Credit/course distribution for 5 year M.Sc. (Integrated Chemistry)

Total Number of credits students should accumulate: 192

Suggested soft core courses are only departmental recommendations. It is not mandatory for the students to register the suggested courses. Students are free to choose any course they like from other schools/departments offer during a particular semester. All students are encouraged to consult his/her faculty advisor before choosing soft core courses

Semester 1: (Hard: 19 + Soft: 3)
Required Credits: 22

S. No.	Course	Hard/Soft core	Credits
1	CHEM100 General Chemistry Laboratory I	Hard Core	2
2	CHEM101 General Chemistry I	Hard Core	3
3	PHYS 130 Physics Laboratory I	Hard Core	2
4	PHYS 131 Mechanics	Hard Core	3
5	ENGL 111 Functional English	Hard Core	3
6	MATH 111 Differential Calculus	Hard Core	3
7	EASC 111 Earth and Environment	Hard Core	3

Suggested Soft Core Course:

Sl. No.	Course	Hard/Soft	Credits
1	PHED 111 Practical Course in Physical Education	Soft Core	3

Semester 2: (Hard: 19 + Soft: 3
Required Credits: 22

S. No	Course	Hard/Soft	Credits
1	CHEM 102 General Chemistry II	Hard Core	3
2	CHEM 120 General Chemistry Laboratory II	Hard Core	2
3	PHYS 140 Physics Laboratory II	Hard Core	2
4	PHYS 141 Thermal Physics and Kinetic Theory	Hard Core	3
5	MATH 121 Integral Calculus	Hard Core	3
6	ENGL 121 Functional English II	Hard Core	3
7	BIOL 121 General Biology I	Hard Core	3

Suggested Soft Core Course:

Sl. No.	Course	Hard/Soft	Credits
1	EASC 121 Paleontology	Soft Core	3

Semester 3: (Hard: 17 + Soft: 3)
Required Credits: 20

S. No	Course	Hard/Soft	Credits
1	CHEM 201 Inorganic Chemistry I	Hard Core	3
2	CHEM 241 Physical Chemistry I	Hard Core	3
3	CHEM 200 Chemistry Laboratory III	Hard Core	2
4	BIOL 211 General Biology II	Hard Core	3
5	EASC 211 Crystallography and mineralogy	Hard Core	3
6	A language course (other than English)	Hard Core	3

Suggested Soft Core Courses:

Sl. No	Course	Hard/Soft	Credits
1	PHYS 232 Electricity and Magnetism	Soft Core	3
2	MATH 231 Multivariable Calculus	Soft Core	3

Semester 4: (Hard: 17 + Soft: 3)
Required Credits: 20

S. No	Course	Hard/Soft	Credits
1	CHEM 210 Chemistry Laboratory IV	Hard Core	2
2	CHEM 222 Organic Chemistry I	Hard Core	3
3	PHYS 241 Modern Physics I	Hard Core	3
4	MATH 242 Linear Algebra	Hard Core	3
5	A Course in Computer Science	Hard Core	3
6	A course from School of Management	Hard Core	3

Suggested Soft Core Courses:

Sl. No	Course	Hard/Soft	Credits
1	PHYS 242 Electric Circuits Theory	Soft Core	3
2	A course from School of Social Sciences	Soft Core	3

Semester 5: (Hard: 15 + Soft: 6)
Required Credits: 21

S. No	Course	Hard/Soft	Credits
1	CHEM 300 Chemistry Laboratory V	Hard Core	3
2	CHEM 321 Organic Chemistry II	Hard Core	3
3	CHEM 341 Physical Chemistry II	Hard Core	3
4	MATH 351 Elements of Differential Equations	Hard Core	3
5	A course from Social Science (philosophy/History)	Hard Core	3

Suggested Soft Core Courses:

Sl. No	Course	Hard/Soft	Credits
1	PHYS 332 Electronic Devices and Circuits*	Soft Core	3
2	PHYS 333 Modern Physics II	Soft Core	3
3	PHYS 331 Classical Optics	Soft Core	3

Semester 6: (Hard: 15 + Soft: 3)
Required Credits: 18

S. No	Course	Hard/Soft	Credits
1	CHEM 310 Chemistry Laboratory VI	Hard Core	3
2	CHEM 302 Inorganic Chemistry III	Hard Core	3
3	CHEM 322 Organic Chemistry III	Hard Core	3
4	CHEM 352 Analytical Chemistry	Hard Core	3
5	PHYS 341 Computational Physics	Hard Core	3

Suggested Soft Core Courses:

Sl. No	Course	Hard/Soft	Credits
1	PHYS 343 Modern Optics	Soft Core	3
2	MATH 361 Fundamentals of Complex Analysis	Soft Core	3
3	PHYS 342 Basics of Materials Science	Soft Core	3

Semester 7: (Hard: 15 + Soft: 3)
Required Credits: 18

S. No	Course	Hard/Soft	Credits
1	CHEM 400 Chemistry Laboratory VII	Hard Core	3
2	CHEM 403 Advanced Inorganic Chemistry I	Hard Core	3
3	CHEM 422 Advanced Organic Chemistry I	Hard Core	3
4	CHEM 443 Symmetry and Group Theory in Chemistry	Hard Core	3
5	CHEM 463 Quantum Chemistry I	Hard Core	3

Suggested Soft Core Courses:

Sl. No	Course	Hard/Soft	Credits
1	PHYS 434 Electronic Devices, Circuits, and Microprocessors	Soft Core	3
2	PHYS 435 Numerical Methods and MATLAB	Soft Core	3
3	A Course from other schools	Soft Core	3

Semester 8: (Hard: 15 + Soft: 3)
Required Credits: 18

S. No	Course	Hard/Soft	Credits
1	CHEM 410 Chemistry Laboratory VIII	Hard Core	3
2	CHEM 404 Advanced Inorganic Chemistry II	Hard Core	3
3	CHEM 424 Spectroscopic Identification of Organic compounds	Hard Core	3
4	CHEM 444 Statistical Thermodynamics and Reaction dynamics	Hard Core	3
5	CHEM 463 Quantum Chemistry I	Hard Core	3

Suggested Soft Core Courses:

Sl. No	Course	Hard/Soft	Credits
1	PHYS 434 Electronic Devices, Circuits, and Microprocessors	Soft Core	3
2	PHYS 435 Numerical Methods and MATLAB	Soft Core	3
3	A course from other schools	Soft Core	3

Semester 9: (Hard: 15 + Soft: 3)
Required Credits: 18

S. No	Course	Hard/Soft	Credits
1	CHEM 500 Advanced Laboratory Techniques	Hard Core	3
2	CHEM 503 Advanced Inorganic Chemistry III	Hard Core	4
3	CHEM 524 Advanced Organic Chemistry II	Hard Core	4
4	CHEM 544 Spectroscopy: Theory and Applications	Hard Core	4

Suggested Soft Core Courses:

Sl. No	Course	Hard/Soft	Credits
1	CHEM 527 Advanced Organic Chemistry III	Soft Core	3
3	A course from other schools	Soft Core	3

Semester 10: (Hard: 6 + Soft: 9)

Required Credits: 15

S. No	Course	Hard/Soft	Credits
1	CHEM 580 Project Work	Hard Core	4
2	CHEM 582 Comprehensive Evaluation/Viva	Hard Core	2

Soft Core Courses (three courses have to be registered)

Sl. No	Course	Hard/Soft	Credits
1	CHEM 504 Inorganic Photochemistry	Soft Core	3
2	CHEM 506 Ligand Field Theory	Soft Core	3
3	CHEM 508 Supra-molecular Chemistry	Soft Core	3
4	CHEM 524 Natural Products Chemistry	Soft Core	3
5	CHEM 528 Asymmetric Synthesis	Soft Core	3
6	CHEM 542 Advanced Magnetic Resonance and Solid state Chemistry	Soft Core	3
7	CHEM 546 Electro Analytical Techniques	Soft Core	3
8	CHEM 548 Nano-materials and Photo-catalysis	Soft Core	3
9	A course from other Schools	Soft Core	3

Total Credits: 192

CHEM100 General Chemistry laboratory 0-1-4-2

Experiments related to the courses of this semester

CHEM 101: General Chemistry – I 3-1-0-3

Unit I (Fundamental concepts; Measurements in Chemistry; Language of Chemistry)
Chemistry: Matter, Energy, Chemical and Physical Properties, Classifying Matter; Atoms and Molecules; Fundametal concepts and language of chemistry. (Chapter 1 and 2 of Robinson)

Unit II (Atoms and molecules)
Atomic and Molecular Masses: molecular formula and determination
Stoichiometry and Chemical Change, quantitative analysis, Thermochemistry: enthalpy and its consequences
Atoms: Structure and spectra, introduction to quantum theory, The Periodic Table: Electron Configuration and general properties (Chapters 3,4, and 5 of Robinson)

Unit – III (Chemical bonding; chemical reactions and periodic table)
Ionic Bonding, covalent bonding: oxidation states and Lewis symbol, Valence Bond Theory: Hybridization of Atomic Orbitals: sp Hybridization, sp2 Hybridization, sp3 Hybridization, sp3d and sp3d2 Hybridization, Assignment of Hybrid Orbital to central atoms, Hybridization involving double and triple bonds. Molecular Orbital Theory: Molecular Orbitals, Molecular Orbital energy diagrams, Bond order, H2 and He2 Molecules, Diatomic Molecules of the Second Period. (Chapters 6, 7, and 8 of Robinson)

Unit – IV: (Gases, intermolecular forces, liquids and solids; solutions and colloids)
The Macroscopic Behavior of Gases: Temperature, gas laws.
The Microscopic Behavior of Gases: Kinetic and molecular theory of gases, inter molecular forces
Properties of Liquids and Solids: forces between molecules, properties of liquids and solids, structure of crystal and solids
The nature of solutions: The formation of solutions, dissolutions of ionic compounds, dissolution of molecular electrolytes.
Macroscopic Properties of Solutions: Solutions of gases in lipids, solutions of liquids in lipids, the effect of temperature on the solubility of solids in water, solid solutions.
Expressing Concentration: Percent composition, molarity, molality, mole fraction. Colligative Properties of Solutions, colloids chemistry (Chapters 10, 11, and 12 of Robinson)

Unit – V (Chemical kinetics and equilibrium)
Rate of reaction: Rate of reaction and rate laws
The Microscopic Explanation of Reaction Rates: Introduction to collision theory of reaction rates, activation energy and the Arrhenius equation, elementary reaction, reaction Mechanisms, Catalysis.

An introduction to Equilibrium: The state of Equilibrium, reaction quotients and equilibrium constants, Le Chatelier`s Principle, Predicting the direction of a reversible reaction, calculation of equilibrium constants
Kinetics and Equilibrium: The relationship of reaction rates and equilibrium, reaction mechanisms involving equilibrium.

Ionic equilibrium: monoprotic, diprotic, and triprotic acids; properties of Bronsted bases in aqueous solutions, pH, pOH: measurements and significance, solubilityr products
The Lewis concept of Acids and Bases: Definitions and examples.
Precipitation and Dissolution (Chapters 13, 14, 15, 16, and 17 of Robinson)

Text Books:
1. General Chemistry, W. R. Robinson, J. D. Odom, H. F. Holtzclaw, Jr., Tenth Edition, AITBS Publishers, New Delhi.

Further Reading:
2. General Chemistry, D. D. Ebbing, 7th Edition, AITBS Publishers, New Delhi.

CHEM120 General Chemistry Laboratory II 0-1-4-2

Experiments related to the courses of this semester

CHEM 102: General Chemistry – II 3-1-0-3

Unit – I (Chemical thermodynamics; Electrochemistry; Oxidation – Reduction)
The first law of thermodynamics, state functions. Work and heat Galvanic Cells and Cell Potentials: Galvanic cells, cell potentials, standard electrode potentials, circulation of cell potentials, relationship of the cell potential and the equilibrium constant.- Batteries: Primary cells, secondary cells, fuel cells, corrosion.
Electrolytic cells: The electrolysis of molten sodium chloride, the electrolysis of aqueous solutions, electrolytic disposition of metals, Faraday's Law of electrolysis. (Chapters 18 and 19 of Robinson)

Unit – II (Introduction to nuclear chemistry)
Stabilty of nuclei, nuclear reactions, nuclear energy, nuclear series, and other applications (Chapter 20)

Unit – III (Chemistry of metals and semi-metals; co-ordination compounds)
The elemental representative metals: Periodic relationships among groups, preparation of representative metals, chemical compounds - The semi-metals: The chemical behavior and structures of the semi-metals, occurrence and preparation of boron and silicon, boron and silicon hydrides, boron and silicon halides, boron and silicon oxides and derivative.
The transition elements, properties of the transition elements, preparation of the transition elements, compounds of the transition elements, copper oxide superconductors.
Coordination compounds: Basic concepts, the naming of the complexes, the structures of complexes, isomerism in complexes, uses of complexes. - Introduction to bonding: VSEPR, crystal field theory, properties and bonding (Chapter 22 and 23 of Robinson)

Unit – IV (Introductory organic chemistry: Structure and bonding at carbon; stereochemistry)
Organic Compounds of Carbon: Alkanes, nomenclature, Hydrocarbons. Derivatives of aromatic and non-aromatic hydrocarbons - Polymers: Factors that affect properties of polymers, polymer properties, kinds of polymers - Stereochemistry of carbon compounds: stereo-structures – ways of representing stereo chemistry, stereo chemistry of simple hetero nuclear rings - Stereoisomerism: enantiomers and diastereomers; concept of chirality, priority rules. (Chapters 9 and 24 of Robinson)

Unit – V (Organic reaction mechanisms)
Types of organic reactions - addition, substitution, elimination reactions - interpretation of reaction profiles – Introductory treatment. (Chapter 9 of Robinson)

Text Book:

1. General Chemistry, W. R. Robinson, J. D. Odom, H. F. Holtzclaw, Jr., Tenth Edition, AITBS Publishers, New Delhi.

Further Reading:
2. General Chemistry, D. D. Ebbing, 7th Edition, AITBS Publishers, New Delhi.

CHEM200 Chemistry Laboratory III 0-1-4-2

Experiments related to the courses of this semester

CHEM 201 Inorganic Chemistry I 3-1-0-3

Unit – I (Hydrogen and Hydrides, Alkali and Alkaline earth Metals)

Hydrogen and Hydrides: Electronic structure, abundance, preparation and properties, isotopes, ortho- and para hydrogen; Hydrides: ionic, covalent, metallic and intermediate hydrides; Hydrogen bonding.

Alkali metals: Introduction, halides, oxides and hydroxides, salts of oxo-acids, aqueous solution chemistry, complexes and organometallic compounds.

Alkaline Earth metals: Introduction, halides, oxides and hydroxides, salts of oxo-acids, aqueous solution chemistry, complexes and organometallic compounds.

Unit – II (Boron and Carbon group – Basic treatment)

Boron group: Introduction, diborane and hydrogen compounds of the other elements, metal borides, halides and complex halides of B, Al, Ga, In and Tl, oxides, oxo-acids, oxo-anions and hydroxides; nitrogen derivatives; Al, Ga, In and Tl salts of oxo-acids and aqueous solution chemistry, organometallic compounds.

Carbon group: Introduction, Intercalation compounds of graphite, hydrides, carbides and silicides, halides and complex halides; oxides and oxo-acids of carbon; oxides and oxo-acids and hydroxides of Si, Ge, Sn and Pb; Silicates; Silicones; Sulfides; Cyanogen, its derivatives and silicon nitride; aqueous solution chemistry and oxo-acid salts of Sn and Pb; Organometallic compounds.

Unit – III (Nitrogen and Oxygen group- Basic treatment)

Nitrogen group: Introduction; hydrides; nitrides, phosphides and arsenides; halides, oxo-halides and complex halides; Oxides, oxo-acids and sulfides of N, P, As, Sb and Bi; Phosphazenes; Aqueous solution chemistry; Organic derivatives.

Oxygen group: Introduction; Hydrides; Halides, Oxohalides and complex halides, Oxides, Oxo-acids and their salts; Sulphur-nitrogen compounds; Aqueous solution chemistry of S, Se and Te; Organic derivatives.

Unit – IV (Halogens and noble gases- Basic treatement)

Introduction; hydrogen halides; general considerations of halides; interhalogen compounds and polyhalogen ions; oxides and oxyfluorides of Cl, Br and I; oxo-acids of halogens and their salts; aqueous solution chemistry; organic derivatives.

Noble gases: Introduction; compounds of Xe, Kr and Rn.

Unit V (Nuclear Chemistry- Basic treatment)

Introduction; nuclear binding energy; radio-activity and nuclear reactions; nuclear fission and fusion; spectroscopic techniques based on nuclear properties; separation of stable isotopes and unstable isotopes; applications of isoptopes.

Recommended Books:
1. A. G. Sharpe, Inorganic Chemistry, 3rd Edition, Addison-Wesley, 1999.
2. J. D. Lee, A New Concise Inorganic Chemistry, 3rd Edition., ELBS, 1987.
3. D. F. Shriver, P. W. Atkins, C. H. Langford, Inorganic Chemistry, ELBS. 1990.

CHEM 241: Physical Chemistry I 3-1-0-3

Unit I (Solutions)
Gibbs - Duhem equation - thermodynamics of mixing - Henry's & Raoult's laws - liquid mixtures - colligative properties - mixture of volatile liquids - distillation - azeotropes - solvent & solute activity,

UNIT – II (Phase transformations)
Stability of phases - Clapeyron equation - Clasius-Clapeyron equation. Thermodymamics of phase transition; classification of phases - bubbles, cavities and droplets-Kelvin equation, capillary action.

UNIT – III (Phase diagrams)
One component systems - two component systems - reactive systems - three component systems - Chemical equilibrium - equilibrium response to pressure - van't Hoff relation - Ellingham diagram.

UNIT – IV (Equilibrium electrochemistry-Ions in solution- 1)
Activities in solutions - mean activity coefficient - Debye - HÜckel theory - role of electrodes - electrochemical potential - types of electrodes - kinds of cell - emf and electrode potentials - standard electrode potentials - thermodynamics of emf of cells – potentiometric titrations - pK & pH - acid base titrations – buffers.

UNIT – V (Equilibrium electrochemistry-Ions in solution- 2)
Ion transport and molecular diffusion: Ion motion - conductivity - mobilities - transport numbers and measurement - Debye Huckel Onsager theory - diffusion - Fick's laws - diffusion and convection.

Text Book:

Physical Chemistry, P. W. Atkins, 6th edition, Oxford Publications
Further Reading:
Physical Chemistry, Alberty
Physical Chemistry, Thomas Engel and Reid

CHEM 210 Chemistry Laboratory IV 0-1-4-2

Experiments related to the courses of this semester

CHEM. 222: ORGANIC CHEMISTRY I 3-1-0-3

Unit I (Introduction to Organic Chemistry)
Introduction to functional groups, structure and bonding; isomers, nomenclature, and resonance; Intermolecular forces
(Organic Chemistry by P.Y Bruice Chapter 1 and Chapter 2)

Unit II (Chemical reactivity of organic molecules)
Reaction Classification by Structural Change by Reaction Type; Acid-Base reactions, Oxidations & Reductions, Reaction Variables, Reactants & Reagents, Product Selectivity, Other Variables, Reaction Rate ,Intermediates, Reaction Energetics, Bond Energy, Electronic Effects, Steric Effects, Solvent Effects, Reaction Mechanisms, Curved Arrow Notation, Reactive Intermediates, Reaction Illustrations, Nucleophilicity & Basicity, Acid-Base Catalysis
(Organic Reactivity; Virtual text of organic chemistry)

Unit III (Stereochemistry)
Stereoisomers: Alkene Configurational Isomers, Cycloalkane Configurational Isomers
Conformational Isomers: Ethane,Butane, Cycloalkanes, Substituted Cyclohexanes
Chirality & Symmetry: Symmetry Elements, Enantiomorphism, Optical Activity, Configurational nomenclature, Compounds Having Two or More Stereogenic Centers, Fischer Projection Formulas, achiral diastereomers, Other Configurational Notations, Resolution Conformational Enantiomorphism
(Chapter 2.9 – 2.15 and chapter 4 upto 4.13 of Bruice).

Unit IV (Chemistry of non aromatic hydrocarbons)
Nomencalture, synthesis and reactions of alkanes
Nomenclature , synthesis and reactions of alkenes.
Nomenclature , synthesis and reactions of alkynes
Nomenclature , synthesis and reactions of dienes
(Chapters 8,3, 5,6 and 7 of Bruice)

Unit V (Chemistry of aromatic hydrocarbons)
Aromaticity, Huckel Rule, resonance energy, Benzene structure and reactions, Naphthalene structure and reactions, Activity and orientation of substituted benzenes.
(Chapters 14 and 15 of Bruice)

Text book:
Organic Chemistry, P. Y. Bruice, Pearson Education, 3rd edition, 2006

Further Reading
1. Organic Chemistry; Wade

2. Organic Chemistry, Clayden

CHEM 300 Chemistry Laboratory V 0-1-6-3

Experiments related to the courses of this semester

CHEM 301: Inorganic Chemistry II 3-1-0-1

Unit – I (Coordination Compounds 1)
Introduction, physical and chemical properties of transition elements; Introduction to coordination compounds; coordination numbers and geometries in transition metal complexes; nomenclature; isomerism in transition metal complexes – structural, geometrical and optical isomerism.

Unit – II (Coordination Compounds 2)
Double salts and coordination compounds; Werner's work; effective atomic number; bonding in transition metal complexes – valence bond theory, crystal field theory (octahedral and tetrahedral complexes); magnetism.

Unit – III (Transition Metals of the First Series)
Introduction and the chemistry of Scandium, Titanium, Vanadium, Chromium, Manganese, Iron, Cobalt, Nickel, Copper and Zinc.

Unit – IV (Transition Metals of the Second and Third Series)
Introduction and the chemistry of Yttrium & Lanthanum, Zirconium & Hafnium, Niobium & Tantalum, Molybdenum & Tungsten, Technetium & Rhenium, Ruthenium & Osmium, Rhodium & Iridium, Palladium & Platinum, Silver and Gold, Cadmium & Mercury.

Unit – V (Lanthanide and Actinide Elements)
Lanthanides: Introduction, occurrence, separation, oxidation states and general chemistry.
Actinides: Introduction, isolation and general chemistry.

Text Book:
D. F. Shriver, P. W. Atkins, C. H. Langford, Inorganic Chemistry, ELBS. 1990.

Recommended Books:
1. A. G. Sharpe, Inorganic Chemistry, 3rd Edn., Addison-Wesley, 1999.
2. J. D. Lee, A New Concise Inorganic Chemistry, 3rd Edn., ELBS, 1987.
3. B. Douglas, D. McDaniel, J. Alexander, Concepts and Models of Inorganic Chemistry, 3rd Edn., John Wiley, 2001.

CHEM.321: Organic chemistry II 3-1-0-3

Unit I (Reactions at sp3 hybridized carbon)

Substitution reactions - SN1, SN2 reaction mechanism, factors influencing SN1 and SN2 reactions, elimination reaction E1, E2, E1cb reaction mechanisms factors affecting, substitutions vs eliminations.
[Chapters 9, 10 and 11 of Bruice]

Unit II (Organometallics of Groups I and II, boron, silicon, sulphur)
Alkyl and aryl lithiums preparation and reactions, Grignard reagent synthesis and reactions, sulpur stabilized anions, sulphonium salts, sulphonium ylids, sulphur stabilized cations carbonyl compounds, sulphoxides, borons - hydroborations, allyl and crotyl boranes, silicon - reactions of silanes and silyl enol ether.
[Chapter 46 and 47 of Clayden]

Unit III (Reactions of aldehydes and ketones)
Reactions of carbonyl compounds with carbon, hydrogen, oxygen and nitrogen nucleo philes, reactions of α, β and unsaturated carbonyl compounds, reactions at the α-carbon.
[chapters 17 and 19 of Bruice]

Unit IV (Reactions of carboxylic acids and their derivatives)
Reactions of carboxylic acids and their derivatives with oxygen and nitrogen nucleophiles – relative reactivities of carboxylic acid and its derivatives – general machanism of acylation reaction.
[Chapter 16 of Bruice]

Unit V (Introduction to spectroscopic identification of organic molecules)
Mass spectrometry, infrared spectroscopy UV- Visible spectroscopy and NMR spectroscopy (Chapter 12 and 13 of Bruice)

Text book:
Organic Chemistry, P. Y. Bruice, Pearson Education, 3rd edition, 2006

Further Reading
1. Organic Chemistry; Wade
2. Organic Chemistry, Clayden

CHEM 341: Physical Chemistry II 3-1-0-3

Unit I (Chemical Kinetics – 1)
Rates of reaction - order and molecularity of reactions - rate law and rate constants - determination of rate law - first, second, third and fractional order of reactions - half lives - Arrhenius theory - types of reactions: approaching equilibrium, consecutive reactions, - steady state approximation - pre equilibria.

Unit II (Chemical Kinetics – 2)

Introduction to collisional theory of reactions - Lindemann Hinshelwood unimolecular reactions - complex reactions: reversible, parallel, competitive reactions, chain reactions - polymerization - explosion - oscillations - rapid reactions –.

Unit III (Reaction in solutions)
Comparison of rate between gas phase and in solution – factors governing rates of reaction in solution – theories of reaction rates applied to reactions in solutions – influence of liquid medium in rate – kinetic isotope effect – solvent isotope effect – linear free energy relationship

Unit IV (Surface and Colloids)
Surface tension, capillarity-structure of surface films-surfactants and micelles. Adsorption on surfaces - physisorption & chemisorption - desorption - adsorption isotherms: Gibbs, Langmuir, BET, other isotherms - measurement of surface area using adsorption isotherms, kinetics of homogeneous catalytic reaction - colloids: classification – preparation, purification, and stability of colloids

Unit V (Reaction in the excited states)
Photochemical reactions – excited electronic states – intermolecular and intramolecular deactivation kinetics of excited states - types of photochemical reaction – photoelectron-chemistry

Textbook:
Physical Chemistry, P.W. Atkins, 6th edition, Oxford publication, 1998

Further Reading:
1. G. L. Agarawal, Basic Chemical Kinetics, Tata McGraw Hill, 1990.
2. J. Rajaram, J. Kuriakose, Kinetics and chemical transformation, MacMillan India Limited, 1993.
3. G. M. Barrow, Physical Chemistry, McGraw Hill, 1979.

CHEM 310 Chemistry Laboratory VI 0-1-6-3

Experiments related to the courses of this semester

CHEM 302 Inorganic Chemistry III 3-1-0-3

Unit I (Chemistry and Periodic Trends among Metals)
General periodic trends among metals; alkali metals; alkaline earth metals; coinage metals; zinc subgroup; scandium family and rare earths; actinide metals; transition metals - group 4 to 7, group 8 to 10.

Unit II (Acids and Bases)
Bronstat acids and bases: Bronstat acidy, periodic trends in Bronstat acidy, polyoxo compound formation; Lewis acids and bases: definitions, strengths, representative Lewis acids, heterogeneous acid-base reactions.

Unit III (Solid State Chemistry)
Inorganic Solids: Ionic solids, close packing, radius ratio, Structure of ionic crystals, ionic radii, lattice energy; crystal structure, defects structures, insulators, semiconductors and superconductivity.

Unit IV (Main group Organometallics)
Classification and structure, ionic and electron deficient compounds of groups 1, 2 and 12.; Electron deficient compounds of the boron group; Electron-precise compounds of the carbon group. Electron-rich compounds of the nitrogen group.
Unit V (Introduction to Bio-inorganic Chemistry)
Pumps and transport proteins: Ion pumps, Oxygen transport; Enzymes and catalysis: Oxaloacetate decarboxylase, carboxy peptidase; Redox catalysis: cytochromes, nitrogen fixation, photosynthesis.

Text book:
D. F. Shriver, P. W. Atkins, C. H. Langford, Inorganic Chemistry, ELBS. 1990.

Recommended Books:
1. A. G. Sharpe, Inorganic Chemistry, 3rd Edn., Addison-Wesley, 1999.
2. J. D. Lee, A New Concise Inorganic Chemistry, 3rd Edn., ELBS, 1987.
4. B. Douglas, D. McDaniel, J. Alexander, Concepts and Models of Inorganic Chemistry, 3rd Edn., John Wiley, 2001.
5. W. L. Jolly, Modern Inorganic Chemistry, 2nd Edn., McGraw-Hill, 1991.

CHEM: 322 ORGANIC CHEMISTRY III 3-1-0-3

Unit I (Heterocycles)
Chemistry of five and six–membered aromatic heterocycles with one hetero atom-synthesis and reactions of pyrrole, furan, thiophene, pyridine, indole, quinoline and isoquinoline and biologically important heterocycles
(Chapter 27 of Bruice)

Unit II (Carbohydrates and Lipids)
Carbohydrates: Classification, configuration of aldoses and ketoses, reactions of monosaccharides, chain elangation, chain shortening, stereochemistry of glucose, the Fischer proof, cyclic structure of mono saccharides, formation of glycosides, reducing and non-reducing sugar, determination of ring size, di-saccharides and poly-saccharides.
(Chapter 20 of Bruice.)
Lipids: Fatty acids, waxes, fats and oils, membranes .
(Chapter 24 of Bruice)

Unit III (Amino acids, peptides and proteins)
Classification and nomenclature of amino acids – configuration of amino acids, acid-base amino acids—isoelectric points—primary structure of peptides – end terminal analysis – peptides synthesis—secondary structure of proteins tertiary and quaternary structure of proteins.

(Chapter 21 of Bruice.)

Unit IV (Nucleosides, nucleotides and nucleic acids)
Nucleosides and nucleotides, nucleic acids, helical forms of DNA, DNA replication. (Chapter 25 of Bruice).

Unit V (Polymers and drugs)
Introduction to synthetic polymers: General classes of synthetic polymers, chain growth polymers, stereo chemistry of polymerization, polymerization of dienes, co-polymers, step-growth polymers, physical properties of polymers, bio-degradable polymers. (Chapter 26 of Bruice)
Introduction to organic chemistry of drugs: Naming drugs, lead compounds, molecular modification, random screening, serendipity in drug development, receptors, drugs as enzyme inhibitors, QSAR, anti-viral drugs (Chapter 30 of Bruice.)

Text book:
Organic Chemistry, P. Y. Bruice, Pearson Education, 3rd edition, 2006
Further Reading
1. Organic Chemistry; Wade
2. Organic Chemistry, Clayden

CHEM 352: Analytical Chemistry 3-1-0-3

UNIT I (Tools and Data Handling)
Balances, burettes, volumetric flasks, pipettes, calibration of tools, sampling. Errors and Statistics: significant figures, rounding off, accuracy and precision, determinate and indeterminate errors, standard deviation, propagation of errors, confidence limit, test of significance, rejection of a result.

UNIT II (Separation Techniques)
Solvent Extraction: distribution Coefficient, distribution ratio, solvent extraction of metals, multiple batch extraction, counter current distribution. - Chromatographic Techniques: classification, theory of chromatographic separation, distribution coefficient, retention, sorption, efficiency and resolution. - Column, ion exchange, paper, TLC & HPTLC: techniques and application. - Gas Chromatography: retention time or volume, capacity ratio, partition coefficient, theoretical plate and number, separation efficiency and resolution, instrumentation and application.

UNIT III (Spectroscopic Techniques)
Electromagnetic radiation, absorption, and emission of radiation – instrumentation: sources, monochromators, detectors. - Flame spectrometry: flame emission, AAS, ICP, instrumentation and application. - Absorption spectrometry: UV-VIS, IR, instrumentation, techniques and applications.

UNIT – IV Thermal and Radiochemical Techniques:

Thermogravimetry: instrumentation and techniques, TGA curves, DTA and DSC, applications. Radiochemical methods: decay reactions, growth of radioactivity, radiation detectors, tracer techniques.

UNIT V (Electroanalytical Techniques)
Electrogravimetry, coulometry, voltam- metry, polarography, conductometry, instrumentation, techniques and application.

Textbook:
D. C. Harris, Quantitative Chemical Analysis, 4th Ed., W. H. Freeman, 1995

Further reading:
2. G. D.Christian & J. E. O'Reily, Instrumental Analysis, 2nd Ed., Allyn & Balon, 1986.

CHEM 400 Chemistry Laboratory VII 0-1-6-3

Synthesis and Characterization of selected inorganic and organic compounds
Experiments related to the courses of this semester

CHEM 403 Advanced inorganic chemistry I 3-0-0-3

UNIT I (Inorganic Solids)
Types of solids, covalent, ionic, molecular and metallic solids, lattice energy, cohesive energy and Medelung constants, Van der Waals forces, hydrogen bonding, unit cell, crystal lattices, structure of simple ionic compounds, radius ratio and close packed structures. Imperfections in crystals (point defects and F centers).

UNIT II (Boron and Silicon)
Synthesis, properties and structures of Boron and Silicon compounds: Boron hydrides (small boranes and their anions, B1B4), carboranes, metalloboranes, metallocarboranes; boron halides, boron-nitrogen compounds; silicates, silicones, zeolites; diamond, graphite.

UNIT III (Nitrogen, Phosphorous, Sulphur)
Hydrides, oxides and oxy acids of nitrogen, phosphorous, sulphur; phosphines, phosphazines, sulphur-nitrogen compounds.

UNIT IV (Interhalogen compounds)
Pseudo halogens; oxides and oxoacids of halogens. Noble gas compounds: Synthesis & structure of Xe compounds. Poly anions and isopoly anions of Phosphorous, Vanadium, Chromium, Molybdenum and Tungsten, heteropoly anions of Molybdenum and Tungsten.

UNIT V (Nuclear chemistry)
Radioactive decay and equilibrium. nuclear reactions, Q value, cross sections, types of reactions, chemical effects of nuclear transformations; fission and fusion, fission products

and fission yields; radioactive techniques, tracer technique, neutron activation analysis, counting techniques such as G. M. ionisation and proportional counter.

Textbook:
F. A. Cotton, G. Wilkinson, Advanced Inorganic Chemistry, 5th Edn., John Wiley.

Further Reading:
1. J. E. Huheey, Inorganic Chemistry, 4th Edn., Harper International.
2. N. N. Greenwood, A. Earnshaw, Chemistry of the Elements, 2nd Edn., BH, 1997.
3. D. F. Shriver, P. W. Atkins, C. H. Langford, 3rd Edn. Inorganic Chemistry, ELBS. 1999.
4. W. L. Jolly, Modern Inorganic Chemistry, 2nd Edn., McGraw-Hill, 1991.

CHEM 423 Advanced organic chemistry I 3-0-0-3

Unit I (Structure and bonding: introductory physical organic chemistry)
Review of structure and bonding in organic compounds – VB and MO theory - Concept of hybridization, resonance, aromaticity, anti-aromaticity, frontier orbitals, hardness and softness. Application of HMO theory.
Introductory Physical Organic Chemistry: Acids and bases, HASA, equilibrium constant thermodynamic effect, kinetic effects - Thermodynamic and kinetic control of organic reactions. Hammond postulate, Curtin-Hammett principle - Hammett equation - Application to organic reactions.

Unit II (Stereochemistry and reactivity)
Review of basic principles of stereochemistry, axial chirality, planar chirality, helicity, prochirality, other stereochemical descriptors, Configurational and conformational effects on reactivity - Stereospecific and stereoselective reactions and diastereoselective reactions. Introduction to asymmetric synthesis.

Unit III (Reactive intermediates)
Reactive carbon species – structure stability, formation and reactivity of carbanion, cabocation, radicals, carbene and benzynes.
Reactive heteroatom intermediates – structure, stability, generation and reactions of heteroatom electrophiles and nucleophiles.

Unit IV (Organic reaction mechanism – I)
Types of reactions, mechanism of reactions. Substitution at saturated and unsaturated reaction center (carbon) by radical, nucleophile, electrophile addition - elimination, elimination – addition mechanism

Unit V (Organic reaction mechanism –II)
Addition reactions to carbon – carbon, carbon – hetero atom multiple bonds – isolated and conjugated multiple bonds. Elimination reactions-generating carbon – carbon and carbon – heteroatom multiple bonds.

Textbook:
F. A. Carey and R. J. Sundberg (Part A and B) Kluwer Academic / Plenum Publishers (2000)

Further Reading:
2. E. L. Eliel, Stereochemistry of carbon compounds. John Wiley (1997)
3. C. J. Moody and G. H. Whitham, Reactive intermediates Oxford chemistry Primers (1992).
4. S. Ege, Organic Chemistry, AITBS (2001)
5. Reinhard Bruckner (Academic Press) 2003 Advanced Organic Chemistry – Reaction Mechanisms.
5. Warren et.al Advanced organic chemistry.
6. Organic Chemistry, Clayden et al
7. P.Sykes, A Guidebook to Mechanism in Organic Chemistry (6th Edn)

CHEM 443: Symmetry and group theory in chemistry 3-0-0-3

UNIT I (Basic Group theory)
Algebraic Systems – Common properties of Operators – Levels of Abstraction – Subsystems – Direct Products – Isomorphisms - Axioms and theories of group – Abelian and cyclic groups – Finite sub-groups and Homomorphisms - Similarity Transformation and Classes - Cosets and Permutation Groups.

UNIT II (Molecular symmetry, Symmetry Groups)
Symmetry Elements and operations – Planes – Axes - Inversions – Improper Axes – Products of Symmetry Operations – Equivalence symmetry elements and operations – Relations between symmetry operations – Classes – Symmetry groups with multiple higher order axes – Symmetry Point groups – Matrix representation of symmetry operations

UNIT III (Group Theory in Molecular Quantum Chemistry)
Representation of groups - Character - Reducible and Irreducible Representations - Great Orthogonality Theorem - Construction of Character Tables – Cyclic groups - Double groups - Direct Products – Complete and Incomplete Projection Operators – Constructions of Symmetry adapted Linear Combinations.

UNIT IV (Applications)
Symmetry properties of Hamiltonian operator - Wave functions as basis for Irreducible Representations - Transition moment integrals - selection rule for spectral transitions - Mutual exclusion principle – LCAO – MO Approximation – Symmetry factoring of secular equations-Ligand field theory – Molecular Vibrations – Woodward-Hoffmann Cyclization rules.

UNIT V (Crystallographic Symmetry)
Point symmetry Operations – Hexagonal Coordinates – Crystals systems – Lattice – Primitive unit cell – Bravais Lattices – Centering of Lattices – Wigner-Seitz and other

unit cells- 2d lattices – Crystallographic point groups – Schoenflies approach – Laues groups – space groups – symmorphic and non-symmorphic operations – Derivation of Space groups

Textbook:
F. A. Cotton: Chemical Applications of Group Theory, Wiley Eastern, 1985.

Further Reading:
(2) A. M. Lesk, Introduction to symmetry and group theory for chemists, Kluwer, NY, 2004.
(3) A. Vincent, Molecular Symmetry and Group theory, A Programmed Introduction to chemical applications, Wiley, New York, 2001.
(4) R. L. Carter, Molecular Symmetry and Group theory, Wiley, NY, 1997.
(6) R. B. Woodward and R. Hoffmann, Conservation of Orbital symmetry, Verlag Chemie GmbH, NY, 1970.
(8) G. burns and A. M. Glazer, Space groups for Solid State Scientists, Acadamic press, NY, 1978.

CHEM 463: Quantum Chemistry I 3-0-0-3
Prerequisite: PHYS 241: Quantum mechanics or B.Sc (Chemistry)

Unit 1 (Hydrogen atom)
Review of Hydrogen atom – Schrödinger equation and nature of its solutions – Othogonality and Normalization – Energies and Degeneracies - Spherical harmonics - Angular Momentum – Quantum Numbers and their interdependence – Radial and Radial distribution plots – Angular plots - Atomic units.

Unit II (Variation Theory)
Variation theorem and its proof – Linear Variation – Matrix formulation of linear variation method - Secular determinant - Non-Linear variation – Illustrative examples - Particle in a box with finite and varying potential energy – Anharmonic oscillator – Hydrogen atom – Polarizability of Hydrogen atom.

UNIT III (Perturbation Theory)
Time Independent Perturbation theory – Non-degenerate states - First order perturbation – Correction to Energy and Wave functions – Second and higher order perturbations – Illustrative Examples - Degenerate States – Hydrogen atom in an electric field - Zeeman effect – Introductory Time Dependent Perturbation theory.

Unit IV (Many Electron Wave functions)
Non-relativistic Atomic Hamiltonian - Independent Electron Model – Effect of interelectron repulsion - Product wave functions – Antisymmetry of wave functions– Nature of exchange – Electron spin – Spin operators and Spin Eigen Functions – Pauli's Principle - Slater Determinants – singlet and triplet states of excited Helium.

Unit V (Atomic Structure)

Theory of Self-consistent Field – Hartree Theory – Hartree Fock Theory –SCF total electronic energy – Slater type Orbitals – Aufbau principle – Electronic configuration - Electron Angular momentum in atoms – Spectroscopic Term symbols – Spin-Orbit coupling – selection rules for atomic spectra – Periodic properties.

Textbook:
D. A. McQuairrie: Quantum Chemistry, Viva books Pvt. Ltd., Chennai, 2003.

Further Reading:
1. J. P. Lowe and K. A. Peterson, Quantum Chemistry, Elsevier Acadamic Press, New York, 2006.
2. 3. P. W Atkins and R. S. Friedman: Molecular Quantum Mechanics, Oxford University Press, 2005.
4. I. N. Levine, Quantum Chemistry, Prentice Hall, 2000.
5. A. K Chandra, Introduction to Quantum Chemistry, Tata McGraw Hill, 1988.
6. R K. Prasad, Quantum Chemistry Through Problems and Solutions, New Age International, 1997.
7. R. Anantharaman, Fundmantals of Quantum Chemistry, Macmillan India Ltd., 2001.
8. F. L. Pilar: Elementary quantum chemistry, Mc-Graw Hill International, 2nd ed. 1990.

CHEM 410 Chemistry Laboratory VIII 0-1-8-3

Computational chemistry and analytical techniques
Experiments related to the courses of this semester

CHEM 404 Advanced Inorganic Chemistry II 3-0-0-3

UNIT I (Introduction to transition metal complexes)
Brief review of the general characteristics of transition elements, types of ligands, nomenclature of coordination complexes, chelates, chelate effect, geometry and isomerism, Werner, Sidzwick and Valence bond theory.

UNIT II (Electronic structure of transition metal complexes 1)
Crystal field theory, crystal field splitting, application of d-orbital splittings to explain magnetic properties, low spin and high spin complexes, crystal field stabilization energy, spectrochemical series, weak and strong field complexes, thermodynamic and related aspects of crystal fields, ionic radii, heats of ligation, lattice energies, site preference energies.

UNIT III (Electronic structure of transition metal complexes 2)
MO theory of complexes (quantitative principles involved in complexes with no pi and with pi bonding) and ligand filed theories and molecular symmetry, angular overlap model, Jahn Teller effect, electronic spectra of transition metal complexes, Orgel and Tanabe-Sugano diagrams, charge transfer and d-d transitions, nephelauxetic series.

UNIT IV (Inorganic reaction mechanisms)
Inert and labile compounds, substitution reactions of octahedral complexes, dissociative, associative, aquation, conjugate base mechanism; substitution reactions of square planar

complexes, trans effect, trans effect series, theories of trans effect; electron transfer reactions.

UNIT V (Magnetism)
Types of magnetism - dia, para, ferro and antiferro magnetism, quenching of orbital angular moment, spin orbit coupling; Chemistry of lanthanides and actinides: lanthanide contraction, oxidation states, spectral and magnetic properties, use of lanthanide compounds as shift reagents.

Textbook:
D. F. Shriver, P. W. Atkins, C. H. Langford, Inorganic Chemistry, 3rd Edn. ELBS. 1999.

Further reading:
1. F. A. Cotton, G. Wilkinson, Advanced Inorganic Chemistry, 5th Edn., John Wiley.
2. J. E. Huheey, Inorganic Chemistry, 4th Edn., Harper International.
3. B. Douglas, D. McDaniel, J. Alexander, Concepts and Models of Inorganic Chemistry, 3rd Edn., John Wiley, 2001.
5. N. N. Greenwood, A. Earnshaw, Chemistry of the Elements, 2nd Edn., BH, 1997.
6. W. L. Jolly, Modern Inorganic Chemistry, 2nd Edn., McGraw-Hill, 1991.

CHEM 424 Spectroscopic identification of organic compounds 3-0-0-3

Unit I (Application of UV – Visible and IR spectroscopy to organic structure elucidation)
Introduction to spectroscopic techniques of structure elucidation. Electromagnetic radiation, energy and electromagnetic spectrum, units, absorption of energy by organic compounds, types of spectroscopic methods to organic structure elucidation.
UV – Visible Spectroscopy: Basic principles, application of UV – Visible spectroscopy to organic structure elucidation, Woodward – Fisher rules, Octant rule, Application of ORD – CD to stereochemical assignments.
IR – Spectroscopy – Basic principles, characteristic frequencies of common functional groups.

Unit II (Application of NMR Spectroscopy)
Basic principles. Introduction to NMR techniques – CW and FT NMR techniques.
1H NMR Spectral parameters – intensity, chemical shift, multiplicity, coupling constant, factors affecting,. Analysis of first order and second - order spectra. Structure determination of organic compounds by 1H NMR spectra.

Unit III (Multinuclear NMR (with specific emphasis on 13C NMR))
13C NMR: Proton coupled; off–resonance decoupled; proton noise decoupled 13C NMR spectra. Assignment of chemical shifts, additively effect, characteristic chemical shifts of common organic compounds and functional groups, DEPT and SEFT spectra.
NMR of common heteroatoms present in organic compounds (N, F, O, P, S and D)
2D NMR techniques 1H – 1H COSY, 1H – 13C COSY – HMBC, NOESY and INADEQUATE spectra.

Unit IV (Application of mass spectroscopy to organic structure elucidation)
Basic principles, techniques of ion production and ion and daughter ions, molecular ion and isotope abundance, nitrogen rule, energetics of fragmentation - metastable ions, common fragmentation pathways – fragmentation pattern of common chemical classes.
Unit V (Problem solving exercises involving UV, IR NMR & MS data)
Problems involving interpretation of spectral details of organic compounds

Textbook:
R. M. Silverstein and F. X. Webster, Spectrometric identification of organic compounds., John Wiley and Sons.Inc., Sixth edition (1997).

Further reading:
1. W. Kemp, Organic Spectroscopy, Third Edition , MacMillon (1994).
2. Pavia, Lampman and Kriz, Introduction to Spectroscopy, 3rd Edn., Brooks/Cole Pubs. Co.
2. D. H Williams and Ian Fleming, Spectroscopic methods in organic chemistry, Tata McGraw Hill, (1998).
4. William Kemp, Introduction to multinuclear NMR.

CHEM 444: Statistical thermodynamics and reaction dynamics 3-0-0-3

Unit I (Statistical Thermodynamics – Introduction)
Probability, Bose-Einstein, Fermi-Dirac, Boltzmann statistics and distribution and sterling's approximation

Unit II (Statistical Thermodynamics – Partition function and implications)
Partition function and thermodynamic properties - Partition function- translational, rotational, vibrational, electronic,- entropy, energy and heat capacity – heat capacity of solids – equilibrium constant

Unit III (Non-equilibrium Thermodynamics)
Entropy production, flux-force relationship, Onsager reciprocal relationship, electrochemical potential, steady state entropy

Unit IV (Reaction Dynamics)
Potential energy surfaces-electronically excited molecules, bimolecular collisions, Molecular beam Scattering, statistical approach of reaction dynamics to transition state theory, unimolecular reaction dynamics, transition state theory of solution reactions, kramers's theory,

Unit V (Electrode Kinetics)
Electrical double layer, Aspects of electrochemical reactions, elucidation of mechanism of an electrode reaction

Textbook
Physical chemistry – McQuirre,

Further Reading:

CHEM 464: Quantum Chemistry II 3-0-0-3
Prerequisite: CHEM 463

Unit I (Diatomics)
Born-Oppenheimer approximation – MO Theory – LCAO approximation – Orthogonality of MOs – MOs of H2+ and H2 –- Excited states of H2 -VB theory – Comparison of VB vs MO methods - non-crossing rule, correlation of homo and hetero nuclear diatomics, MO configuration, Electronic states and Term symbols.

Unit II (Empirical MO theory)
The simple Huckel method –Assumptions – Determinant, Energies and Wave functions – Extended Huckel Method - Overlap – Population analysis - FMO theory – Interaction and Walsh diagrams – Non-crossing rule – s-p mixing – hybridization - Conjugation and Hyperconjugation – FMOs of functional groups – Isolobal analogy.

Unit III (Basics of Popular Quantum Chemical Calculations)
Hamiltonian and Wave functions – Roothan's equations – Fock matrix – SCF procedure - Interpretation of LCAO-MO-SCF Results – unrestricted open-shell Hertree-Fock theory - Basis sets – Semi-empirical methods – Density Functional Theory – Hellmann-Feynmann theorem.

Unit IV (Properties of Molecules)
Normal modes - Vibrational Analysis and Characterization of Stationary Points – Electrical Properties (dipole moments, optical activity, Polarizability)– Magnetic Properties (NMR chemical shifts, shielding, spin-spin coupling and Hyperfine interactions) – Thermodynamic properties – IRC and excited state studies,

Unit V (Advanced Topics in Quantum chemistry)
Electron correlation – Configuration Interaction (CI) – Truncated and Direct CI – Multi configuration SCF – Complete Active Space SCF – Multi Reference CI – Many body perturbation theory – Coupled Cluster Methods – Quantum Chemistry of Solids – Band Structure and Density of State Calculations – Population Analysis.

Recommended Books:
1. J. P. Lowe and K. A. Peterson, Elsevier Acadamic Press, New York, 2006.
2. P. W Atkins and R. S. Friedman: Molecular Quantum Mechanics, Oxford, 2005.
3. T. A. Albright, J. K. Burdett, M. H. Whangbo, Orbital Interactions in Chemistry, John-Wiley & sons, 1985.
4. F. Jensen, Introduction to computational chemistry, Wiley, NY, 2007.
5. D. C. Young, Computational Chemistry, John-Wiley and Sons, NY, 2001.
6. C. J. Cramer, Essentials of Computational Chemistry, John-Wiley & Sons, 2004.
7. N. W. Ashcroft, N. D. Mermin, Solid State Physics, Cornell University, NY, 1976.
8. A. Szabo and N. S. Ostlund, Modern Quantum Chemistry, Dover, NY, 1996.
9. R. Hoffmann, Solids and Surfaces, Wiley-VCH, NY, 1988.

CHEM 500 – Advanced laboratory techniques 0-0-8-3
Experiments related to advanced synthetic and analytical techniques

CHEM 503 Advanced Inorganic chemistry III 4-0-0-4

UNIT I (Organometallic Chemistry 1)
Compounds with transition metal to carbon bonds: classification of ligands, nomenclature, eighteen electron rule; transition metal carbonyls: range of compounds and structure, bonding, vibrational spectra, preparation, reactions; transition metal organometallics: square planar complexes, metal alkyls, metal alkylidenes and metal alkylidynes; Structure and bonding: metal-olefin bond and arene metal bond.

UNIT II (Organometallic Chemistry 2)
Compounds with ligands having extended pi systems: bis(cyclopentadienyl) compounds, cyclopentadienyl carbonyl compounds, bis(arene) compounds, arene carbonyl compounds; isolobal analogy, metal-metal bond, transition metal clusters; clusters and catalysis; hydride and dihydrogen complexes; fluxionality.

UNIT III (Organometallic Chemistry 3)
Organometallic reactions and catalysis: oxidative addition, reductive elimination, insertion, hydride elimination, abstraction; olefin hydrogenation, hydroformylation, Wacker process, Ziegler-Natta polymerisation, cyclo oligomerisation, olefin isomerisation, olefin metathesis, Monsanto acetic acid synthesis, Fischer-Tropsch process, hydrosilylation.

UNIT IV (Bioinorganic Chemistry 1)
Metal ions in biological systems: heme proteins, hemoglobin, myoglobin, hemerythrin, hemocyanin, ferritin, transferrin, cytochromes and vitamin B12; Iron-sulphur proteins: rubredoxin, ferredoxin and model systems.

UNIT V (Bioinorganic Chemistry 2)
Metalloenzymes: active sites, carboxy peptidase, carbonic anhydrase, superoxide dimutase, xanthine oxidase, peroxidase and catalase; photosynthesis, water oxidation, nitrogen fixation, nitrogenase; ion pump, metallodrugs.

Text books:
P. Powell, Principles of Organometallic Chemistry, 2nd Edn., ELBS, 1991.
J. E. Huheey, Inorganic Chemistry, 4th Edn., Harper International, 2001.

Recommended Books:
3. C. Elschenbroich, A. Salzer, 2nd Edn., VCH, 1992.
4. M. F. Purcell, J. C. Kotz, Inorganic Chemistry, Saunder, 1977.
5. F. A. Cotton, G. Wilkinson, Advanced Inorganic Chemistry, 5th Edn., John Wiley.
6. R. W. Hay, Bio Inorganic Chemistry, Ellis Horwood, 1987.
7. Lehninger, Principles of Biochemistry, Van Eikeren, 1982.

8. T. M. Loehr, Iron carriers and Iron proteins, VCH, 1989.

CHEM 523 Advanced organic chemistry II 4-0-0-4

Unit I (Concerted Reactions)
Cycloaddition, electrocyclic and sigmatropic and related pericyclic reactions - Explanations based on frontier orbital, Woodward-Hoffman and Huckel-Mobius theories - Application of concerted reactions in organic synthesis.

Unit II (Organic Photochemistry)
Introduction to organic photochemistry - Frank Condon Principle - Jablonski diagram and energetics of excitation - Photochemistry of alkene, diene, aromatic, carbonyl and conjugated systems - Application of photochemical reactions in organic synthesis.

Unit III (Modern reagents in organic Synthesis)
Introductory treatment to the application of silicon, phosphorus, selenium, palladium, ruthenium, rhodium, indium, titanium and samarium reagents in organic synthesis.

Unit IV (Rearrangement reactions in Organic Synthesis)
Review of rearrangement reactions and their application in organic synthesis (emphasis on reactions rather than reactivity)

Unit V (Oxidation and Reduction Reactions in Organic Synthesis)
Oxidation of organic compounds with reagents based on peroxides, peracids, ozone, osmium, chromium, ruthenium, silver, dimethyl sulfoxide, iodine, and selenium dioxide. Reduction of organic compounds with reagents based on alkali and alkaline earth metals, boron, aluminum, hydrogen, hydrazine, formic acid and dissolving metals.

Recommended Books:
1. R.O.C. Norman and J. Coxon, Principles of Organic Synthesis - ELBS, 1994.
2. Smith, Organic Synthesis - Magrew-Hill, 1996.
3. J.D. Coyle, Organic Photochemistry - Wiley, 1985.
4. Carruthers, Modern Methods in Organic Syntheis, Academic Press, 1989.

CHEM: 527 Advanced organic chemistry III 3-0-0-3

Unit I (Heterocyclic chemistry – I)
Nomenclature, Non-aromatic heterocyclic compounds – three, four, five, six membered rings with one hetero atom (N,O,S), structure, synthesis and reactions.

Unit II (Heterocyclic chemistry – II)
Aromatic heterocyclic compounds – five and six membered heterocyclic systems with two hetero-atoms (N, O, S). Benzo fused heterocyclic systems – structure, synthesis and reactivity.

Unit III (Biochemical Reactions and Reagents)

Fixation of carbondioxide and other photosynthetic reactions – Kerb's cycle – structure and reactions of important coenzymes – Biosynthesis of amino acids – Kelvin cycle – Urea cycle – introduction to biosynthetic pathways to secondary metabolites

Unit IV (Green Chemistry)
Green Chemistry – Genesis and concept of Green Chemistry, Principles, Strategies
Alternative Techniques in Organic Synthesis
Use of microwave, ultrasound, ionic liquids, super-critical solvents in organic synthesis; Multi-component reactions

Unit V (Synthetic Methodology)
Synthesis of Target Molecules based on synthon approach, disconnection approach; retro-synthetic analysis; synthesis using chiral molecules.

Recommended Books
1. T.L.Gilchrist, Heterocyclic Chemistry. John Wiley & Sons, (1987)
2. J.A Joule and K.Mills, Heterocyclic Chemistry, Fourth edition, Blackwell Science Ltd, (2000).
3. E.E Conn, P.K Stumpf and Doi, Biochemistry, John Wiley , (1992).
4. Clayden Organic Chemistry
5. S. Warren, Organic Synthesis, Disconnection Approach, John Wiley, 1985.
6. Rashmi Sinhi and M.M. Srivastava;(Ed) Narosa Publications Green Chemistry Environmentally Friendly Alternatives

CHEM 543 Spectroscopy- Theory and application 4-0-0-4

Unit I (Microwave and IR spectroscopy)
Electromagnetic radiation, interaction of electromagnetic radiation with matter, quantum mechanical approach - transition probabilities: Einstein coefficients - pure vibrational and rotational spectra, selection rules, vibrational and rotational spectra of polyatomic molecules, normal modes, anharmonicity, selection rules - Raman effect: classical and quantum theory of Raman effect, rotational and vib-rotational Raman spectra

UNIT II (Electronic spectroscopy)
Transition moments, assignment of electronic transitions of N2, H2O and formaldehyde using group theory, fluorescence and phosphorescence, ESCA, PES, AUGER techniques

UNIT III (Magnetic Resonance I: introduction to theory of NMR)
Origin of magnetic moments in matter, electronic and nuclear moments, interaction with magnetic field, Larmor equation - conditions for magnetic resonance absorption, relaxation times, line widths and line shapes, chemical shifts, ring currents, diamagnetic anisotropy, spin-spin splitting, high resolution NMR spectra of simple molecules, first and second order treatment of AB systems - FT techniques

UNIT IV (Magnetic Resonance II)

EPR, NQR and mossbauer spectroscopic techniques - Electron spin resonance: g value, hyperfine structure, esr of organic free radicals, esr of solids, esr of inorganic ions, esr of simple free radicals in solutions - NQR and Mossbauer spectroscopy.

UNIT V (Introductory solid state chemistry)
Crystal morphology, Mi1ler indices - x-ray diffraction - close packing, factors affecting crystal structure, defects, vacancies and dislocations - LEED, neutron diffraction and electron diffraction.

Recommended Books:
1. P. W. Atkins, Physical Chemistry, Oxford, London, 6th edition, 1998.
2. R. Sindhu, Molecular Spectroscopy, Tata McGraw Hill, 1986.
3. Banwell, Molecular Spectroscopy, Tata McGraw Hill, 1998.
4. A. Carrington and Machlachlon, Magnetic Resonance, Harper & Row, 1967.
5. Graebeal, Molecular Spectroscopy, Prientice Hall, 1968.
6. G. M. Barrow, Introduction to Molecular Spectroscopy, McGraw Hill, 1964.

CHEM 580 PROJECT 0-0-16-5

Students are allotted to various faculties of the department according to their CPI and / or choice. They will be working on specialized problem related to the research interests of the respective guides.

CHEM 504 Inorganic photochemistry 4-0-0-4
Pre-requisite: CHEM 402, CHEM 501

UNIT I (Basic principles)
Absorption of light –photochemical laws – photostationary states – rate law – photolysis – quantum yields – actinometry – scavenging of reaction intermediates – flash photolysis – single photon techniques – flow techniques – picosecond transient kinetics.

UNIT II (Kinetics of photoluminescence)
Thermal effects of photoluminescence – luminescence yield – time resolved detection of excited states – radiative and non radiative transitions – energy transfer.

UNIT III (Photoredox reactions)
Charge transfer complex – theory of electron transfer reactions – reactivity of CTTM, CTTL excited states – medium effects

UNIT IV (Ligand field photochemistry)
General features of ligand field photochemistry – reaction of excited states of dn metal complexes.

UNIT V (Organometallic photochemistry)
Excited states in organometallic compounds – metal carbonyls – compounds with □ or □ M – C bonds – hydride complexes.

Recommended Books:
1. K.K. Rohatgi-Mukherjee, Fundamentals of Photochemistry, Tata-McGraw Hill, 1981.
2. J. Calvert and J.N. Pitts, Photochemistry
3. Collected readings in inorganic photochemistry, J. Chem. Edn. 1983
4. G. J. Ferraudi, Inorganic photochemistry, 1973
5. A.W. Adamson, E.D. Fleishcer, Concepts in inorganic photochemistry, 1963

CHEM 506 Ligand Field Theory 4-0-0-4
Pre-requisites: CHEM 463 &CHEM 464

UNIT I (Introduction)
Qualitative basis of crystal fields, Atomic spectroscopy (free ion, free ion terms, term wave functions, spin-orbit coupling), Thermodynamic aspects of crystal fields.

UNIT II (Ions in Crystal Field)
Free ions in weak crystal fields (effect of a cubic crystal field on S,P,D,F,G,H, and I terms), Free ions in Medium and strong crystal fields.

UNIT III (MO theory of complex ions)
Bonding in Oh/Td complexes, qualitative calculations of 10Dq, Electronic spectra of complex ions.

UNIT IV (Magnetic properties of complex ions)
Complexes of non-cube stereochemistry, Actinide element compounds

UNIT V (ESR of complex ions)
Theory and evaluation of spin Hamiltonian parameters for systems with s=1/2 and s >1/2.

Recommended Books:
1. B.N. Figgis, Introduction to Ligand Fields, Wiley Eastern Ltd., New Delhi/Bangalore, 1976.
2. A. B. P. Lever, Inorganic Electronic Spectroscopy, Elsevier, 1986.

CHEM 508 Supra-molecular chemistry 4-0-0-4

Unit I (Concepts of Supramolecular Chemistry)
Definition, Nature of supramolecular interactions, Host-guest interaction, Molecular recognition, Types of recognition, Self-assembly.

Unit II (Cation-binding Hosts)
Concepts, Cation receptors, Crown ethers, Cryptands, Spherands, Calixarens, Selectivity of cation complexation, Macrocyclic and template effects.

Unit III (Binding of Anions and Neutral molecules)

Concepts, Anion host design, Anion receptors, Shape and selectivity, Neutral receptors, clathrates, cavitands, cyclodextrins, cyclophanes.

UNIT IV (Applications of Supramolecular Chemistry)
Rational Design, Molecular Paneling, Supramolecular reactivity and catalysis, Supramolecular devices, Nanoscience applications.

UNIT V (Supramolecular Chemistry in Biology)
Membranes, Macrocyclic systems, Photosynthesis, Oxygen transport, Biological mimics, Enzymes, Metallobiosites, Heme analogues.

Recommended Books:
1. J. M. Lehn, Supramolecular Chemistry, Concepts and Perspectives, VCH, 1995.
2. H. Dodziuk, Introduction to Supramolecular Chemistry, Kluwer Academic, 2002.
3. F. Vogtle, Supramolecular Chemistry, An Introduction, John Wiley & Sons, 1991.
4. J. W. Steed, J. L. Atwood, Supramolecular Chemistry, A Concise Introduction, John Wiley, 2000.
5. A. Bianchi, K. B. James, E. G. Espana, Supramolecular Chemistry of Anions, Wiley-VCH, 1997.
6. M. Fujita, Molecular Self-assembly, Organic Versus Inorganic Approaches, Springer, 2000.
7. J. L. Atwood, J. E. D. Davies, D. D. MacNicol, F. Vogtle, J. M. Lehn, Comprehensive Supramolecular Chemistry, Pergamon, 1996.

CHEM 524 Natural products chemistry 3-0-0-3
Pre-requisite: CHEM 527

Unit I (Chemistry of Terpenes)
Biosynthesis of Terpenoids - Monoterpenes - Sesquiterpenes - Diterpenes (structure of terpenoids such as pinene, camphor, hirsutene, abietic acid, squalene etc),

Unit II (Steroids)
Biosynthesis of Steroids - Structure of common steroids such as cholesterol, ergosterol, stegmasterol, Cholic acid - Steroidal hormones; Estrone, Progesterone - Testosterone - Synthetic strategies towards steroids

Unit III (Poly-phenolics and other plant coloring molecules)
Chemistry of flavones; isoflavones and aurones, Biosynthesis and role of polyphenolics

Unit IV (Alkaloids and antibiotics)
Biosynthesis and structure determination of representative examples of pyrrolidine, piperidine, indole, quinoline, and isoquinoline alkaoids; Structure of □-lactam antibiotics (penicillin)

Unit V(Introduction to Marine Natural Products)

Recommended Books:
1. K. Nakanishi, Natural Product Chemistry Blackie Publications, 3 Vols.
2. R.H. Thomson, Chemistry of Natural Products - Wiley, New York, 1996.
3. I.L. Finar, Advanced Organic Chemistry, ELBS, New Delhi, 1975.

CHEM 528 Asymmetric synthesis 3-0-0-3

Unit I (Introduction to asymmetric synthesis)
Asymmetric synthesis – Definition, importance of asymmetric synthesis, conditions for an efficient asymmetric synthesis, energetic considerations, strategies for asymmetric synthesis- advantages and limitations of each strategy, analytical methods for determining enantiomeric excess. Resolving agents and resolution of common functional groups. Resolution of priviledged chiral ligands- BINOL, trans 1,2-diaminocyclohexane

Unit II (Substrate and reagent control of stereoselectivity) Asymmetric synthesis with chiral substrate: Nucleophilic addition to α –chiral carbonyl compounds, Electrophilic addition to α – chiral olefins - epoxidation, cyclopropanation, hydroboration – oxidation, alkylation of enolates of β-chiral carbonyl compounds. Asymmetric synthesis using chiral reagents: Chiral organo boranes ,- application in hydroboration, reduction and allylation reactions, T.S models, Chiral lithium aluminium hydride application in reduction of prochiral ketones T.S model, chiral organo cuprates, Michael addition to α ,β – unsaturated carbonyl compounds T.S model, chiral lithium amides – enantioselective deprotonation.

Unit III (Reaction between chiral substrate and chiral reagent)
Double stereo differentiation Matched pair and mismatched pair example from aldol reaction and hydroboration reactions. Kinetic resolution

Unit IV (Asymmetric synthesis using chiral auxiliary)
Champhor derived auxiliaries, menthol derived auxiliaries chiral pyrrolidines, oxithiane, oxazolidine-2-one, oxazoline, 2-phenylcyclohexanols, 8-phenylmenthol, SAMP, RAMP hydrazones Structure, Functional group for which it is an auxiliary, selected reactions.

Unit V (Asymmetric synthesis using chiral catalyst) Organometallic catalysts : Hydrogenation catalyst, Sharpless epoxidation catalyst, semicorin catalyst, Jacobson catalyst, selected reactions. Organo caltalysts : Chiral proline and proline derived compounds, tertiary amines, phosphanes, phosphoramides, ureas amidines, imines, diols, sulphides in asymmetric reactions – selected examples.

Recommended Books
1.Eliel Stereochemistry of Organic Compounds
2.R.E.Gawley and J.Aube; Principles of Asymmetric Synthesis, Pergaman, 1996
3.G.Q.Lin, Y.Li and A.S.Cchan Principles and applications of asymmetric synthesis; Wiley-Interscience; 2001.

CEM 542: Advanced Magnetic Resonance and solid state chemistry 4-0-0-4

Unit I(Magnetic Resonance-I)
Classical and quantum mechanical description of resonance, Bloch's equations and solution for a weak rf-field, complex susceptibilities, nuclear induction, FT techniques, 900and 1800 pulses, spin echoes, measurements of T 1 and T 2 by pulse techniques, NOE, 2D-J-resolved NMR, COSY.

Unit II (Magnetic Resonance-II)
Spin-Hamiltonian for hydrogen atom, first and second order perturbation treatment, isotropic and anisotropic hyperfine interactions. Mechanism of hyperfine interactions in aromatic radical ions in solutions, spin density, McConnel relation. EPR in solids: g- and A- matrices, effective spin Hamiltonian, treatment for p1 and dl ions. Single crystal and powder EPR lineshapes, S >1/2 systems with emphasis on zero-field splitting. }

Unit III (Solid State Chemistry-1)
Imperfactions and related phenomena- Defects in Solids: Point defects, line defects and plane defects. Thermal properties- Heat capacities of Solids: Dulong-Petit law, Einstein and Debye theories, thermal conductivity of insulators and thermal expansion coefficient. Electrical conductivity- origin of band gap, Fermy energy, density of states, thermal conductivity of metals, semiconductors and superconductivity.

Unit IV (Solid State Chemistry-2)
Magnetic properties: classification of magnetic materials, quantum mechanical theory of paramagnetism, nuclear paramagnetism, ferro- antiferro- and ferrimagnetism. Solid state transformations, solid state reactions, theory and techniques of crystal growth.

Unit V (Solid State Chemistry-3)
Diffusion in solids: diffusion mechanisms, Ficks laws of diffusion, diffusion as a random walk problem. Optical properties: thermionic emmission, photovoltaic effect, optical absorption of semiconductors. Dielectric properties: dielectric constant and related properties, behaviour of dielectric materials in ac fields, Clausius-mosotti equation. Thermoelectric effects: Thompson effects, peltier effect, Seebeck effect, thermocouples and Hall effect. Hopping semiconductors, polarons , liquid crystals, and glasses. Pauling's rules in polyhedral structural chemistry

Recommended Books
1. H. V. Keer, Principles of Solid State, Wiley Eastern Limited, 1993
2. W. R. West, Solid State Chemistry and its Applications, John Wiley and Sons, New York, 1984.
3. A Carrington and A. D. Mclachlan, Introduction to Magnetic Resonance, Harper & Row, New York, 1979.
4. A Derome, Modern NMR Technique, Pergamon, 1983.
5. Farrar and E. D. Becker, Pulsed FT NMR Spectroscopy.
6. Wertz and Bolton, Electron Spin Resonance, McGraw Hill.

CHEM 546 – Electro analytical techniques 3-0-0-3

Unit I (Kinetics of Electrode Reactions)
Mass transfer by Diffusion and Migration – models of electrode reactions – current potential characteristics – general mass transfer equation , migration and diffusion

Unit II (Potential Step Methods)
Types of techniques, step under diffusion control, Ilkovic equation – polarographic analysis – sampled current voltammetry: reversible, irreversible processes, multicomponent systems

Unit III (Chrono Methods)
Chronoamperometry, chronocoulometry – pulse polarographic methods: Tast pulse, normal pulse, differential pulse

Unit IV (Potential Sweep Methods)
Cyclic Voltammetry: Nernstian reversible, totally irreversible, quasi-reversible processes, multicomponent systems – convolute or semi-integral techniques

Unit V (Bulk Electrolysis Techniques)
Classification of methods – Controlled Potential methods: current – time behaviour, electrogravimetry, electroseparation – Coulometric measurements: controlled current methods: characteristics, coulometric methods – Electrometric end point detection: classification, potentiometric, amperometric methods.

Recommended Books:
1. A. J. Bard and L. R. Faulkner, Electrochmical Methods, Fundamentals and applications, John Wiley, 1980
2. Bockris and Reddy, Electrochemistry, vol 1 & 2, Plenum, 1973.
3. H. Kissinger, Electroanalytical Techniques, John wiley, 1998
4. P. H. Reiger, Electrochemistry, Prientice Hall, 1987.

CHEM 548 Nanomaterial and Photo-catalysis 4-0-0-4

Unit I (Nanomaterials)
Nano-science, Fullerene, types of Nanotubes, Molecular Computers

Unit II (Nano-biometrics)
Lipids, templates, proteins, optical memory and DNA, information and Probes, Photodynamic therapy

Unit III (Photonics and Solar Energy)
Photon trapping, nanoholes and photons, formation imaging, solar absorbers, nanostructural polymers, photonic crystals

Unit IV (Nano-electronics and Quantum electronics)
Semiconductors, Transistors, Nanofabrication of Quantum Computers.

Unit V (Nanomaterial Photo-catalysis)
Nanostructured materials, energy conversion and storage

Recommended books:
1. Nanotechnology Basic Science and Energy Technologies, Mich Wilson, Kamali Kanengara, Geoff smith, Michelle Simmons and Burkherd Raguk, Overseas press (I), N.D. 2005.