synthesis, structure, bonding and reactivity.
 - (c) Applications of organometallics in organic synthesis: C-C bond coupling reactions (Heck, Sonogoshira, Suzuki etc). C-N bond coupling reactions. Reduction reactions using transition metal hydrides; asymmetric hydrogenation.

Recommendend Books:

1. Organometallics: A Concise Introduction, C. Elschenbroich and A. Salzer, 3rd Edn. 1999.
2. Chemistry of the Elements, N. N. Greenwood and A. Earnshaw, 2nd Edn., Elsevier, 2005.
3. Modern Inorganic Chemistry, W. L. Jolly, McGraw Hill, New York, 2nd Edn., 1991.
4. Concepts and Models of Inorganic Chemistry, B. Douglas, D. McDaniel and J. Alexander, John Wiley, New York, 3rd Edn., 1993.
5. Organometallic Chemistry of the Transition Metals, R. H. Crabtree, Wiley, New York, 1988.

C206: Quantum Chemistry I

1. **Origin of quantum mechanics :** Historical perspective, The photoelectric effect, Wave-particle duality, electron diffraction, black body radiation, uncertainty principle. [5]
2. **Wave Functions:** Concepts of wave function, operators, eigen values and eigen functions, commutation relations. Introduction to linear algebra and matrix representation of operators. [6]
3. **Basic postulates of quantum mechanics :** Time dependent Schrödinger equation, Stationary states, time independent Schrödinger equation, concept of quantization. [6]
4. **Simple exactly solvable systems:** Particle in one dimensional box and extensions to two and three dimensions, One dimensional harmonic oscillator, Rigid rotor, Angular momentum, concept of space quantization. [8]
5. **Applications to atomic systems:** Hydrogen atom, orbitals, shapes of orbitals, radial distribution function, electron spin. [6]
6. **Many electron atoms:** Helium atom and many electron wave functions, concept of screened nuclear charge, spin orbitals, Pauli Exclusion Principle and Slater determinants to represent many-electron wave functions. Introduction to variational and perturbation methods. [11]

Recommended Books:

1. Physical Chemistry : A Molecular Approach, D. A. McQuarrie and J. D. Simon, Viva Books, New Delhi, 1998.
2. Introduction to Quantum Chemistry, A. K. Chandra, Tata McGraw Hill, 1997.
3. Molecular Quantum Mechanics, P. W. Atkins and R. S. Friedman, 3rd Edn., Oxford University Press, 1997.
4. Quantum Chemistry, D. A. McQuarrie and J. D. Simon, Viva Books, New Delhi, 1998.
5. Quantum Chemistry, I. N. Levine, 5th Edn., Pearson Education, 2003.
6. Elementary Quantum Chemistry, F. L. Pilar, McGraw-Hill Book Company, New York, 1968.

C301: Physical Organic Chemistry

1. **Stereoelectronic Effects:** Anomeric & Related Effects; Acetals, Esters, Amides and Related Functions; Reactions at sp^3 , sp^2 , and sp Carbons; Examples in Synthesis and Biological Processes; Felkin-Ahn Model, Houk Model, Cieplak Model, EFOE Model, and Cation-Complexation Model as Applied to π -Facial Selectivity; Baldwin's Rule. [10]
2. **Pericyclic Reactions:** The Nature of Pericyclic Reactions; The Woodward-Hoffmann Rules and Molecular Orbitals; Cycloaddition reactions; Electrocyclic Reactions; Sigmatropic Rearrangements-[1,2], [1,3], [1,5], [2,3] and [3,3]; Cheletropic Reactions; Cope Rearrangements; Claisen Rearrangements; Enantioselective Pericyclic Reaction. [16]
3. **Photochemistry:** Electronic Configurations-Multiplicity, S_0 , S_1 , T_1 ; Electronic Transitions - π to π^* , n to π^* ; Selection Rules and Solvent Effect on π to π^* , n to π^* Transitions; Photochemistry of Olefins, Dienes and Carbonyl Compounds; Chemistry of Vision. [10]
4. **Radical Reactions:** Generation and Characterization of Free Radicals; Nucleophilic and Electrophilic Radicals; Substitution Reaction; Addition Reactions; Radical Coupling; Barton Reaction. [6]

Recommended Books:

1. F. A. Carey, R. J. Sundberg "Advanced Organic Chemistry Part B: Structure and Mechanisms" 5th Edition, Springer, 2007.
2. R. Bruckner "Organic Mechanisms: Reactions, Stereochemistry and Synthesis" Springer, 2010.
3. J. Clayden, N. Greeves, S. Warren, P. Wothers "Organic Chemistry" Oxford University Press, 2001.
4. M. B. Smith, J. March "March's Advanced Organic Chemistry" 6th Edition, Wiley-VCH, 2007.
5. E. V. Anslyn, D. A. Dougherty "Modern Physical Organic Chemistry" California University Science Books, 2006.
6. I. Fleming "Molecular Orbitals and Organic Chemical Reactions" Wiley-VCH, Student Edition, 2010.
7. J. M. Coxon, B. Halton "Organic Photochemistry" Cambridge University Press, 1974.
8. C. H. Depuy and O. L. Chapman "Molecular Reactions and Photochemistry", Prentice Hall of India, 1975.

C302: Molecular Spectroscopy and Group Theory

1. **Group Theory :** Symmetry Elements, Symmetry Operations, Point Groups, Symmetry Representations, Applications of symmetry to Molecular Orbital diagrams of simple molecules (examples: H_2O , BeH_2 , BF_3 ($\sigma + \pi$)). Definition of a group and basic theorems, molecular symmetry groups and classes, Great orthogonality theorem, Matrix representation of groups, irreducible representations and Character Tables. Symmetry properties of wave functions, orbitals as basis sets for irreducible representations, symmetry adapted linear combinations. Assignment of symmetry representations of d -orbitals for specific geometries. [12]
2. **Introduction to Spectroscopy:** Interaction of light with matter, transition moments and transition probabilities, Einsteins coefficients, oscillator strength. [2]
3. **Diatomic Molecules:**
 - (a) **Electronic Spectra:** Born-Oppenheimer approximation, Potential energy curves of diatomic molecules, Frank-Condon principle, electronic transitions in homonuclear and heteronuclear diatomics. [4]
 - (b) **Microwave and Infrared Spectroscopy:** Simple harmonic oscillator and rigid rotor model, Rotational spectra of diatomic molecules, Stark effect, vibrational spectra of diatomic molecules, anharmonic corrections, selection rules, fundamental and overtone bands, Isotope effects, vibrational rotational coupling. [6]
4. **Polyatomic Molecules:**
 - (a) **Electronic Spectra:** Electronic structure, electronic spectra of polyatomic molecules - linear conjugated molecules, aromatic molecules, transition metal compounds, fluorescence, phosphorescence, internal conversion and charge transfer. [9]
 - (b) **Rotational, Vibrational and Electronic Spectroscopy of Polyatomic Molecules :** Symmetric and asymmetric top molecules, normal modes of vibration and their classification by group theory, coupling between rotational and vibrational degrees of freedom. Symmetry and normal modes of vibration. Rovibrational spectra, Concept of anisotropic polarizability and Raman spectra. [9]

Recommendend Books:

1. Chemical Applications of Group Theory, F. A. Cotton, John Wiley, 3rd Edn., 2003.
2. Symmetry and Spectroscopy: An Introduction to Vibrational and Electronic Spectroscopy, D. C. Harris and M. D. Bertolucci.
3. Fundamentals of Molecular Spectroscopy, C. N. Banwell and E. M. McCash, Tata McGraw Hill, 1995.
4. Molecular Spectroscopy, G. M. Barrow, McGraw Hill, 1985.
5. Spectra of Atoms and Molecules, P. F. Bernath, Oxford Univ. Press, 2005.
6. Modern Spectroscopy, J. M. Hollas, John Wiley, 4th Edn., 2004.
7. Molecular Symmetry and Group Theory, R. L. Carter, John Wiley and Sons, 1998.

C303: Statistical Mechanics

1. Basic assumptions, concept of microscopic and macroscopic states, ensembles and averages. Calculation of distribution functions in canonical ensemble and the canonical partition function. Relations between the canonical partition function and thermodynamic functions. Calculations in other ensembles like microcanonical and grand canonical ensembles. [12]
2. Calculations of partition functions and thermodynamic properties for ideal systems of monatomic and diatomic molecules. Calculations of fluctuations and equivalence of ensembles. [7]
3. Calculation of heat capacity of solids, Einstein and Debye theories, study of chemical equilibrium in terms of partition functions. [4]
4. **Quantum Statistics:** Maxwell-Boltzmann, Bose-Einstein, and Fermi-Dirac statistics. Systems of Fermions and Bosons in weak and strong degenerate limits. [7]
5. **Classical Statistical Mechanics:** partition functions as integrals over phase space coordinates, Systems of interacting particles, imperfect gases, concept of radial distribution functions of liquids and applications to ionic solutions using Debye-Huckel theory. [6]
6. **Non-equilibrium Statistical Mechanics:** Onsager regression hypothesis and fluctuation-dissipation theorem, calculations of transport coefficients like diffusion, conductivity. [6]

Recommendend Books:

1. Physical Chemistry : A Molecular Approach, D. A. McQuarrie and J. D. Simon, Viva Books, New Delhi, 1998.
2. Statistical Mechanics, D. A. McQuarrie, University Science Books, 2nd Edn., 2000.
3. Introduction to Modern Statistical Mechanics, D. Chandler, Oxford Univ. Press, 1987.
4. Statistical Thermodynamics of Non-Equilibrium Processes, J. Kaizer, Springer, 1st Edn., 1987.
5. Statistical Physics II: Non-Equilibrium Statistical Mechanics, R. Kubo, M. Toda and N. Hashitsume, Springer, 2003.

C304: Coordination Chemistry

1. **Theories of bonding:** CFT (including Jahn-Teller). Effects of ligand field (spectrochemical series, enthalpies of hydration, spinel structures. Shortcomings of CFT. MO theory of coordination complexes. Electronic Spectra of complexes including Orgel diagrams and Tanabe - Sugano diagrams. [10]
2. **Magnetism:** Introduction to Magnetism. Origin of diamagnetism. Paramagnetism: Van Vleck formula and its approximated forms, Curie law. Magnetic susceptibility, orbital quenching and spin-only moment. Magnetic exchange interactions in coordination compounds: ferrimagnetism and antiferromagnetism. Bulk magnetic properties and ferromagnetism. Molecule-based magnetic materials: organic magnets and single molecule magnets. [10]
3. **Mechanisms of reactions of transition metal complexes:** Substitution (Kinetic effects: labile vs inert) and electron-transfer reactions (Outer-sphere, Self-exchange; Inner-sphere). [7]
4. **Bioinorganic Chemistry:** Basic principles (why specific metal ions are present in certain proteins/enzymes): Heme proteins, types, structure and function (including mechanism of function): Hemoglobin, myoglobin, Cytochrome C, Cytochrome P450, Catalases, Peroxidases. Non-Heme Proteins: Hemeerythrin, Ribonucleotide reductase, Methanol monooxygenase (a) Iron-Sulfur Proteins: Ruberodoxin, Ferredoxin; (b) DNA / RNA : Ribozymes. [10]
5. **Transition metal based supramolecular structures :** Ligand design and applications. [5]

Recommendend Books:

1. Advanced Inorganic Chemistry, F. A. Cotton, C. A. Murillo, and M.Bochmann, Wiley Interscience, 2001.
2. Inorganic Chemistry, D. F. Shriver and P. W. Atkins, Oxford University Press, 1999.
3. Supramolecular Chemistry: Concepts and Perspectives, J. M. Lehn, VCH, 1995.
4. Principles of Bioinorganic Chemistry, S. J. Lippard and J. M. Berg, Panima Publications, New Delhi, 1997.
5. Bioinorganic Chemistry ; Inorganic Elements in the Chemistry of Life. Kaim, B. Schwederski Wiley, 1994
6. Biological Inorganic Chemistry: Structure and Reactivity Harry B. Gray, Edward I. Stiefel, Joan Selverstone Valentine, Ivano Bertini University Science Book; 2006
7. Reaction Mechanism of Inorganic and Organometallic Systems , R B Jordan, 2nd Edn., Oxford University Press, 1991.

References:

1. Bioinorganic Chemistry, Asim K. Das, Allied Books, Kolkata, 2004.
2. Molecular Symmetry and Group Theory: A Programmed Introduction to Chemical Applications, A. Vincent, John Wiley, 2001.
3. Mechanism of Inorganic Reactions, F. Basolo and R. G. Pearson, 2nd Edn. Wiley, 1967
4. Inorganic Reaction Mechanisms, M L Tobe and J Burgess, 1st Edn., Wesley Longmans Ltd. 1999.
5. Inorganic Chemistry- Principles of Structure and Reactivity, J.E. Huheey, E. A. Keiter, R.L. Keiter and O. K. Medhi, Pearson Education, 2007.

C305: Chemical Binding

1. **Introduction:** Review of basic principles of quantum mechanics, atomic structure, variation and perturbation methods. [3]
2. **Electronic structure of diatomic molecules:** Born-Oppenheimer approximation, H_2^+ ion, molecular orbitals of ground state and excited states of H_2^+ (LCAO-MO), homo and heteronuclear diatomic molecules, electronic term symbols, valence bond theory of diatomic molecules, comparison of valence bond and molecular orbital theories. Term Symbols for diatomic molecules. [12]
3. **Self-consistent Field Methods:** Hartree-Fock theory of atoms and molecules, post-Hartree-Fock theories, configuration interaction wave functions. [8]
4. **Electronic structure of polyatomic molecules:** SCF-MO treatment of closed shell systems and applications to molecules (H_2O , NH_3 , CH_4) ; Potential energy surface and equilibrium geometry, molecular vibrational frequencies. Brief introduction to density functional theory. [9]
5. Virial theorem and chemical bonding. The Hellman-Feynman theorem. [4]
6. Semi-empirical and molecular mechanics treatment of molecules, Huckel molecular orbital theory for conjugated organic molecules and its applications to ethylene, butadiene, benzene; delocalization energy and stability. [6]

Recommendend Books:

1. Modern Quantum Chemistry: Introduction to Advanced Electronic Structure, A. Szabo and N. S. Ostlund, Dover, 1996.
2. Molecular Quantum Mechanics, P.W. Atkins and R.S. Friedman, OxfordUniversity Press, 3rd Edn., 1997.
3. Quantum Chemistry, I. N. Levine, 5th Edn., Pearson Education, 2000.

C306: Physical Methods in Chemistry I

1. **General Introduction to spectroscopy:** Electromagnetic radiation and its interaction with atoms and molecules. Holistic view of spectroscopy. [2]
2. **Ultraviolet Spectroscopy:** Electronic Transition; definitions of related terms and designation of UV-absorption band. Studies of conjugated and extended conjugated systems. WoodwardFieser rules. Analytical use of UV-spectroscopy. [8]
3. **Infrared and Raman Spectroscopy:** Molecular Vibrations, Instrumentation of IR and Raman spectroscopic techniques. Interpretation of infrared and Raman spectra, Identification of functional groups, hydrogen bonding, Complexity of IR spectra, Utility of IR spectroscopy in structural elucidation. Raman spectroscopy in material science; SERS. [8]
4. **Fluorescence spectroscopy:** Phenomena of fluorescence. Photochemical laws, general characteristics, Quantum yield and its measurements. Radiationless transitions. Spin states and their interconversion. Kashas rule and solvent effect. Spin orbit coupling. Energy transfer processes. Donoracceptor complexes, excimers, exiplexes. Fluorescence quenching (static and dynamic). SternVolmer analysis, Timescale of molecular processes in solution. Steadystate and timeresolved fluorescence. Fluorescence anisotropy. Biochemical fluorophores. New fluorescence technologies: Multiphoton Excitation, Fluorescence correlation Spectroscopy, Single-molecule detection. [12]
5. **Photoelectron spectroscopy:** Experimental methods, Ionisation processes and Koopmans theorem. Photoelectron spectra and their interpretation. Applications. [5]
6. **Mass Spectrometry:** Basic concepts. Instrumentation, Fragmentation and rearrangements (including McLafferty rearrangement) of different classes of organic molecules. Isotope effects. [5]

Recommendend Books:

1. Modern Spectroscopy J. M. Hollas.Wiley, 2004.
2. Physical Methods in Chemistry, R. S. Drago, 2nd Ed., Saunders, 1992.
3. Essentials of Photochemistry, A. Gilbert and J. Baggot, Blackwell Scientific Publications, 1992.
4. Fundamentals of Photochemistry, K. K. RohatgiMukherjee, Wiley Eastern Ltd., 1978.
5. Molecular Fluorescence, Bernard Valeur, WileyVCH, 2002.
6. Principles of Molecular Photochemistry: An Introduction, P. Walsh, N. J. Turro, V. Ramamurthy, J. C. Scaiano, University Science Books, 2008.
7. Principles of Fluorescence Spectroscopy. Joseph R. Lakowicz, 3rd Edition, Springer, 2006.
8. Interpretation of Mass Spectra, F. W. McLafferty, 1980.
9. Spectrometric Identification of Organic Compounds, R. M. Silverstein, G. C. Bassler and T. C.Morrill, John Wiley, New York, 5th Ed., 1991.

C401: Physical Methods in Chemistry II

1. **Nuclear Magnetic Resonance Spectroscopy:** Basic Principles, Chemical shifts, Spin-spin interactions. Application of ^1H and ^{13}C NMR spectroscopy including NOE, COSY, NOESY, and other 2D techniques in the structure determination of bioorganic compounds. Application in conformational analysis. Multinuclear (^{31}P , ^{19}F , ^{29}Si) NMR of various inorganic and organo-metallic compounds. Instrumental aspects. NMR of paramagnetic sample: Contact shifts and pseudo contact shifts, shift reagents. Pulsed NMR: modern multiple-pulsed experiments including 2D NMR. [20]
2. **Electron Spin Resonance Spectroscopy (ESR):** A brief review of theory. Analysis of ESR spectra of systems in liquid phase, radicals containing single set, multiple sets of protons, triplet ground states: Transition metal ions; Fe, Cu, Mo, Cr, Mn, VO^{2+} containing systems: g values, symmetry. The practical interpretation of ESR spectra, in solid state and solution states. Multiple electron systems; Triplet ground state, Zerofield splitting, Kramers degeneracy, Spectral line-shapes when $D \ll h\nu$, $D \sim h\nu$ and $D \gg h\nu$. EPR of photoexcited triplet states. [7]
3. **Doubleresonance Techniques (ENDOR):** ENDOR in liquid solution, ENDOR in powders and nonoriented solids. ENDOR spectra of free-radicals coupled to multiple sets of nuclei with spin. ENDOR of paramagnetic metals and complexes. Biological Applications: Substrate free radical, Flavins and metal free flavin proteins, Photosynthesis, Heme proteins, Iron-Sulfur proteins, Spin labels. [7]
4. **Mossbauer Spectroscopy:** Basic physical concepts, spectral line shape, isomer shift, quadrupole splitting, magnetic hyperfine interaction. Interpretation of Mossbauer parameters of ^{57}Fe , ^{99}Ru , ^{101}Ru , ^{195}Pt , ^{193}Ir and ^{110}Sn . Some special applications: Solid state reactions, thermal decomposition, ligand exchange, electron transfer, isomerism, surface studies and biological applications. [7]

Recommend Books:

1. NMR Spectroscopy: Basic Principles, Concepts and Applications in Chemistry, H. Gunther, 2nd Ed., John Wiley & Sons, 1995.
2. Spectrometric Identification of Organic Compounds, R. M. Silverstein, G. C. Bassler and T. C. Morrill, John Wiley, New York, 5th Ed., 1991.
3. Basic ^1H and ^{13}C NMR Spectroscopy, M. Balci, Elsevier Science, 2005.
4. Electron Paramagnetic Resonance: Elementary Theory and Practical Applications, J. A. Weil, J. R. Bolton and J. E. Wertz, Wiley Interscience, New York, 1994.
5. Physical Methods in Chemistry, R. S. Drago, 2nd Ed., Saunders, 1992.
6. Mossbauer Spectroscopy : An Introduction for Inorganic Chemists and Geochemists, McGraw Hill, UK, 1973.
7. Mossbauer Spectroscopy, N. N. Greenwood and T. C. Gibb, Chapman & Hall, 1971.
8. Electron Spin Resonance : Elementary Theory and Practical Applications, J. E. Wertz and J. R. Bolton, McGraw Hill, 1984.

C403: Chemistry of Heterocycles and Natural products

1. **Chemistry of Heterocycles:** Introduction and Application of Heterocycles; Nomenclature of Aromatic and Non-aromatic Heterocycles; Synthesis and Reactivity of 5&6-membered Aromatic Heterocycles with One or Two Hetero Atoms. [12]
2. **Chemistry of Natural Products:** Introduction and Application of Carbohydrates; Steroids, Terpenoids, Fatty Lipids, Prostaglandins and Alkaloid; Biogenesis and Total Synthesis of Selected Natural Products. [20]
3. **Chemistry of Biomolecules:** Classification and Structures of Amino Acids; Peptides, Proteins and Nucleic Acids; Solid Phase Synthesis; Nucleic Acids Synthesizer. [10]

Recommended Books:

1. J. A. Joule, K. Mills "Heterocyclic Chemistry" 5th Edition, Blackwell, 2010.
2. T. Eicher, S. Hauptmann "The Chemistry of Heterocycles" 2nd Edition, Wiley-VCH, 2003.
3. R. J. Simmonds, "Chemistry of Biomolecules: An Introduction" RSC, 1992.
4. I. L. Finar, "Organic Chemistry" Vol. II, ELBS, 1990.
5. S. V. Bhat, B. A. Nagasampagi, M. Sivakumar "Chemistry of Natural Products" Springer, 2005.
6. E. J. Corey, X.-M. Cheng "The Logic of Chemical Synthesis" Wiley-Interscience, 1995.
7. T. Hudlicky, J. W. Reed "The Way of Synthesis: Evolution of Design and Methods for Natural Products" Wiley-VCH, 2007.

C402: Chemical Rate Processes

1. **Kinetic Measurements:** General features of fast reactions; study of fast reactions by flow techniques, relaxation methods (T-Jump, P-Jump, ultrasonic, pulse radiolysis, NMR); flash photolysis; salt and solvent effects on reactions in solutions. [5]
2. **Chain Reactions :** Features of chain reactions; thermal and photochemical reactions (hydrogen-bromine reaction, decomposition of aldehydes and ketones). [5]
3. **Kinetics of oscillatory reactions :** Introduction to oscillatory reactions; Belousov-Zhabotinsky and Field-Koros-Noyes models. [4]
4. **Rate Theory:** Concept of potential energy surfaces, transition state theory including its statistical mechanical treatment, Phenomenological theories of unimolecular reactions (Lindemann, Hinshelwood), statistical mechanical theories of unimolecular reactions (RRKM). [10]
5. **Chemical Dynamics:** Collision theory and Reaction Dynamics, Reaction Cross section and rate constant, Brief idea of Molecular Beam Scattering, Dynamics in condensed phase. [10]
6. **Femtochemistry :** Concepts and perspectives; applications to studies of dynamics and control of chemical reactions. [6]

Recommendend Books:

1. Physical Chemistry, I. Levine, Tata McGraw Hill, 5th Edn., 2007.
2. Physical Chemistry : A Molecular Approach, D. A. McQuarrie and J. D. Simon, University Science Books, 1997.
3. Chemical Kinetics and Dynamics, J. I. Steinfeld, J. S. Francisco and W. L. Hase, Prentice Hall, 1999.
4. Chemical Dynamics in Condensed Phases: Relaxation, Transfer and Reactions in Condensed Molecular Systems, A. Nitzan, Oxford Univ. Press, 2006.

References:

1. Basic Chemical Kinetics, H. Eyring, S. H. Lin and S. M. Lin, John Wiley & Sons, New York, 1980.
2. The World of Physical Chemistry, K. J. Laidler, Oxford University Press, 1993.

2 Elective Courses

C351: Photochemistry

1. **Introduction:** Importance of Photochemistry; Electromagnetic Radiation; Colour Perception and the Colour Circle; Beer-Lambert Law; Electronic Configurations: Multiplicity, S_0 , S_1 , T_1 etc.; Electronic Transitions and Solvent Effects: π to π^* , n to π^* etc. Molecular Orbitals (FMO Approach). [6]
2. **Unimolecular Photophysical Processes:** Jablonski Diagram; Frank-Condon principle; Fluorescence; Inter-System Crossing; Phosphorescence; Delayed Fluorescence; Quantum Yield. [6]
3. **Bimolecular Photophysical Processes:** Thermodynamics and Kinetics of Excited State Bimolecular Interactions; Excimer and Exciplex; Photosensitization and Quenching; Heavy Atom Effect; Photoinduced Electron and Charge Transfer; Resonance Energy Transfer: Coulombic and Exchange mechanisms. [8]
4. **Fluorescence Spectroscopy:** Characteristics of Excitation and Emission Spectra; Basic Theories Involving Various Fluorescence Spectral Parameters; Fluorescence Anisotropy; Introduction to Fluorescence Probing Techniques and Applications; Fluorescent Molecular Sensors of Ions and Molecules. [10]
5. **Photochemistry of Organic Compounds:** Photochemistry of Alkenes; Pericyclic Reactions; Photo-oxidation and Photo-reduction; Photochemistry of Carbonyl Compounds. [8]
6. **Applied Photochemistry:** Chemistry of Vision; Photochemistry in Nature; Photochemistry in Atmosphere; Supramolecular Photochemistry; Solar Cell; Fuel cell. [4]

Recommendend Books:

1. Fundamentals of Photochemistry, K. K. Rohatgi Mukherjee, Wiley Eastern Ltd., 1978.
2. Modern Molecular Photochemistry, N. J. Turro, University Science Books, 1991.
3. Molecular Fluorescence, B. Valeur, Wiley-VCH, 2002.
4. Principles of Molecular Photochemistry: An Introduction, P. Walsh, N. J. Turro, V. Ramamurthy, J. C. Scaiano, University Science Books, 2008.
5. Organic Photochemistry, J. M. Coxon and B. Halton, Cambridge University Press, 1974.
6. Molecular Reactions and Photochemistry, C. H. Depuy and O. L. Chapman, Prentice Hall of India.
7. Photochemistry and Pericyclic Reactions, J. Singh and J. Singh, New Age International Publishers, 2003.
8. Pericyclic Reactions, Ian Fleming, Oxford Science Publications 1998.

C352: Pharmaceutical Chemistry

1. **Drug discovery and development:** The why and wherefore of drugs; Stereochemistry and solubility factors; Principles of drug design (molecular and biochemical); 'Lead' modification approach, SAR/QSAR; Computer-aided drug design; Natural products drug discovery. [15]
2. **Basic Principles of medicinal chemistry:** Drug action at enzymes; Drug action at receptors; Physico-chemical aspects of drug molecules; Selected examples of drugs and natural products. [15]
3. **Pharmacodynamics and Pharmacokinetics:** Drug distribution and survival; Concept of Prodrug; Pharmacokinetic models; Drug metabolism. [10]

Recommendend Books:

1. Essentials of Pharmaceutical Chemistry, D. Cairns, Pharmaceutical Press, 2nd Edition 2003.
2. Fundamentals of Medicinal Chemistry, G. Thomas, Wiley-Blackwell, 1st Edition, 2003.

C353: Classics in Molecules

1. Introduction, Understanding Structural Diagrams of Organic Molecules, Protein and Three-Dimensional Protein Structure, Nucleic Acids, Synthesis, Biosynthesis. [7]
2. Urea & Acetic Acid, Glucose, Aspirin, Camphor, Terpeneol, Tropinone, Haemin, Quinine, Morphine, Steroids & the Pill, Strychnine, Penicillin, Longifolene, Prostaglandins & Leukotrienes, Vitamin B12, Erythronolide B & Erythromycin A, Monensin, Avermectin, Amphotericin B, Ginkgolide B, Cyclosporin, FK506 & Rapamycin, Calicheamicin γ 1, Palytoxin, Taxol, Mevacor, Zaragozic Acids & CP Molecules, Brevetoxin B, Ecteinascidin 743, Epothilones, Resiniferatoxin, Vancomycin, Thiostrepton. [20]
3. Modern Drug Discovery and Developments, Designed Small Drug Molecules for Mental Illness, Viral Infections, Gastrointestinal Disorders, Heart diseases and Sexual Dysfunction. [12]
4. DNA Technologies, Vaccines, Antibodies, Diabetes, Anemia, Rheumatoid Arthritis, Breast Cancer, Biologics. [7]

Recommendend Books:

1. K.C. Nicolaou and Tamsyn Montagnon, "Molecules that Changed the World", VCH, 2008.
2. E.J. Corey, László Kürti and Barbara Czakó, "Molecules and Medicine", VCH, 2008.
3. J. Block and J. M. Beale "Wilson and Gisvold's Textbook of Organic Medicinal and Pharmaceutical Chemistry", 11th Ed., Lippincott Williams & Wilkins, 2003.

C551: Molecular Modeling

1. **Introduction:** What is molecular modeling? Computable quantities. [1]
2. **Concept of Potential Energy Surface:** Stationary points, Born-Oppenheimer approximation, Geometry optimization, Normal modes of vibration. [3]
3. **Molecular Mechanics:** Basic principles, Properties that can be calculated, Strengths and weaknesses. [3]
4. **Quantum Mechanics:** Hartree-Fock-Self-Consistent-Field theory, post-Hartree-Fock (Electron correlation) methods, Density functional theory, Semi-empirical methods. [7]
5. **Chemical Dynamics:** Unimolecular and Bimolecular reactions, Reaction path and transition states, Classical trajectories, Direct dynamics, Quantum dynamics. [6]
6. **Simulations of Molecular Ensembles:** Properties as ensemble and time averages, Molecular dynamics simulations, Monte Carlo simulations. [10]
7. **Modeling Lab:** Hands-on experience for using different simulations methods and algorithms pertaining to the course. [10]

Recommendend Books:

1. C. J. Cramer, Essentials of Computational Chemistry, Wiley, 2004.
2. I. N. Levine, Quantum Chemistry, Prentice-Hall of India, 2006.
3. P. W. Atkins, Molecular Quantum Mechanics, Oxford, 2008.
4. M. P. Allen and D. J. Tildesley, Computer Simulation of Liquids, Oxford, 1987.
5. A. R. Leach, Molecular Modelling, Prentice Hall, 2001.
6. F. Jensen, Introduction to Computational Chemistry, John Wiley & Sons, 2007.

C552: Solid State Chemistry

1. **Crystal Chemistry:** A brief introduction to crystallography, Lattices, unit cells, symmetry, point groups, space groups.
Packing: CCP, HCP, voids, radius ratio rules.
Bonding in crystals: ionic, covalent, metallic, van der Waals, hydrogen bonds.
Description of crystal structures: metallic & nonmetallic structures, AB, AB₂, AB₃ (ReO₃), spinels, pyrochlores, perovskites, K₂NiF₄ etc.
Paulings rules for ionic crystal structures and the concept of bond valence.
Methods of crystallography: powder, single crystals, X-ray, neutron and electron diffraction. [7]
2. **Defects in solids:** Origin of defects in crystals; Perfect and imperfect crystals; thermodynamics of defect formation; types of defects : point defects, line defects, plane defects; Schottky and Frenkel defects; thermodynamics of Schottky and Frenkel defect formation; crystal classifications; Madelung constant and lattice energy. [7]
3. **Electronic structure of solids:** Atoms to molecules to crystals; orbitals to bonds to bands; Electronic structure of crystalline solids, elementary band theory: metals, insulators and semi-conductors., Solid state ionics; intrinsic and extrinsic semiconductors. Transport property measurement techniques: electrical resistivity, thermopower, Hall effect Magnetism of d vs. f metal compounds. [8]
4. **Critical Phenomena:** Phase transitions (Order-disorder, Martensite-austenite, Spinoidal decompositions); liquid crystals; structure-property relations (magnetic, electrical, superconductivity, optical and thermal). Powder synthesis by conventional and modern chemical methods, reactivity of solids, decomposition mechanisms, powder processing (sintering and diffusion processes), tailoring of solids, special methods for single crystal growth and thin film depositions. [10]
5. **Synthesis of solids:** Chemistry behind synthesis; intercalations; synthesis/preparation of single crystals; hydrothermal methods. Framework Solids; Zeolites, Aluminophosphates and related structures; Metal-organic framework compounds - their structures and properties. [6]
6. **Superconductivity:** Superconductivity : General aspects of superconductivity; effects of magnetic field; BCS Theory; oxide Superconductors. [4]

Recommendend Books:

1. Solid State Chemistry and Its Applications, A. R. West, John Wiley, 1987.
2. Solid State Chemistry, L. Smart and E. Moore, Chapman and Hall, 1992.
3. Principles of the Solid State, H. V. Keer, Wiley Eastern Ltd., 1994.
4. New directions in solid state chemistry, C.N.R. Rao and J. Gopalakrishnan, Cambridge University Press, 2008.
5. The Electronic Structure and Chemistry of Solids, P. A. Cox, Oxford University Press, 2005.
6. Ionic crystal, lattice defect and non-stoichiometry, N.N. Greenwood, Chemical Pub. Co., New York, 1970.
7. An Introduction to crystal chemistry, R.C. Evans, Cambridge University Press, 1964.

C554: Crystallography

1. Origin of X-rays, Filters, monochromators, sealed tube, rotating anode synchrotron radiation, safety considerations. [5]
2. Crystals and their properties- Concepts of symmetry, direct and reciprocal lattice, planes, indices, unit cell, Braggs law in direct and reciprocal lattices. Primitive and non-primitive lattices, point and space groups, equivalent positions, systematic absences and space group determination, occupancy factors. [15]
3. Theory of structure factors, Argand diagram and its use, Lorentz and polarization corrections, absorption corrections, absolute scale of intensities; unit cell determination, data collection parameters, data reduction, phase problem and structure solution by Patterson and direct methods. [15]
4. Structure refinement techniques, presentation and interpretation of structural data, examination of CIF file and critical evaluation of a structure. Errors and pitfalls, twinning and disorder, Renninger effect, extinctions, anomalous scattering and its use. [10]

Recommended Books:

1. X-ray structure determination: A practical guide, G.H. Stout and L.H. Jensen, Springer, 1992.
2. Fundamentals of crystallography, C Giacavazzo, Oxford University Press
3. X-ray analysis and the structure of organic molecules, Jack. D. Dunitz, Wiley, 1996.
4. Crystal Structure Determination, Werner Massa, Springer.
5. Structural Inorganic Chemistry, A. F. Wells, Clarendon Press, 1986.

C555: Principles of Drug Action

1. **Pharmacodynamic Phase in Drug Action:** Introduction to Pharmacodynamics, Biochemical Basis of Drug Action, Drug absorption, distribution and bioavailability, Passive diffusion, Active transport mechanisms, Excretion and reabsorption of drugs. [7]
2. **Pharmacokinetic Phase in Drug Action:** General classification of pharmacokinetic properties, Pharmacokinetic models, Intravascular administration, Extravascular administration, Estimation of pharmacokinetic parameters, The use of pharmacokinetics in drug design. [7]
3. **Novel Therapeutic Agents:** Synaptic Pharmacology: Cholinergic- and adrenergic systems, CNS Agents: Antipsychotics, antidepressants, CVS Agents: Antihypertensives, Antineoplastic agents, Analgesic and anti-inflammatory agents, Drug toxicity. [12]
4. **Concepts in Drug Metabolism:** Basic principles and factors affecting drug metabolism, Secondary pharmacological implications of metabolism, Phase I metabolic reactions, Phase II metabolic reactions, Drug metabolism and drug design, Prodrugs, Metabolic pathways for common drugs. [7]
5. **Stability of Drugs and Medicines:** Oxidation and stability of free-radicals, Prevention of oxidative deterioration, Autoxidation of fats and oils, Examples of drugs susceptible to ageing and hydrolysis, Other mechanisms of degradation. [6]
6. **Drug Development:** Clinical trials (Phase-I to Phase-IV), Formulation development, Quality control aspects (methods of assay). [6]

Recommended Books:

1. Thomas G. (2003) Fundamentals of Medicinal Chemistry, Wiley.
2. Cairns D. (2008) Essentials of Pharmaceutical Chemistry (3rd Ed.), Pharmaceutical Press.
3. Block J and Beale JM. (2003) Wilson and Gisvold's Textbook of Organic Medicinal and Pharmaceutical Chemistry (11th Ed.), Lippincott Williams & Wilkins.
4. Rang HP, Dale MM et al. (2007) Rang & Dale's Pharmacology (6th Ed.), Churchill Livingstone.
5. Hardman JG, Limbird LE et al. (2001) Goodman & Gilman's The Pharmacological Basis of Therapeutics, McGraw-Hill Professional.

C556: Advanced Bio-inorganic Chemistry

1. **Principles of bioinorganic chemistry** (Justification of why certain protein/enzyme contains a particular metal ion) [3]
2. **Heme Proteins:** Types, function and mechanisms , Myoglobin, Hemoglobin, Cytochrome c, Cytochrome P450, Peroxidases (Horseradish Peroxidase, Chloroperoxidase), Catalase, Cytochrome c Oxidase, Synthetic porphyrins of biological relevance. [5]
3. **Iron-Sulfur Proteins:** Types, function and mechanisms , Rubredoxin, Ferredoxins, Aconitase [3]
4. **Non-Heme Proteins:** Types, function and mechanisms, Mononuclear Systems (Catechol-1,2-Dioxygenases, Transferrin, Ferritin, Superoxide Dismutase, IsopenicillinN-Synthase) Dinuclear Systems (Hemerythrin, Ribonucleotide Reductase, Methane Monooxygenase, Purple Acid Phosphatases) [6]
5. **Copper Proteins (Type I, II, and III):** Types, function and mechanisms, Blue Copper Proteins; Hemocyanin, Tyrosinase, Catechol Oxidase; Superoxide Dismutase; Ascorbase Oxidase, Laccase; galactose oxidase [5]
6. **Molybdenum Enzymes:** Types, function and mechanisms, Oxo-Transfer Enzymes; Xanthine Oxidase; Nitrogenase. [5]
7. **Manganese:** Photosynthesis (Photosystem I and Photosystem II); function and mechanisms. [4]
8. **Zinc Enzymes:** function and mechanisms, Hydrolytic Enzymes (Carbonic Anhydrase; Carboxy Peptidase A; Alkaline Phosphatase). [5]
9. **DNA/RNA:** Types, function and mechanisms, DNA nicking enzymes; DNA Polymerase; Ribozymes. [5]
10. **Environmental & Medicinal Aspects:** Acid-rain; Green-house Effect etc. Radiopharmaceuticals; Photo-Dynamic Therapy; Anti-Tumor Drugs (cis-Platin, Carboplatins; Bleomycins); ion-pumps. [5]

Recommended Books:

1. Principles of Bioinorganic Chemistry; S. J. Lippard and J. M. Berg, Panima Publications, New Delhi, 1997.
2. Bioinorganic Chemistry ; Inorganic Elements in the Chemistry of Life; W. Kaim, B. Schwederski Wiley, 1994
3. Biological Inorganic Chemistry: Structure and Reactivity; Harry B. Gray, Edward I. Stiefel, Joan Selverstone Valentine, Ivano Bertini, University Science Book; 2006
4. Specific Review Articles to be collected from Internet.

C557: Nuclear Magnetic Resonance

1. **Classical NMR Spectroscopy:** Nuclear magnetism, Bloch equations, chemical shift, linewidth, scalar coupling [4]
2. **Theoretical description of NMR spectroscopy:** Expectation value of magnetic moment, density matrix, pulses and rotation operator, chemical shift and coupling Hamiltonians, concept of coherence, one pulse experiment. [5]
3. **Product Operator Formalism:** Operator spaces, basis operators, free precession, pulses, single and multiple quantum coherences, application of POF to study spin echo and standard polarization transfer protocols like INEPT. [6]
4. **Practical aspects of NMR spectroscopy:** Tuning, matching, shimming, temperature calibration, spectrum referencing, sampling theorem, quadrature detection, Fourier transformation, zero filling, apodization, phasing, signal to noise ratio, spin decoupling, pulse field gradients, water suppression, one dimensional experiments. [14]
5. **Two dimensional NMR experiments:** Two dimensional spectroscopy, coherence transfer, COSY, double quantum filtered COSY, TOCSY, NOESY, HSQC, HMQC, sensitivity enhanced HSQC. [10]
6. **Higher dimensional NMR experiments:** Need for higher dimensional experiments, HNCA, HN(CO)CA, introduction to the new trend of fast multidimensional experiments: GFT, spatially spatial encoding. [3]

Recommended Books:

1. Protein NMR Spectroscopy, 2nd Ed, John Cavanagh, W. J. Fairbrother, A. G. Palmer III, M. Rance and N. J. Skelton, Elsevier academic press, 2007
2. Spin dynamics 2nd Ed., Malcolm H. Levitt, John Wiley and sons Ltd., 2008

C558: Advanced Functional Materials

1. **Introduction to Materials in Modern Technology:** Materials as an enabling element of technological progress. Functions that materials perform. The properties - structure - processing connection. [2]
2. **Semiconductor Materials:** Intrinsic semiconductors, Band Structure of Semiconductors, Impurity Semiconductors, II-V and II-VI compounds, Hall effect, SC devices. Charge carrier dynamics in semiconductor nanomaterials. [10]
3. **Dielectric Materials:** Dielectric constant and polarizability, Insulating materials, Ferroelectrics, Piezoelectrics, Measurement of Dielectric properties, Applications. [6]
4. **Nanosized Magnetic Materials:** Basic concepts of magnetism. Types of magnetic behavior, Magnetic domains, soft and hard magnets, Classification Magnetic Nanomaterials, Ferrofluids, Single-domain particles, Physical Properties of Magnetic Nanostructures, Nanomagnetism for Biological Applications. [6]
5. **Polymer materials and nano-composites:** Classification of Polymers, Structure-Property Correlation, Molecular weights, Conduction in polymers, Natural composites, Incorporation of Nanomaterials into Polymer Media, Organic Polymer nanocomposites, Metal and Ceramic composites, Clay Nanocomposite Materials, Polymer-Clay Nanocomposites, Polymer/graphite nanocomposites, Polymer Composites with Carbon Nanotubes. [10]
6. **Amorphous and Porous Materials:** Crystalline vs. Amorphous Solids, Glass Formation, Structural Models of Amorphous Materials, Properties of Metglasses, Evolution and Development of Porous Materials, Chemistry of Microporous Materials, Mesoporous Materials, Semiconductor Nanoparticles in Zeolites, Polymers and Carbon Materials in Zeolites. [10]

Recommended Books:

1. Fundamental of Nanotechnology, Gabor L. Hornyak, John J. Moore, Harry F. Tibbals, Joydeep Dutta, CRC press, Taylor & Francis Group, 2009
2. Optical Properties and Spectroscopy of Nanomaterials, Jin Zhng Zhang, World Scientific Publishing Co. Pte. Ltd, 2008.
3. Science of Engineering Materials and Carbon Nanotubes, C. M. Srivastava, C. Srinivasan, New Age International Publishers.
4. Optimization of Polymer Nanocomposite Properties, Edited by Vikas Mittal, WILEY-VCH Verlag GmbH & Co. KGaA, Weinheim, 2009.
5. Chemistry of Zeolites and Related Porous Materials: Synthesis and Structure RUREN XU, WEN-QIN PANG, JIHONG YU, QISHENG HUO, JIESHENG CHEN, John Wiley & Sons (Asia) Pte Ltd, 2007.
6. Polymer Nanocomposites Handbook Rakesh K. Gupta Elliot Kennel Kwang-Jea Kim, CRC press, Taylor & Francis Group, 2008.

C559: Supramolecular Chemistry

1. **Introduction:** Understanding of Supramolecular Chemistry (Multidisciplinary Nature, Complementarities in biology); Selectivity; Supramolecular Interactions; Chelate and Macrocyclic Effects; Characterizing Supramolecular Systems; Structural, Kinetic and Thermodynamic. [6]
2. **Molecular Self-assembly:** Non-Covalent Interactions: Electrostatic, Hydrogen Bonding, $\pi-\pi$ Stacking, Dispersion and Induction Forces, Hydrophobic or Solvophobic Effects, π -Electron Donor-Acceptor Systems, Catenanes and Rotaxanes, Transition Metal Directed Assemblies; Molecular Macrocycles and Boxes: Locked and Unlocked Molecular Boxes, Ladders and Grids, Cages; Hydrogen Bond Directed Assemblies: Rosettes and Ribbons, Peptide Nanotubes; Self-Replicating Molecular Systems. [12]
3. **Synthesis of Macrocycles:** High Dilution Technique; Coordination Template Effects; Cation Binding and De-Metallation; Porphyrins; Corrins; Crown Ethers; Cryptands; Spherands; Sepulchrates; Siderophores; Calixarenes. [4]
4. **Molecular Sensors of Ions and Molecules:** Anions, Cations and Neutral Molecules Receptor Design Principles: Recognition by Electrostatic and Hydrogen Bonding, Lewis Acidic Hosts Interactions etc.; Introduction to Fluorescence Probing Techniques and Applications: Fluorescent Molecular Sensors of Ions and Molecules, Logic Gate etc.; Expanded Porphyrins, Amide Functionalized Metallo Compounds, Cyclophanes, Electrostatics and Hydrophobicity, Hydrogen Bond Receptors, Chiral Recognition; Hydrophobic Effect: Recognition In Water; Solvent Effect; Cyclodextrins; Calixarenes; Metallo Receptor For Nucleic Acid Bases; Boronic Acid Receptors for Sugars. [20]

Recommended Books:

1. D. J. Cram and J. M. Cram, Container Molecules and their Guest, Monographs in Supramolecular Chemistry, Ed. J. F. Stoddart, The Royal Society of Chemistry, Cambridge, 1994.
2. J. M. Lehn, Supramolecular Chemistry: Concepts and Perspectives, VCH, Weinheim, 1995.
3. Comprehensive Supramolecular Chemistry, Ed. J. L. Atwood, J. E. D. Davies, D. D. MacNicol, F. Vogtle, Volumes 2 and 3, Elsevier Science, Oxford, 1996.
4. Supramolecular Chemistry of Anions, Ed. A. Bianchi, K. Bowman-James, E. Garcia-Espana, John Wiley and Sons, New York, 1997.
5. Supramolecular Chemistry, P. D. Beer, P. A. Gale and D. K. Smith, Oxford University Press, 1999.
6. A Practical Guide to Supramolecular Chemistry, Peter J. Cragg, John Wiley & Sons Ltd, England, 2005.

C560: Chemistry of Nanomaterials

1. **Introduction:** Nano and nature, Fascination and Motivation of Nanoparticle Research, Bottom-up and Top-down approaches [3]
2. **Zero and One-Dimensional Nano structures:** Introduction, Aqueous and Non-aqueous Sol-Gel Chemistry, Surfactant-Assisted Synthesis, Solvent-Controlled Nanoparticles, Assembly: Introduction, Oriented Attachment and Mesocrystals, Superlattices, Core-Shell nanoparticles: Introduction, Types of Systems, Characterization, Properties. [10]
3. **Carbon Nanomaterials:** Fullerenes and their Derivatives, Carbon Nanotubes: Structure and Properties, Nanocrystalline Diamond [8]
4. **Self Assembled Monolayers:** Introduction, Monolayers on Gold, Growth process, Phase transitions, Patterning monolayers, Mixed Monolayers Structure, Electrochemistry and Applications of Self-Assembled Monolayers of Thiols [4]
5. **Nano and Micro-emulsion:** Surface Active Agents, Micellization, Mechanism of emulsion, Characterization of Micro-emulsion [8]
6. **Application of Nanomaterials:** Solar Energy Conversion, Molecular and Nanoelectronics, Nanocatalysis, Biological Applications and other Applications. [12]

Recommendend Books:

1. Nanoparticles: Synthesis, Stabilization, Passivation, and Functionalization, Edited by R. Nagarajan, T. Alan Hatton, ACS SYMPOSIUM SERIES 996.
2. Metal Oxide Nanoparticles in Organic Solvents, Markus Niederberger and Nicola Pinna, Markus Niederberger and Nicola Pinna, Springer-Verlag London Limited 2009 .
3. Fundamental of Nanotechnology, Gabor L. Hornyak, John J. Moore, Harry F. Tibbals, Joydeep Dutta, CRC press, Taylor & Francis Group, 2009.
4. Carbon Nanomaterials, Advanced Materials Series, Edited by Yury Gogotsi, Taylor and Francis Group, LLC, 2006.
5. Carbon Nanotubes and Related Structures, Edited by Dirk M. Guldi and Nazario Martín, WILEY-VCH Verlag GmbH & Co. KGaA, Weinheim, 2010.
6. Nano: The essential, Understanding nanoscience and nanotechnology, T. Pradeep, Tata McGraw-Hill Publishing Company Limited.
7. Applied Surfactants, Thrwat F. Tadros, WILEY-VCH Verlag GmbH & Co. KGaA, Weinheim, 2006.

C561: Advanced Bio-organic Chemistry

1. **Enzymology:** Mechanistic studies of enzymatic reactions. Studies of enzyme kinetic for substrate/inhibitors (reversible/irreversible) and their future aspects in drug design. The role of cofactors and hormones in enzymatic reactions. Enzymes as Catalysts in organic chemistry reaction (Group Transfer Reactions, Reduction and Oxidation; Monooxygenation; Dioxygenation Substitutions, Addition/Elimination; Carboxylations; Decarboxylation; Isomerizations; Aldol and Claisen Reactions; and Retroreactions; Formylations, Hydroxymethylations, and Methylations; Rearrangements. [12]
Application of Enzyme Kinetics: Substrate Kinetics; Kinetics of Enzyme Inhibition; Substrate Inhibition; Nonproductive Binding; Competing Substrates; Multi-substrate Systems; Allosterism and Cooperativity. [5]
2. **Biosynthesis of secondary metabolites:** Polyketide Biosynthesis; Saccharide Biosynthesis; Shikimate Pathway (PDF); Shikimate Pathway Flavonoids ; Alkaloid Biosynthesis; Alkaloid Bioynthesis: Tyrosine Derivatives; Terpene Biosynthesis with example-Taxol, vancomycine, penicillin and other recent discovered natural products. Design and synthesis of modified secondary metabolites analogues. Isotope labeling (radioactive/non radioactive) and their application in biosynthetic pathways. [12]
3. **Non-natural bio-active molecules:** Synthesis and importance of these amino acids (β, γ & δ), non-ribosomal peptides and nucleotides (PNA, LNA, TNA & other stable analogues). [5]
4. **Introduction of vital bio-macromolecule secondary structures:** G-Quadruplex, i-motif, RNAi (mi-RNA & si-RNA) & Collagen and their application in therapeutics. [5]

Recommendend Books:

1. Organic Chemistry of Enzyme-Catalyzed Reactions, Revised Edition by Richard Silverman Published: FEB-2002. ISBN 10: 0-12-643731-9. ACADEMIC PRESS
2. Structure and Mechanism in Protein Science: A Guide to Enzyme Catalysis and Protein Folding by Alan Fersht, Publisher: W. H. Freeman; 1st edition (September 15, 1998)
3. Evaluation of Enzyme Inhibitors in Drug Discovery: A Guide for Medicinal Chemists and Pharmacologists (Methods of Biochemical Analysis); by Robert A. Copeland, Publisher: Wiley-Interscience; 1 edition (March 28, 2005).
4. Dewick, Paul M. Medicinal Natural Products: A Biosynthetic Approach. 2nd ed. New York, NY: John Wiley & Sons, Inc., 2001. ISBN: 9780471496410 (paperback);
5. Structural Diversity of G-Quadruplex Scaffolds; Stephen Neidle and Shankar Balasubramanian, CRC Press Copyright Year-2006.
6. Gene Silencing by RNA Interference: Technology and Application, by Muhammad Sohail (Editor), CRC Press; 1 edition (July 26, 2004).
7. Modified Nucleosides: in Biochemistry, Biotechnology and Medicine (ed P. Herdewijn), Wiley-VCH Verlag GmbH & Co. KGaA, Weinheim, Germany.
8. Natural Products: The Secondary Metabolites , James R. Hanson Copyright Year:2003. ISBN: 978-1-84755-153-5

C562: Polymer Chemistry

1. Classification of polymers, Nomenclature of polymers, Synthesis of polymers using different methods, viz chain polymerization, step polymerization, ring-opening polymerization etc. Polymerization techniques, viz Bulk polymerization, Solution polymerization, Suspension polymerization, Emulsion polymerization etc. [10]
2. Polymer characterization, Molecular weight-number average, weight average; significance of molecular weight; methods of characterizing molecular masses, GPC, Viscosity, Mass analysis, end-group analysis, Thermal properties - melting point, glass transition temperature (T_g), factors influencing T_g, relation between T_g and molecular weight. Crystallinity in polymers - degree of crystallinity in polymers, structural regularity and crystallinity. [15]
3. Kinetics of polymerization, free-radical, cationic and anionic polymerization and polycondensation. [5]
4. Copolymerization, free-radical and ionic copolymerization and copolycondensation [5]
5. Stereochemistry of polymerization, types of stereoisomerism in polymers, properties of stereoregular polymers, different methods for the synthesis of stereoregular polymers. Less traditional approaches: ATRP, RAFT, ROMP, Surface functionalization of polymers [5]
6. Biodegradable polymers: Synthesis and challenges [3]

Recommendend Books:

1. Odian, G. Principles of Polymerization. 4th ed. Hoboken, NJ: Wiley-Interscience, 2004.
2. Allcock, H. R., Lampe, F. W. in Contemporary Polymer Chemistry; Prentice-Hall: Engelwood Cliffs, NJ, 1990
3. Billmeyer Jr. F. W. Textbook of Polymer Science Wiley - Inter Science.

C563: Molecular Reaction Dynamics

1. **Introduction:** The rate constant - History and current view. What is molecular reaction dynamics? [2]
2. **Theoretical Methods I:** Transition State Theory (TST), RRKM Theory. [5]
3. **Theoretical Methods II:** Rate and cross-section, Classical scattering theory, Quantum scattering theory (reactive and non-reactive), Connection to TST and RRKM. [10]
4. **Experimental Methods:** Newton's diagrams, Molecular Beams, State-resolved spectroscopic techniques, Imaging techniques. [8]
5. **Applications:** Photoselective chemistry - photodissociation and photoisomerization dynamics, Dynamics in real time (ps, fs and attosecond regimes), Molecular energy transfer, Control of chemical reactions, Condensed phase dynamics, Dynamics of gas-surface reactions. [15]

Recommend Books:

1. R. D. Levine, Molecular Reaction Dynamics Cambridge University Press, NY 2005.
2. J. I. Steinfeld, J. S. Francisco and W. L. Hase, Chemical Kinetics and Dynamics, Prentice Hall Inc., NJ, 1999.
3. Journal articles.

C564: Theory of Molecular Spectroscopy

1. **Recap:** Introduction and review of basic quantum mechanics, molecular symmetry. [3]
2. **Rovibronic Hamiltonian - Coordinates and momenta:** Euler angles, axis systems, rotational and vibrational angular momentum, normal and internal coordinates, the **G** matrix, the **GF** matrix. [8]
3. **Rovibronic wavefunctions:** Classification of rotational, vibrational, rotation-vibration, and electronic wavefunctions, Hund's cases. [6]
4. **Energy levels and interaction:** Rotation-vibration interactions, vibronic and rovibronic interactions, Renner-Teller and Jahn-Teller effect, Rydberg states, spin effects. [8]
5. **Transition intensities and Optical selection rules.** Electric - magnetic dipole electric quadrupole transitions, multiphoton processes and Raman effect. [7]
6. **Advanced topics** Spectroscopy at high energies, intramolecular vibrational energy redistribution (IVR), wave-packet approach to spectroscopy. [8]

Recommend Books:

1. P. R. Bunker and P. Jensen, Molecular Symmetry and Spectroscopy, NRC Research Press, Ottawa.
2. J. D. Graybeal, Molecular Spectroscopy, McGraw-Hill.
3. P. F. Bernath, Spectra of Atoms and Molecules, Oxford University Press, NY, 1995.
4. E. B. Wilson, J. C. Decius and P. C. Cross, Molecular Vibrations: The Theory of Infrared and Raman Vibrational Spectra, Dover, NY, 1955.

C565: Advanced Organic Chemistry

Review of Basic Bonding Concepts; Conformational Analysis; Stereochemistry; Kinetics and Thermodynamics of Organic Reactions; Reaction Mechanisms and Conformational Effects on Reactivity; Oxidation Reactions; Reductions Reactions; Enolate Chemistry; Metalation Reactions; Key Ring Forming Reactions; Olefin Synthesis; Conjugate Additions; Synthetic Analysis and Design; Total Synthesis of Natural Products; Asymmetric Synthesis; Combinatorial Chemistry.

Recommendend Books:

1. E. V. Anslyn, D. A. Dougherty "Modern Physical Organic Chemistry" California University Science Books, 2006.
2. E. L. Eliel, S. H. Wilen "Stereochemistry of Organic Compounds" Wiley-Interscience, 1994.
3. R. Bruckner "Organic Mechanisms: Reactions, Stereochemistry and Synthesis" Springer, 2010.
4. F. A. Carey, R. J. Sundberg "Advanced Organic Chemistry Parts A & B: Structure and Mechanisms" 5th Edition, Springer, 2007.
5. M. B. Smith, J. March "Marchs Advanced Organic Chemistry" 6th Edition, Wiley-VCH, 2007.
6. E. J. Corey, X.-M. Cheng "The Logic of Chemical Synthesis" Wiley-Interscience, 1995.
7. T. Hudlicky, J. W. Reed "The Way of Synthesis: Evolution of Design and Methods for Natural Products" Wiley-VCH, 2007.
8. P. Wyatt, S. Warren "Organic Synthesis: Strategy and Control" Wiley, 2007.
9. M. Christmann, S. Bräse Eds "Asymmetric Synthesis- The Essentials" 2nd Edition, Wiley-VCH, 2008.
10. K. C. Nicolaou, R. Hanco, W. Hartwig Eds. "Handbook of Combinatorial Chemistry", VCH-Wiley, Weinheim 2002.

C566: Catalysis: Reaction Mechanisms and Applications

1. Introduction to catalysis; fundamental concepts. [5]
2. Survey of ligands; Characteristics of the transition-metal in the complexes; Elementary steps. [10]
3. Reaction mechanisms and applications: Carbonylation, Hydroformylation, Hydrogenation, metathesis reactions, oxidation reactions, Isomerization reactions, Cross-Coupling reactions, and C-H functionalization reactions. [20]
4. Examples of synthetic and industrial applications. [5]

Recommendend Books:

1. The Organometallic Chemistry of the Transition Metals. R. H. Crabtree, John Wiley & Sons, 2005.
2. Industrial Catalysis. J. Hagen, Wiley-VCH, 2006.
3. Homogeneous Catalysis. P. W. N. M. van Leeuwen, Kluwer Academic Publishers, 2004.
4. Homogeneous Catalysis. S. Bhaduri, D. Mukesh, John Wiley & Sons, 2000.
5. Metal-Catalyzed Cross-Coupling Reactions A. de Meijere, F. Diederich (Eds.), 2004.
6. Catalysts for Fine Chemical Synthesis. S. M. Roberts, G. Poignant, John Wiley & Sons, 2002.
7. Catalysis of Organic Reactions, S.R. Schmidt, CRC Press, 2007

C567: Advanced Main Group Chemistry

1. (a) Direct bonds between metal atoms: Mg and Ca compounds with metal-metal bonds (b) Multiple bonded group 13, 14 and 15 elements: Synthesis, reactivity and bonding [12]
2. NHC stabilized low oxidation state main group metal complexes [4]
3. Low oxidation state main group metal hydrides: synthesis and reactivity [4]
4. NHCs analogues with low valent group 13 and 14 elements: Synthesis, structure and reactivity studies; (a) Boron(I), Aluminum(I), Gallium(I), Indium(I) and Thallium(I) heterocycles (b) Silicon(II), Germanium(II), Tin(II), and Lead(II) heterocycles [8]
5. Role of main group compounds in catalysis, organic synthesis and medicinal chemistry [8]
6. Inorganic New Materials: Nanomaterials, polymers and chemical sensors [6]

Recommendend Books:

1. Inorganic Chemistry-Principles of Structure and Reactivity. 4th Edn. Huheey J. E.; Keiter, E. A.; and Keiter, R. L. Harper-Collins, NY, 1993
2. Concepts and Models of Inorganic Chemistry. 3rd Edn. Douglas, B.; McDaniel, D.; and Alexander, J. John Wiley, New York. 1993
3. Chemistry of the Elements. 2nd Edn. Greenwood, N. N.; and Earnshaw, A. Pergamon, Oxford, 1989
4. Organometallics: A Concise Introduction, C. Elschenbroich and A. Salzer, 3rd Edn. 1999
5. Inorganic and Organometallic Polymers. Chandrasekhar, V. Springer-Verlag, Heidelberg, 2005
6. Journal articles

C568: Advanced Fluorescence Spectroscopy

1. Phenomena of Fluorescence and Instrumentation for Fluorescence Spectroscopy: Introduction. Jablonski Diagram, Characteristics of Fluorescence Emission, Fluorescence Lifetimes and Quantum Yields. Spectrofluorometers, Light Sources, Monochromators, Optical Filters, Photomultiplier Tubes, Polarizers. [5]
2. Fluorophores: Intrinsic or Natural Fluorophores; Fluorescence Enzyme Cofactors, Extrinsic Fluorophores; Protein-Labeling Reagents, Membrane Probes, Red and Near-Infrared (NIR) Dyes, DNA Probes, Chemical Sensing Probes, Viscosity Probes, Green Fluorescent Proteins, Long-Lifetime Probes. Quantum Dots. [4]
3. Life-Time Measurements: Time-Domain and Frequency- Domain Measurements. Time-Correlated Single-Photon Counting; Principle and Instrumentation, Alternative Methods for Time-Resolved Measurements; Streak Cameras, Upconversion Methods. Data Analysis. [6]
4. Some Important Photo-processes: Dynamics of Solvent and Spectral Relaxation: Measurement of Time-Resolved Emission Spectra (TRES), Theory for Time-Dependent Solvent Relaxation, Fluorescence Quenching: Theory, Fractional Accessibility to Quenchers, Applications of Quenching to Proteins; Fluorescence Anisotropy: Origin of the Definitions of Polarization and Anisotropy, Measurement of Fluorescence Anisotropies, Causes of Depolarization, Biochemical Applications. Energy Transfer: Theory of Energy Transfer for a Donor-Acceptor Pair, Distance Measurements Using Resonance Energy Transfer (RET), Biochemical Applications of RET. [12]
5. Multiphoton Excitation: Introduction to Multiphoton Excitation, Two-Photon Absorption Spectra, Cross Section for Multi-photon Absorption. [3]
6. Single-Molecule Detection (SMD): Detectability of Single Molecules, Instrumentation for SMD, Single-Molecule Photophysics, Biochemical Applications of SMD. [3]
7. Fluorescence Correlation Spectroscopy(FCS): Principles of Fluorescence Correlation Spectroscopy, Theory of FCS, Examples of FCS Experiments. [3]
8. Fluorescence-Lifetime Imaging Microscopy(FLIM):Early Methods for Fluorescence-Lifetime Imaging, Laser Scanning TCSPC FLIM, Lifetime Imaging of Cellular Biomolecules. [3]
9. Radiative Decay Engineering: Introduction to Radiative Decay Engineering, Review of Metal Effects on Fluorescence, Surface Plasmon-Coupled Emission(SPCE), Applications of Metal-Enhanced fluorescence, Application of SPCE. [3]

Recommendend Books:

1. Principles of Fluorescence Spectroscopy, Joseph R. Lakowicz, 3rd Edition, Springer, 2006
2. Advanced Time-correlated Single photon Counting Techniques, W. Becker, Springer, 2005
3. Molecular Fluorescence Principles and Applications, B. Valeur, WILEY-VCH, 2002
4. Single-Molecule Detection in Solution. Methods and Applications, C. Zander, R. A. Keller, and J. Enderlein, WILEY-VCH, 2001

C569: Bio-macromolecules

1. Buffers (their use in study of biomolecules), pH, pKa of amino acids, D and L amino acid nomenclature [1]
2. Biophysical techniques to purify and study proteins: Dialysis, salting out and precipitation by organic solvents, Ion exchange, gel filtration, reversed phase, affinity chromatography, ultracentrifugation, gel electrophoresis [3]
3. Proteins: protein sequencing by chemical and mass & NMR spectroscopic methods, Use of spectroscopic tools in studying biomolecules. Primary (single letter amino acid codes), Ramachandran plot, secondary structures like helices, parallel and antiparallel -sheets, circular dichroism of secondary structures, tertiary (motifs and domains: some important motifs like Rossmann fold, helix turn helix, 4 helix bundles, beta barrel), quaternary structure (Hemoglobin and Myoglobin) and Enzymes [21]
4. Nucleic acids: A, B and Z-DNA structures, Method of replication, sequencing of nucleic acids (Chemical, dideoxy and fluorescence), Transcription, Translation, genetic code, genomes, Genes, over expression of recombinant proteins, mutagenesis (random and site directed). Polymerase chain reaction (PCR) [9]
5. Carbohydrates and Glycoproteins, proteoglycans, Membranes and lipids, bacterial cell wall synthesis and mechanism of some important antibiotics like penicillin, antibiotic resistance [4]
6. Metabolism: Photosynthesis, Calvins cycle, Glycolysis, Krebs cycle, electron transport, cofactors. [4]

Recommendend Books:

1. Voet, D, Voet, JG, Pratt, CW Fundamentals of biochemistry: life at the molecular level, 2nd Edition, 2006
2. Berg J.M, Tymoczko J.L. and Stryer L. Biochemistry, 6th Edition, 2007
3. Creighton, TE, Proteins: structure and molecular properties, 2nd edition, 1993
4. Lewin B. Genes IX, 2008
5. Branden C and Tooze J., Introduction to protein structure, 2nd Edition, 1999.
6. Fersht A., Structure and mechanism in protein science: a guide to enzyme catalysis and protein folding, 1999

C570: Advanced Heterocyclic Chemistry

1. Introduction: Heterocyclic Chemistry Introduction to heterocycles: Nomenclature, spectral characteristics, reactivity and aromaticity. [2]
2. Synthesis and reactivity of three and four membered heterocycles e.g., aziridine, azirine, azetidine, oxiranes, thiarines, oxetenes and thietanes. [4]
3. Synthesis and reactivity of five membered rings with two heteroatoms: pyrazole, imidazole, oxazole, thiazole, isothiazole and benzofused analogs; Benzofused five membered heterocycles with one heteroatom, e.g., indole, benzofuran, benzothiophene. [8]
4. Synthesis and reactivity of benzofused six membered rings with one, two and three heteroatoms: benzopyrans, quinolines, isoquinoline, quinoxaline, acridine, phenoxazine, phenothiazine, benzotriazine, pteridines. [8]
5. Synthesis and reactivity of seven and large membered heterocycles: azepines, oxepines, thiepinines; spiro heterocycles; bicyclic compounds containing one or more heteroatoms [4]
6. Recent methods of C-H functionalization/activations of heterocyclic derivatives. [16]

Recommendend Books:

1. Carey, F.A. & Sundberg, R. J. Advanced Organic Chemistry, Parts A & B, Plenum: U.S. 2004
2. Thomas. L. Gilchrist, Heterocyclic chemistry, (3rd Edition) 1997
3. Joules, J. A; Mills, K.; Smith, G. F. Heterocyclic Chemistry, 3rd Ed.
4. Advances in Heterocyclic Chemistry, Book series Elsevier Edited by Alan Katritzky
5. Branden C and Tooze J., Introduction to protein structure, 2nd Edition, 1999.
6. Journal articles

3 Laboratory Courses

C141: Chemistry Laboratory I

1. Determination of acid-neutralizing power of commercial antacids.
2. Estimation of phosphoric acid in cola drinks by molybdenum blue method.
3. Element detection and characterization of organic compounds.
4. Extraction of Caffeine, an alkaloid, from Tea Leaves.
5. Synthesis of Aspirin.
6. Identification of unknown mixtures containing 4 radicals, by dry and wet tests.
7. Photochemical reduction of ferric oxalate in cyanotype blue printing.
8. Synthesis of hexamminenickel(II) chloride.
9. Synthesis of paracetamol.
10. Estimation of acid strength in a citrus fruit.

Recommended Books:

1. The Systematic Identification of Organic Compounds, R. L. Shriner, C. K. F. Hermann, T. C. Morrill, D. Y. Curtin and R. C. Fuson, John Wiley, 8th Edn., 2004.
2. Practical Organic Chemistry, A. I. Vogel, ELBS, 2002.
3. Laboratory Manual in Organic Chemistry, R. K. Bansal, Wiley Eastern, 1980.
4. Comprehensive Practical Organic Chemistry : Qualitative Analysis, V. K. Ahluwalia and S. Dhingra, Universities Press (India) Ltd, 2000.
5. A Collection of General Chemistry Experiments, A. J. Elias, Universities Press, 2007.

C142: Chemistry Laboratory II

1. Determination of Critical Solution Temperature (CST) of Phenol-Water system. Study the effect of added impurity (NaCl) on CST.
2. Determine the solubility of oxalic acid (benzoic acid) in water at different temperatures. Calculate the heat of solubilization (ΔH).
3. Determination of partition coefficient of acetic acid in water and butanol.
4. Study the kinetics of acid catalysed hydrolysis of methyl acetate in the presence of HCl and H₂SO₄. Determine the order with respect to [acid], and compare the strengths of the two acids.
5. Standardization of pH meter. Titration of strong acid against strong base, using the pH meter.
6. (i) Calibrate the conductometer by using standard KCl solution. (ii) Titrate a solution of a strong acid; weak acid; and a mixture of the two acids, conductometrically, against a standard alkali.
7. Verification of Debye-Huckel-Onsager equation $\Lambda = \Lambda_0 - S\sqrt{C}$ for strong univalent electrolytes.
8. Estimation of calcium in milk powder through EDTA complexometry.
9. Verification of Beer - Lamberts Law: Determination of the concentration of coloured solutions of copper sulfate and potassium dichromate.
10. Estimation of potassium ions in coconut water, by Flame Photometry.
11. Estimation of cane sugar by polarimetry.

Recommended Books:

1. Experimental Physical Chemistry, R. C. Das and B. Behera, Tata McGraw Hill, 1983.
2. Practical Physical Chemistry, A. Findlay and J. A. Kitchener, 8th Edn., Longmans, 1967.
3. A Collection of Interesting General Chemistry Experiments, A. J. Elias, Universities Press, 2007.

C241: Chemistry Laboratory III

1. Standardisation of sodium thiosulphate solution and volumetric estimation of Cu(II) iodometrically.
2. Volumetric estimation of Zn(II), Ca(II) and Mg(II) by EDTA titration, using Eriochrome black-T indicator.
3. Gravimetric estimation of Nickel(II), using dimethylglyoxime.
4. Estimation of : (a) total manganese content in manganese ore (pyrolusite); (b) total iron content in Fe_2O_3 (haematite).
5. Study of the composition of ferric-sulfosalicylic acid complex by Jobs method of continuous variation, and to determine the stability of the complex, spectrophotometrically.
6. Determination of the composition of a binary mixture (potassium Dichromate and potassium permanganate), spectrophotometrically.
7. To study the luminescence behaviour of quantum dots using Photoluminescence Spectrophotometer.
8. Synthesis of 3,5-dimethyl pyrazole.
9. Synthesis of antipyrene from ethyl acetoacetate.
10. Synthesis and characterization PhNacnacH ligand.
11. Synthesis of 1,3-disubstituted bulky aryl thiourea.
12. Extraction and identification of DNA from green peas and onions.
13. Synthesis of Rinecke Salt, $NH_4[Cr(NCS)_4(NH_3)_2].H_2O$, and study of its UV-Visible and IR spectra.
14. Synthesis of antipyrene from ethyl acetoacetate.
15. TLC

Activity I: Selection of solvent for TLC (known compound/unknown compound).

Activity II : Separation of compounds using TLC (e.g. o- and p- nitroaniline) separation using appropriate solvent systems.

Activity III: Separation of components present in Turmeric powder extract (alcohol) or spinach extract using TLC and Column Chromatography (silica columns at microscale level can be Prepared; 10 ml syringe can be used).

Recommendend Books:

1. Vogels Text Book of Qualitative Chemical Analysis, G. H. Jeffery, J. Bassett, J. Mendham and R. C. Denny, 5th Edn., ELBS, 1991.
2. Vogels Text Book of Quantitative Chemical Analysis, G. H. Jeffery, J. Bassett, J. Mendham and R. C. Denny, 5th Edn. , ELBS, 1991.

C242: Electronics Laboratory

1. Familiarization with multimeters, power supplies, function generators, Oscilloscopes; Identification of various components, e.g. resistors, diodes, capacitors etc.
2. Study of I-V characteristics of a linear and a nonlinear resistor.
3. Study of normal and zener Diode characteristics.
4. Study of passive filters and phase shifting RC series network.
5. Study of Half wave rectifier with filters.
6. Study of Full wave rectifier with filters.
7. Application of zener diode as a voltage regulator in power supply.
8. Study of transistor characteristics (CB, CE mode).
9. Study of a single stage common emitter transistor amplifier.

Recommendend Books:

1. Electronics principles, A. Malvin, D. J. Bates, Career Education, 1998.
2. Electronic devices and circuit theory, R. L. Boylestad, L. Nashelsky, Prentice Hall, 2008.

C243: Physical Chemistry Laboratory I

1. Study of the pH dependence of uv-visible spectrum of 4-nitrophenol/methyl orange and determination of its pK by spectrophotometric method.
2. Study of the kinetics of inversion of cane sugar, catalyzed by acid, polarimetrically.
3. Study of the dimerization of benzoic acid by partition method.
4. Adsorption of acetic acid on activated charcoal, and verification of Freundlich / Langmuir adsorption isotherm.
5. Verification of Beer-Lambert's Law and determination of the dissociation constant (pK_a) of methyl red, spectrophotometrically.
6. Study of the phase diagram of a two-component system (diphenylamine-benzophenone) with congruent melting point.
7. Determination of the isotherm for a three-component system (diphenylamine-acetic acid-water).
8. Determination of glass transition temperature of hydrated calcium nitrate, conductometrically.
9. Estimation of halides in a mixture of halides by potentiometric titrations.
10. Study of the Solvent Effects on the fluorescence of fluorescein and other fluorescent molecules.
11. Synthesis and chemiluminescence of Luminol.
12. Estimation of halides in a mixture of halides, by potentiometric titrations.
13. Study of the kinetics of the iodide - hydrogen peroxide clock reaction.
14. Study of the photochromic and kinetic behaviour of a nitrospiropyran derivative.
15. Determination of the bond lengths of diatomic and triatomic molecules, and functional group determination of small molecules, using the FT-IR spectrometer.
16. Laser : Measurement of wave length of light emitted by He-neon laser from the interference spectrum of Fresnel's biprism and mirror.

Recommendend Books:

1. Experimental Physical Chemistry, R. C. Das and B. Behera Tata McGraw-Hill, 1983.
2. Practical Physical Chemistry, A. Findlay and J. A. Kitchener, 8th Edn., Longmans, 1967.
3. A Collection of Interesting General Chemistry Experiments, A. J. Elias, Universities Press, 2007.

C244: Biomolecular Chemistry Laboratory

1. Analysis of kidney stones by permanganometric titration.
2. Determination of strength of acid in lemon juice.
3. Kinetics of an enzyme catalysed reaction--chymotrypsin catalysed hydrolysis of an ester, p-nitrophenyl trimethylacetate.
4. Identification of sugars present in fruit juice by TLC.
5. Determination of the pKs of an amino acid (pK1 and pK2) by potentiometric titration.
6. Estimation of carbohydrates by anthrone method.
7. Determination of the free amino acid end group of some proteins, using Sangers reagent.
8. Determination of iodine number of a fat.
9. Determination of isoelectric point of glycine.
10. Separation of sugar in a solution by TLC.
11. Estimation of iodine in the iodized common salt by iodometry.
12. Estimation of ascorbic acid content in commercially available celin sample.
13. Paper and column chromatography of plant pigments : Extraction and separation of Chlorophyll a and Chlorophyll b.

Recommendend Books:

1. An Introduction to Practical Biochemistry, D. T. Plumer, Tata McGraw Hill, 2000.
2. A Collection of Interesting General Chemistry Experiments, A. J. Elias, Universities Press, 2007.
3. Experimental Physical Chemistry : A Laboratory Textbook, A. M. Halpern and G. C. McBane, W. H. Freeman and Company, New York, 2006.

C341: Organic Chemistry Laboratory I

Organic Synthesis and Analysis

1. Separation of organic compounds from a mixture of compounds using the techniques of solvent extraction, preparative TLC and column chromatography and identification of the individual components by spectroscopic techniques (IR, NMR, UV-VIS), preparation of dry solvents.
2. Synthesis of the following compounds using name reactions :
 - (a) Diels-Alder reaction of Anthracene and Maleic anhydride
 - (b) Synthesis of Cinnamic acid from Benzaldehyde (Perkin reaction)
 - (c) Synthesis of Triphenyl Carbinol (Grignard Reaction)
 - (d) Synthesis of 2-hydroxy-5-methyl benzophenone (Fries rearrangement)
 - (e) Synthesis of Benzilic acid from Benzil (Benzil- Benzilic acid rearrangement)
 - (f) Synthesis of p-methoxycinnamic acid (Knoevenagel reaction).
3. Synthesis of Benzanilide from benzophenone oxime (Beckman rearrangement)
4. Synthesis of 2-phenylindole from acetophenone phenylhydrazone (Fischer-Indole synthesis)
5. Protection and deprotection technique: Synthesis of a ketal of cyclohexanone with ethylene glycol and regeneration of the ketone from the intermediate.
6. Esterification of p-methoxycinnamic acid.
7. Preparation of o-benzoylbenzoic acid from phthalic anhydride and benzene.

The following activities also will be included. Use of chemical data base (from Merck or CRC Handbook); use of ISIS/Chemdraw or any other software for drawing structures and indicating mechanisms; use of models for drawing various projections.

Recommendend Books:

1. Vogels Textbook of Quantitative Chemical Analysis, G. H. Jeffery, J. Bassett, J. Mendham and R. C. Denny, 5th Edn., ELBS, 1991.
2. Spectrometric Identification of Organic Compounds, R. M. Silverstein, G. C. Bassler and T. C. Morrill, 6th Edn., Wiley, 1998.
3. A Collection of Interesting General Chemistry Experiments, Anil J. Elias, Universities Press, 2007.
4. Laboratory Manual of Organic Chemistry, B. B. Dey and M. V. Sitaraman, Allied Publishers, 1992.
5. Laboratory Manual of Organic Chemistry, R. K. Bansal, New Age International Publishers, 2006.

C342: Inorganic Chemistry Laboratory I

1. a) Synthesis of $\text{Mn}(\text{acac})_3$ and $\text{Fe}(\text{salen})\text{Cl}$ Complexes.
b) Elucidation of Redox behavior of the $\text{Mn}(\text{III})$ and $\text{Fe}(\text{III})$.
c) Elucidation of magnetic properties
2. Preparation and characterization of (mesitylene) tricarbonyl molybdenum (0).
3. a) Synthesis and characterization of 2,6-bis(diphenylmethyl)-4-methylaniline.
b) Synthesis and characterize compound
 N,N -bis(2,6-bis(diphenylmethyl)4-methylphenyl)diazabutadiene.
4. Synthesis and characterization of the monoanionic and bidentate amidine ligand.
5. a) Synthesis of meso tetratolul porphyrin from pyrrole and p-tolualdehyde.
b) Synthesis and characterization of zinc-porphyrin(meso-tetratolyl porphyrin) complex.
6. a) Preparation of dimethyl ester of pyridine 2,6-dicarboxylic acid.
b) Synthesis and Characterization of
7E N-(1-3(E-1-(2,6-diisopropylphenylimino)ethyl)phenyl)ethylidene)2,6 diisopropylbenzenamine
7. Separation of the chromium complexes by using ion exchange column.
8. Synthesis and study of $\text{Mn}^{\text{III}}(\text{Salen})\text{Cl}$ by Cyclic Voltammetry and Differential Pulse Voltammetry (DPV), and determination of the following: the formal reduction potential (E^o); the number of electrons transferred in the redox process (n); the diffusion coefficient (D); electrochemical reversibility; and the effects of varying concentration (C) and scan rate.
9. Synthesis and analysis of Nanoparticles by using Disc Centrifuge.
10. Preparation and determination of the effective magnetic moment and number of unpaired electrons in $\text{Mn}(\text{acac})_3$.
11. Preparation and determination of the aquation rate of $[\text{Co}(\text{NH}_3)_5\text{Cl}]\text{Cl}_2$.
12. Preparation and resolution of the optically active compound $\text{Co}(\text{en})_3^{3+}$.

Recommend Books:

1. Handbook of Preparative Inorganic Chemistry, Vol. I & II (edited by G. Brauer), Academic Press, 1963.
2. Experimental Electrochemistry for Chemists, D.T. Sawyer and J. L. Roberts, Jr., John Wiley & Sons, New York, 1974.
3. Vogels Textbook of Quantitative Chemical Analysis, G. H. Jeffery, J. Bessett, J. Medham and R. C. Denny, 5th Edn., ELBS, 1999.

C343: Physical Chemistry Laboratory II

1. Synthesis and characterization of fluorescein by absorption and fluorescence spectroscopy.
2. Quantum Yield Calculation for Anthracene.
3. Estimation of Halides in a Mixture of Halides by Potentiometric Titration.
4. Fluorescence Quenching by KI.
5. Solvatochromic study of a Donor Acceptor system.
6. Determination of viscosity - average molecular weight of polyvinyl alcohol, and the fractions of head-to-head monomer linkages in the polymer.
7. Static and Dynamic Fluorescence quenching and verification of the Stern-Volmer relationship.
8. Study of the excited state properties of 2-Naphthol : (a) excited state acidity constant; (b) deprotonation and protonation rate constants in the excited state.
9. Visualization of atomic orbitals and molecular orbitals.
10. Modeling of elimination/migration reaction of Isopropylazide.
11. Computation of the transition state for simple reactions.
12. Structure and vibrational frequency analysis of hydrogen bonded clusters: Water dimer and water trimer structures, naphthal-water hetero clusters.
13. Computation of potential energy profile for the isomerization of n-butane.
14. Calculation of thermodynamic parameters (ΔG° , ΔH° , ΔS°) for the equilibrium $\text{N}_2\text{O}_4 \rightleftharpoons 2\text{NO}_2$.
15. Computational studies on the ground state and excited state properties of some simple molecules.
16. Chemical Dynamics Simulations of simple reactions.

Recommendend Books:

1. Experimental Physical Chemistry, R. C. Das and B. Behera, Tata McGraw Hill, 1983.
2. A Collection of Interesting General Chemistry Experiments, A. J. Elias, Universities Press, 2007.
3. Experimental Physical Chemistry, V. D. Athawale, P. Mathur, New Age International Publishers, 2001.
4. Experimental Physical Chemistry: A Laboratory Textbook, A. M. Halpern, Prentice Hall, 2nd edition, 1997.
5. G. C. McBane, 3rd edition., W. H. Freeman and Company, New York, 2006.
6. <http://cdssim.chem.ttu.edu>

C344: Organic Chemistry Laboratory II

Multistep Synthesis of Organic Compounds and Characterization by Spectroscopic Techniques

1. Phenylacetylene from cinnamic acid (via dibromocinnamic acid and phenylpropionic acid).
2. Friedel Crafts Reaction and Wolff Kishner Reduction : 4-Phenylbutyric acid from benzene (via -benzoylpropionic acid, and reduction of the carbonyl group employing hydrazine hydrate).
3. Nitration, reduction and diazotization reaction : m-hydroxyacetophenone from acetophenone (via m-nitroacetophenone and aminoacetophenone).
4. Dimedone from acetone (via mesityl oxide).
5. 3-Hydroxycoumarin from glycine (via hippuric acid).
6. Quinoline-2-carboxylic acid from aniline (via 2-methylquinoline and ω -tribromoquinolidine).
7. 2-Aminobenzothiazole from aniline (via phenyl thiourea).
8. Synthesis of a drug (Uramil) : Aminobarbituric acid (Uramil) from diethylmalonate (via barbituric acid and nitro barbituric acid).
9. Beckmann Rearrangement : 6-Phenanthridone from fluorenone (via fluorenone oxime).
10. Synthesis of N,O-Heterocycle : 2,4,5-Triphenyloxazole from benzoin (via desylbenzoate).
11. 9-Acridone from o-chlorobenzoic acid (via N-phenylanthranilic acid).
12. 3,4-Dihydro-4-oxo-1,2,3-benzotriazine from methyl anthranilate (via anthranilohydrazide).
13. Synthesis of Mesoionic compound (p-chlorophenylsydnone) : p-Chlorophenylsydnone from p-chloroaniline (via N-p-chlorophenylglycine-ethyl ester, N-(p-chlorophenyl) glycine), and N-nitroso-N-(p-chlorophenyl) glycine.
14. Diastereoselective reduction of benzil.

Recommendend Books:

1. Intermediates for Organic Synthesis, V. K. Ahluwalia, P. Bhagat, R. Aggarwal, R. Chandra, I. K. International, New Delhi, 2005.
2. Practical Heterocyclic Chemistry, A. O. Fitton and R. K. Smalley, Academic Press, London, 1968.