CY-101: Stoichiometry, Solutions and Gases (3 credits)

Prerequisite: None

Experimental evidence for the atomic hypothesis. Chemical compounds and their composition - introduction to nomenclature. Chemical reactions and stoichiometric calculations. (8 h)

Solution chemistry - electrolytes and non-electrolytes. Colligative properties. Ideal and non-ideal solutions. Reactions in solution - redox, acid-base, precipitation, ionexchange. Colloids. (14 h)

Properties of gases - Avogadro's hypothesis, the ideal gas law. Kinetic molecular theory. Gas mixtures. Solubility of gases. Gases at high pressure and low temperatures - critical phenomena. (14 h)

Suggested reading:

Will be prescribed by the instructor.

CY-102: Qualitative Analysis Lab. (1.5 credits)

Prerequisite: None

Reactions of common cations and anions. Semimicro analysis of mixtures.

Suggested reading:

Lab Manual

CY-151: Energetics and kinetics (3 credits)

Prerequisite: None

Thermochemistry - enthalpy and enthalpy change - calorimetry - enthalpies of formation and of reactions. Entropy and free energy. State functions. (8 h)

Chemical kinetics - reaction rates - effect of concentration and temperatures. Steady state approximation. Reaction mechanism from rate laws. (8 h)

Chemical equilibrium in the gas phase - equilibrium constants and their relation to free energy - temperature dependence. (6 h)

Equilibrium in the aqueous phase - pH, buffers and indicators - complex ions. Heterogeneous equilibria - adsorption. (6 h)

Electrochemistry - voltage and free energy - standard potentials Batteries, fuel cells. (8 h)

Suggested reading:
Will be prescribed by the instructor.

CY-152: Quantitative Analysis Lab. (1.5 credits)

Prerequisite: None

Titrimetry - acid-base, redox, complexometry.

Gravimetry - determination of water of hydration, estimation of sulphate, chloride, aluminium, manganese, iron, nickel.

Colorimetry - Beer's law, estimation of a metal ion (eg., manganese).

Suggested reading:

Lab manual

CY-201: Structural chemistry (3 credits)

Prerequisite: None

Electrons in atoms - the orbital concept - shapes and size of atomic orbitals - electron configuration and the periodic table. (4 h)

The chemical bond - ionic and covalent bonding. MO and VB pictures - hybridization, resonance. Bond parameters - energy, polarity, length. (8 h)

Shapes of molecules - VSEPR theory. (4 h)

The hydrogen bond. Intermolecular forces and non-bonded intra-molecular interactions. Molecular conformations. Examples of different structures and their stabilities from tri-atomics to bio-molecules. (6 h)

The solid state - molecular, ionic and metallic crystals. Crystal lattices - unit cells. Common crystal structures. Factors influencing crystal structures in ionic/molecular solids. Allotropes (of carbon and sulphur). Network solids - silicates. (8 h)

X-ray diffraction and elementary treatment of Bragg's law - NaCl and KCl. (6 h)

Suggested reading:

Will be prescribed by the instructor.

CY-202: Physical Chemistry Laboratory (1.5 credits)

Prerequisite: CY-101, CY-151, CY-152

Contents:

Molecular weight of a polymer (viscometry)

Stoichiometry of a complex (Job's method : colorimetry)

Conductometric titrations

Thermodynamics

- Heat of solution (calorimetry)
- Phase diagram of a 2-component system
- pK_a of amino acid (pH titration)
- Solubility product
- Paritition coefficient

Kinetics

- Rate constant of acid catalysed ester hydrolysis

Suggested reading:

Lab manual

CY-251: Basic Organic Chemistry (3 credits)

Prerequisite: None

1. Bonding and physical properties of organic molecules (8 h)

Nomenclature of simple organic compounds (acyclic, cyclic). Concept of hybridization, resonance, orbital pictures of bonding (sp3, sp2, sp, C-C, C-N & C-O system). Inductive effect, bond polarization, and polarizability, steric inhibition of resonance. Hückel's rules for aromaticity & antiaromaticity, homoaromaticity. Physical properties of bond distance, bond angles, mp/bp & dipole moment in terms of structure and bonding. Concept of acids and bases: effect of structure, substituent and solvent on acidity and basicity.

2. Basic reaction mechanism and intermediates (8 h)

Mechanism classifications - ionic, radical and pericyclic; heterolytic bond cleavage and heterogenic bond formation, homolytic bond cleavage and homogenic bond formation; representation of mechanistic steps using arrow formalism. Reactive intermediates: carbocation (carbenium and carbonium ions), carbanions, carbon radicals, carbenes-structure using orbital picture, electrophilic/nucleophilic behavior, stability, generation and fate (elementary idea)

3. Optical activity and stereochemistry (8 h)

Representation of molecules in saw-horse, Fischer, flying-wedge and Newman formulae and their inter translations, symmetry element and molecular chirality. Configuration: stereogenic unit i) stereocenters: systems involving 1, 2, 3 centers, stereogenicity, chirotopicity, pseudoasymmetric (D/L and R/S) descriptor, threo/ erythro / meso and syn/anti nomenclature. Stereo axis: chiral axis in allenes & biphenyls, R/S descriptor: cis/trans, syn/anti, E/Z descriptors (at C=C and C=N bonds). Optical activity of chiral compounds: specific rotation, optical purity (enantiomeric excess), racemic compounds.

4. Chemistry of organic functional groups (12 h)

Alkanes, olefins, alkynes, halides, alcohols, phenols, ketones, aldehydes, carboxylic acids, ethers, derivatives of carboxylic acids, amines, nitro and cyano compounds; synthesis and basic reactivity with mechanisms.

Suggested Text Books:

1. R. T. Morrison, R. N. Boyd and S. K. Bhattacharjee, Organic Chemistry, 7th Edition, Pearson Education.
2. P. Y. Bruice, Organic Chemistry, 4th Edition, Pearson Education.
3. T. W. Graham Solomons and C. B. Fryhle, Organic Chemistry, 10th edition, Wiley.
4. I. L. Finar, Organic Chemistry, Vol-1, 6th edition, Pearson Education.
5. E. L. Eliel and S. H. Wilen, Stereochemistry of Organic Compounds, Wiley.

CY-252: Identification of Organic Compounds (1.5 credits)

Prerequisite: None

Separation and purification of organic compounds - melting point - boiling point. Characteristic reactions of functional groups. Identification of unknowns - chemical and spectral methods.

Suggested reading:

Lab manual

CY-253: Introductory Supramolecular Chemistry (2 credits)

Prerequisite: None

Basic concepts using chemistry examples (2 h)

Intermolecular interactions and hydrogen bonds (3 h)

Cation binding hosts, cryptands, crown ethers (3 h)

Anion binding hosts, single and multi-point recognition (3 h)

Crystal engineering of solid architectures (4 h)

Self-Assembly in nature and materials (3 h)

Recent examples from literature (4 h)

Suggested Reading:

1. "Supramolecular Chemistry"by J. W. Steed & J. L. Atwood, 1stEdn John Wiley, 2009.
2. "Crystal Engineering. The Design of Organic Solids" by G.R. Desiraju, Elsevier, 1989.
3. "Crystal Engineering - A Textbook" by G. R. Desiraju, J. J. Vittal, A. Ramanan, World Scientific-IISc Press, 2009.
4. Recent papers from journals and reviews and monographs, etc.

CY-254: Elementary Polymer Chemistry (2 credits)

Prerequisite: None

History of macromolecular science. (1 h)

Definition of polymer, monomer, repeat unit, polymerization. Classification of Polymers based on source and polymerizations-polymer composition and structure. Nomenclature- IUPAC, Non-IUPAC, structure-based, and trade names. Types of polymers based on their molecular structure (linear, branched, cross-linked, block) and stereochemistry of repeating units (Tacticity in polymers) (5 h)

Molecular Weights and Sizes: Solubility parameters, Thermodynamics of mixing, Polymer shape and size, measurement techniques-viscosity, colligative properties, chromatography (5 h)

Physical State: Crystalline and Amorphous state, Thermal transitions, Glass-Rubber transition, Mechanical properties- stress-strain behaviour, Elastomer, Fibers and Plastics (5 h)

Polymer Synthesis: step, chain and miscellaneous polymerizations, Kinetics of polymerization (7 h)

Application of Synthetic Polymers: Materials and Biological importance and uses. (3 h)

Suggested Reading:

1. Principles of Polymerization by Geroge Odian
2. Introduction to Physical Polymer Science by L. H. Sperling
3. Polymer Chemistry: An Introduction by M. P. Stevens

CY-301: Inorganic Chemistry (3 credits)

Nuclear Chemistry: Origin of the elements - Nuclear stability and nuclear binding energy - Nuclear forces - Nuclear Reactions - Artificial radioactivity - Transmutation of elements - Fission, fusion and spallation - Nuclear energy - Separation and uses of isotopes - Radiochemical methods - Principles of determination of age of rocks and minerals- Radio-carbon dating - Hazards of radiation and safety measures (6h)

Acids, Bases and Buffers: Arrhenius, Brönsted-Lowry, and Lewis concepts of acids and bases - Factors affecting strengths of acids and bases - K_a, K_b, K_w, pH etc.- Buffers, Henderson's equation - Hydrolysis of salts - Common ion effect (3h)

Non-aqueous Solvents: Physical properties of a solvent for functioning as an effective reaction medium - Types of solvents and their general characteristics - Reactions in liquid ammonia and liquid sulfur dioxide (3h)

Chemistry of selected main group elements: Hydrogen bonds, Hydrates and water clathrates - Hydrides and dihydrogen - Alkali metal solution in liquid ammonia - Complexation of alkali metal ion by crown ether and cryptands, Alkali metal anions. Diborane – structure and bonding - Noble gas compounds (4h)

Coordination Compounds and Transition elements: Werner's theory – Nomenclature- Chelates- Stereochemistry of coordination numbers 4, 5 and 6 - Various types of isomerism in coordination complexes- Theories of metal-ligand bonding in transition metal complexes – Effective atomic number concept- Valence bond theory of coordination compounds - Limitations of valence bond theory - Crystal-field theory and crystal-field splitting in octahedral and tetrahedral complexes - CFSE and its calculation in different stereochemistries - Weak field and strong field- Low spin and high spin complexes - Pairing energy - Spin cross-over region - Brief account of transition elements (14h)

Organometallic chemistry: Definition, nomenclature and classification of organometallic compounds- Alkyl and aryls of Li, Al, Hg and Sn- Metal-ethylenic complexes (3h)

Bioinorganic chemistry: Essential and trace elements in biological processes- Oxygen transport in myoglobin and haemoglobin- Biological function of alkali metal ions (3h)

Suggested reading: F. A. Cotton, G. Wilkinson, P. G. Gauss, Basic Inorganic Chemistry, 3rd Edition, John Wiley, 1995

CY-302: Organic Chemistry: Synthesis and Reactions (3 credits)

1. Addition to C=C bonds and organometallics (8 h)

Electrophilic addition to C=C bonds: Mechanism, reactivity, regioselectivity and stereoselectivity. Reactions: halogenation, hydrohalogenation, hydration, hydrogenation, epoxidation, hydroxylation, ozonolysis, electrophilic addition to dienes (conjugated dienes and allenes). Cycloaddition.

Radical addition: HBr addition, dissolving metal reaction of alkynes and benzenoid aromatics (Birch).

Organometallics: preparation of Grignard reagent, organo lithium and Gilman cuprates and their reactions, 1,2- and 1,4-additions. Reformatsky reaction.

2. Chemistry of carbonyl compounds (9 h)

Chemistry of -carbon of carbonyls-acidity of □-hydrogen (pKa of different carbon acids), keto-enol tautomerism, base and acid catalyzed keto-enol tautomerism. Halogenation, haloform reaction, Hell-Volhardt-Zelinski reaction, □-alkylation, aldol reaction [mixed and directed (metal enolate, enamine)], Michael reaction, Robinson annulation, Knoevenagel condensation, Claisen ester condensation, Dieckmann condensation, Perkin reaction, Stobbe condensation, Darzens reaction, acyloin condensation, McMurry coupling, Wittig reaction.

Malonic and acetoacetic esters: Characteristic reactions of active methylene group, synthetic uses of malonic, acetoacetic and cyanoacetic ester.

Addition of nucleophile to carbonyl adjacent to stereogenic center: Cram and Felkin-Anh model. Umpolung using dithiane.

3. Reagents for reduction and oxidation: Classical methods. (6 h)

4. Substitution, and elimination reactions (13 h)

Substitution at sp3 carbon center- SN1, SN2 and SN2′ mechanisms), effect of solvent, substrate structure, leaving group and nucleophiles, including ambident nucleophiles (e.g. cyanide & nitrite). Mechanism: E1, E2 and E1cB; reactivity. Substitution involving NGP, relative rate & stereochemical features [systems: alkyl halides, allyl halides, alcohols, ethers, epoxides]. Substitution at sp2 carbon. BAC2, AAC2, AAC1 and AAL1 mechanisms (in connection with acids and esters), nucleophilic substitution (SN1, SN2 NGP) cyclohexane system. Elimination (E2) in cyclohexane system. Stereoselective approach to E1, E2 and E1cB mechanisms; reactivity/ orientation (Saytzeff/Hofmann).

Electrophilic aromatic substitution: mechanism orientation and reactivity. Reaction: nitration, nitrosation, sulfonation, halogenation, Friedel-Crafts reaction, chloromethylation, Gatterman, Hoesch, Vilsmeier-Haack reaction, Reimer-Tiemann, Kolbe-Schmidt. Nucleophilic substitution reaction: Addition-elimination reaction. SN1 mechanism, benzyne mechanism.

Suggested Text Books:

1. R. T. Morrison, R. N. Boyd and S. K. Bhattacharjee, Organic Chemistry, 7th Edition, Pearson Education.
2. P. Y. Bruice, Organic Chemistry, 4th Edition, Pearson Education.
3. T. W. Graham Solomons and C. B. Fryhle, Organic Chemistry, 10th edition, Wiley.
4. I. L. Finar, Organic Chemistry, Vol-1, 6th edition, Pearson Education.
5. S. N. Ege, Organic Chemistry: Structure and Reactivity, 5th edition, Houghton Mifflin College Div, 2003.
6. E. L. Eliel and S. H. Wilen, Stereochemistry of Organic Compounds, Wiley.

CY–303: Analytical Chemistry (3 credits)

Errors in Chemical Analysis – (6 h)
Errors and types - Accuracy and precision, Absolute and relative errors, Determinate (systematic) and indeterminate (random) errors,
Statistical treatment of random errors – source and distribution, sample and populations, mean, deviations and standard deviation. Propagation of errors, criteria for rejection of a data (q-test), significant figure and computation rules for significant figures, method of least squares.

Acid-base Titrations – (6 h)
Terminology– equivalence point and end point, primary and secondary standards, reactions used for titrations, molarity and normality, some examples of stoichiometric calculations.
Acid-base titration– Acid-bas indicators, theory of acid base indicators, calculation of pH values at different stages of the acid base titration and titration curve.

Precipitation and ComplexometricTitration– (6 h)
Precipitation titrations- mohr, volhard and fajans methods with examples and indicator theory.
Complexometric titrations- principle, effect of complexing agents and their advantages, examples including EDTA based titration and titration curve, definition of pM^+ (-log M^+), Back and blank titration with examples, direct and indirect determinations, masking and demasking with examples

Gravimetric Method of Analysis – (4 h)
Gravimetry– principle and use with example, Von weimern theory of relative supersaturation, digestion-ostwald ripening, coprecipitation, post precipitation, precipitation from homogeneous solution, organic precipitants.

Electrochemistry in Analysis – (8 h)
Redox titrations – Redox indicators, their use in volumetric analysis, iodometry and iodimetry, example of titration from other redox systems.
Electrochemical methods – electrodes and electrochemical cell, standard electrodes, electrochemical series, glass electrode and pH measurement, electrogravimetry, potentiometric titration, DME and polarography, cyclic voltammetry.

Separation Techniques– (8 h)
Solvent extraction, gas-liquid chromatography (GC), liquid chromatography (LC), high performance liquid chromatography (HPLC), ion exchange chromatography, gel permeation chromatography.

Suggested reading:
(1) “Qualitative Analysis” – Day and Underwood, 5th edition, Prentice-Hall (1986).
(2) “Fundamentals of Analytical Chemistry” – Douglas A. Skoog, Donald M. West, F. James Holler and Stanley R. Crouch, 9th Edition,Cengage Learning(2013).

CY-304: Surface Chemistry and Electrochemistry (3 credits)

Surfaces and interfaces: surface free energy and surface tension, contact angles and wetting, work of adhesion and cohesion, curved interface, Young's equation, capillary action, surfactants and surface pressure, surface excess, Gibbs isotherm, surface double layer and potential. (6 h)

Structure of solid surfaces: Adsorption and desorption of molecules, physisorption and chemisorption, Langmuir Isotherm, BET and other isotherms, dissociative adsorption, temperature dependence of adsorption, sticking probability. Surface analytical techniques, spectroscopies (Auger, photoelectron, vibrational) temperature programmed techniques. Surface imaging electron microscopy. (6 h)

Reactions at surfaces: heterogeneous catalysis, Langmuir-Hinshelwood and Eley-Rideal mechanisms, activation energy. (3 h)

Relevance of surfaces and interfaces: colloids, nanomaterials & biology. (2 h)

Conductance and Ionisation: ionic conductance, electrical force, field and flux, molar conductivity, strong and weak electrolytes and their molar conductance, law of independent migration of ions: Kohlrausch’s law, Ostwald’s dilution law, conductometric titrations. (4 h)

Theory of Electrolytic Conductance (qualitative description only): ionic atmosphere, electrophoretic effect - Debye-Hückel-Onsager equation, Effect of high potential gradient (Wien effect) and high frequency (Debye-Falkenhagen effect). (4 h)

Migration of Ions: Ionic mobility, drift speed, Transport number and its relation with concentration and ionic mobility, Experimental procedures for measuring transport numbers (Hittorf's rule, Moving boundary method), Abnormal transport numbers: Grotthuss mechanism. (3 h)

Ion Activities and Debye-Hückel Theory (qualitative descriptions only): Activity and activity coefficients, Ionic strength, Debye-Hückel limiting law, Debye-Hückel theory for concentrated solution. (3 h)

Electrochemical Cells: Daniell Reversible and irreversible cells, cell representations and half-cell reactions, E.M.F., Thermodynamics of electrochemical systems: Nernst equations, varieties of electrodes, standard electrode potential. (3 h)

Type of boundary between half cells and Liquid junction potentials, Concentration cells, Applications of EMF measurements- potentiometric titrations, determination of activity coefficient, composition of complex ions, solubility product, measurement of pH and pKa (Hydrogen, Quinhydrone, Glass electrodes), Polarization, Overvoltage (3 h)

Application of Electrochemical Cells- Dry cells, Lead Batteries, Alkaline cells (Edison Cell), Fuel cells, Biological energy conversions. (3 h)

CY-305: Organic Chemistry: Conformation and Reactivity (3 credits)

1. Thermodynamic and kinetic principles (11 h)

Reaction thermodynamics: free energy and equilibrium, enthalpy and entropy factors, intermolecular and intramolecular reaction. Heat of hydrogenation and heat of combustion. Application of thermodynamic principle in tautomeric equilibria [keto-enol tautomerism, composition of the equilibrium in different systems (simple carbonyls, 1,3- and 1,2-dicarbonyl systems, phenols, and related systems), substituent and solvent effects]. Reaction kinetics; transition state theory, rate constant and free energy of activation, free energy profile for one step and two step reactions, catalytic reactions, kinetically controlled and thermodynamically controlled reactions, isotope effect, primary kinetic isotopic effect (kH/kD), principle of microscopic reversibility. Crossover experiments.

2. Conformation and stereochemistry (13 h)

Racemization (through cationic, anionic and radical intermediates), resolution of acids, bases and alcohols via diastereomeric salt formation.

Topicity of ligands and faces; Pro-R, Pro-S, and Re/Si descriptors.

Conformation : nomenclature, eclipsed, staggered, gauche and anti, dihedral angle, torsion angle, energy barrier of rotation, relative stability of conformation on the basis of steric effect , dipole-dipole interaction, H-bonding; conformational analysis of ethane, propane, n-butane, haloethane, 1,2-haloethane, 1,2-glycol, 1,2-halohydrin; invertomerism of trialkylamine.

Cyclic stereochemistry: Baeyer strain theory, conformational analysis: cyclohexane, mono and disubstituted cyclohexane, symmetry properties, and optical activity.

3. Photochemistry (4 h)

Primary photochemical processes, Jablonskii diagram, photochemical reactions of carbonyl compounds: Norrish type I and II reactions. Photochemistry of olefins: cis-trans isomerism, Paterno-Buchi reaction.

4. Aromatic and Heterocyclic compounds (8 h)

Naphthalene, anthracene and phenanthrene. Heterocyclic compounds: synthesis, structure, reactivity, orientation and important reactions of epoxide, aziridine, furan, pyrrole, thiophene, and pyridine.

Suggested Text Books:

1. R. T. Morrison, R. N. Boyd and S. K. Bhattacharjee, Organic Chemistry, 7th Edition, Pearson Education.
2. P. Y. Bruice, Organic Chemistry, 4th Edition, Pearson Education.
3. M. B. Smith and J. March, March's Advanced Organic Chemistry, 6th edition, Wiley, 2007.
4. 5. Jonathan Clayden, Nick Greeves, Stuart Warren: Organic Chemistry 2nd Edition, Oxford, 2014

CY-306: Organic Chemistry Lab (2 credits)

Preparation of organic compounds using classical organic reactions such as nitration, bromination, acetylation, condensation and oxidation.

Estimation of selected organic compounds.

Suggested reading:

1. A.I. Vogel, Textbook of Practical Organic Chemistry, 4th edition.
2. Laboratory manual.

CY-307: Analytical Chemistry Lab (2 credits)

Food, Fertilizer and cosmetics analysis

1. Determination of the amount of calcium in milk powder by EDTA complexometric titration.

2. Estimation of iodine in iodized common salt using iodometric titration.

3. Estimation of phosphoric acid in cola drinks (coke, thums up and pepsi) by blue phosphomolybdic acid method (spectrophotometry).

4. Analysis of phosphorous (as phosphate) from phosphorous containing fertilizer.

5. Analysis of sulfur (as sulfate) from sulfur containing fertilizer.

6. Gravimetric analysis of aluminum in commercially available deodorants.

7. Preparation of $[Ni(NH_3)_6]^{2+}$ and analysis of its nickel content by gravimetric method.

8. Extraction and identification of DNA from green peas.

9. Analysis of kidney stones by permanganometric titration.

10. Determination of hardness of tap water.

Suggested reading:

Lab Manual

CY-351: Instrumental Methods of Analysis (3 credits)

Introductory treatment of the following techniques, including basic instrumentation and illustrative applications from all branches of chemistry.

Absorption and emission spectroscopy – (8 h)
Atomic spectroscopy – instrumentation of AAS, AES, ICP-MS/AES
Molecular spectroscopy – instrumentation of UV-Vis, IR and CD spectroscopy

Mass spectrometry – (8 h)
Basic treatment of ionization methods – FD, EI, CI, ESI, MALDI, FAB
Mass analyzers – sectors, quadruple, TOF, ion trap
Detectors – electron multiplier, Faraday cup, array detectors
Applications – small molecules, inorganic complexes, polymers, proteins

NMR spectroscopy – (8 h)
Basics – Larmor precession, resonance absorption, magnetic fields, shielding and chemical shifts, chemical equivalence, relaxation processes
Solution state (^{1}H, ^{13}C) and solid state techniques
Instrumentation – block diagram, magnets, sample probe, RF generation and detection, FT NMR

ESR spectroscopy – (6 h)
Introduction – g factor, hyperfine coupling, fine structure
Instrumentation – microwaves, waveguides, magnetic field modulation
Applications – free radicals, metal complexes, reaction intermediates

Diffraction Techniques – (8 h)
X-ray diffraction – Crystal lattices and Miller planes, Bragg condition, Ewald's sphere
Instrumentation – X-ray sources including synchrotron, filters, detectors including CCD
Powder diffraction techniques – Debye-Scherrer
Single crystal data collection – 4-circle method, Laue method, rotating crystal

Reading material:

1. *Undergraduate Instrumental Analysis* by James W. Robinson, Eileen M. Skelly Frame, George M. Frame II, Sixth Ed, Marcel Dekker, New York, 2005.
2. *Introduction to Spectroscopy* by Donald L. Pavia, Gary M. Lampman, George S. Kriz, James R. Vyvyan, Fourth Ed., Brooks/Cole Thomson Learning 2009.
3. *Physical Chemistry* by Peter Atkins and Julio de Paula, 9th Ed., Oxford University Press, 2010.
4. *Mass Spectrometry of Inorganic, Coordination and Organometallic Compounds* by William Henderson and J. Scott McIndoe, John Wiley & Sons Ltd, 2005.

CY-352: Industrial and Environmental Chemistry (3 credits)

Fuels: Classification, solid, liquid, and gaseous forms. Occurrence, purification, composition and calorific value. (2 h)

Petrochemicals and petroleum products. (3 h)

Catalysis: Relevant to industrial applications. (2 h)

Industrial organic synthesis: Synthesis of methanol, ethanol, acetic acid, acetone, glycerol and ethyl acetate etc. (3 h)

Silicates, glass, ceramics, refractories, cement. (3 h)

Fertilizers: Nitrogenous and phosphate fertilizers. (3 h)

Industrial acids and bases. (2 h)

Active pharmaceutical intermediates and drugs. (4 h)

Polymers, plastics, rubber, synthetic fibers, and paper. (4 h)

Soaps and detergents (2 h)

Insecticides and pesticides. (2 h)

Dyes, paints and pigments. (2 h)

Tanning of leather. (1 h)

Environmental aspects: Global warming, acid rains, smog, ozone depletion, toxic metals, carcinogens. Green chemistry. (3 h)

Suggested reading:

1. P. J. Chenier, Survey of industrial chemistry, 3rd Edition, Kluwer Academic/Plenum Publishers, 2002.
2. B. K. Sharma, Industrial Chemistry including Chemical Engineering, Krishna Prakashan Media (p) Ltd, 2006.
3. S. E. Manahan, Fundamentals of Environmental Chemistry, 3rd edition, CRC press, 2008.

CY-353: Organic Rearrangements and Natural Products (3 credits)

1. Rearrangements (8 h)

Classification as anionotropic, cationotropic, free radical, inter and intramolecular processes. Wagner-Meerwein, Pinacol-pinacolone, Beckmann, Baeyer-Villiger, Dakin, Hoffmann, Curtius, Schmidt, Lossen, Wolff and benzilic acid, Claisen, para Claisen, Cope and oxy-Cope, Favorskii and Fries rearrangements. Migration from nitrogen to ring carbon (Hofmann-Martius, Fischer-Hepp, N-azo to C-azo, Bamberger, Orton, benzidine).

2. Synthesis Planning (3 h)

Retrosynthesis-principles, synthons, disconnections (1/2 bond). Three to four steps synthesis using common and basic organic reactions. Introduction to protection techniques. Problem solving.

3. Natural products (23 h)

Types of natural products. Isolation techniques. Classifications, synthesis and structural aspects. Terpenes- cyclic and acyclic mono-terpenes and their rearrangements; alkaloids, carbohydrates: Monosaccharides: Aldose up to 6 carbons, structure of D-glucose & D-fructose (configuration & conformation), anomeric effect, mutarotation,. Reaction: osazone formation, bromine- water oxidation, stepping-up and stepping–down of aldoses. Disaccharides: glycosidic linkages, structure of sucrose. Maltose, cellobiose, polysaccharides, starch, cellulose, end-group analysis, cyclodextrin. steroids, amino acids, peptides.

4. Selected biosynthetic pathways (2 h)

Suggested Text Books:

1. R. T. Morrison, R. N. Boyd and S. K. Bhattacharjee, Organic Chemistry, 7th Edition, Pearson Education.
2. P. Y. Bruice, Organic Chemistry, 4th Edition, Pearson Education.
3. I. L. Finar, Organic Chemistry, Vol-2, 6th edition, Pearson Education.
4. M. B. Smith and J. March, March's Advanced Organic Chemistry, 6th edition, Wiley, 2007.
5. Jonathan Clayden, Nick Greeves, Stuart Warren: Organic Chemistry 2nd Edition, Oxford, 2014.

CY-354: Computer Programming and Numerical Methods (3 credits)

Computer: brief description of Hardware & Software.

Programming in FORTRAN: Program design (algorithm), organization of program, data types and integer constants, complex constanta, logical constants, variables, implicit and explicit data typing, expressions and hierarchy of operations, mix-mode arithmatic, library functions, input/output specification, formatting, unconditional transfers, conditional statements and constructs, GO TO/ IF statements, relational operators, block if structure, else if construct, do loops, nesting, variables and arrays, parameter/data statements, common blocks, read/write by opening files, subroutines and construction of large program.

Programming Laboratory (Linux OS, vi editor): Students are instructed to write programs on some of the numerical methods taught.

Numerical Methods: Taylor's theorem, Expansion of functions, Remainder, Mean value and Extremevalue theorems, Discrete average value theorem. Numerical Differentiation (first, second and higher derivatives)- Truncation and Roun-off errors, Stepsize dilema, Difference table (Pascal's triangle). Numerical Integration- Riemann sum, Quadrature rule, Interpolating polynomials (Lagrange's), Weights, Mid-point, Trapezoidal, Simpson's rule of integration, Adams' Predictor-Corrector method. Roots of equations- Newton-Raphson and Secant methods, Bisection and False-point methods, Bracketing method. Numerical solution of ordinary differential equations- Initial value problems, Euler's method, Taylor and Runge-Kutta methods, Modified Euler and Huen's method, Error estimates. Curve fitting- Least square fit algorithm, Monotone and convex data. Linear systems- Forward, Backward substitution, LU- factorization, pivoting (only basics), Gaussian Elimination, Gauss-Jordan Elimination, Jacobi and Gauss-Seidel methods. Eigenvalue problems. Statistical analysis of data.

Suggested reading:

1. Numerical Analysis: a Mathematical Introduction, M. Schatzman, Oxford University Press.
2. Numerical Methods in Fortran, J. M. McCormick and M. G. Salvadori, Prentice Hall of India Private Limited.
3. Numerical Analysis, R. L. Burden and J. D. Faires, Brooks/Cole Thomson Learning.
4. An Introduction to Numerical Methods and Analysis, J. F. Epperson, John Wiley and Sons, Inc.
5. Numerical Analysis: A Practical Approach, M. J. Maron, Macmillan Publishing Co. Inc.
6. Introduction to Numerical Analysis, F. B. Hildebrand, McGraw Hill Book Company, New York.
7. Numerical Methods for Engineers, D. V. Griffiths and I. M. Smith, Oxford University Press.
8. Fortran 77 and Numerical Methods, C. Xavier, New Age International Publishers.
9. Computer Programming in Frotran, V. Rajaraman, PHI Learning Private Limited.
10. Numerical Analysis and Computational Programming, S. A. Mollah, Books and Allied (P) Ltd.
11. Numerical Recipes in Fortran: The art of Scintific Computing, W. H. Press, S. A. Teukolsky, W. T. Vellerling and B. P. Flannery, Cambridge University Press.

CY-355: Inorganic Chemistry Laboratory (2 credits)

Synthesis of a variety of Inorganic Compounds: Complexes of 3d metal ions and rare earth ions and main group compounds by using common experimental techniques.

Study of the related literature (UG level).

Preparation of Scientific Reports.

CY-356: Industrial Chemistry Laboratory (2 credits)

Experiments based on major industrial processes, operations and methods of analysis of Industrial Chemicals and materials.

1. Synthesis of allobarbital
2. Synthesis of warfarin
3. Synthesis of paracetamol
4. Synthesis of oil of wintergreen
5. Synthesis of indigo and dyeing of cloth
6. Extraction of casein from milk
7. Estimation of iron in tablet
8. Extraction of curcumin from turmeric
9. Preparation of soap
10. Laboratory preparation of shaving gel
11. Preparation of nylon 6 6
12. Preparation of super absorbent polymer and exploration of its properties
13. Synthesis of molecular sieve – zeolite X and cobalt exchange reaction with it
14. Synthesis of biodiesel

CY-357: Open-ended Laboratory (2 credits)

In this course, students are assigned a task and are expected to try various approaches to solve it. For example, enzyme kinetic studies, study of the gel-fluid phase transition of lipids using fluorescence and synthesis of giant inorganic metal oxide clusters and their reactions. The students are assessed based on the practical skills in the lab, originality and the written report at the end of the course. Since the course in the nature of short projects, the experiments chosen may vary from year to year.

FN-106: Symmetry and Mathematics (3 credits)

Symmetry elements and operations, point groups. Matrix representation of symmetry operations-Great Orthogonality Theorem-Character tables. Direct product representations. Projection operators and symmetry adapted linear combinations. Applications.

Numbers: Real and Complex number algebra. Vector algebra.

Functions & Variables: Differential calculus-first- and higher-order derivatives, evaluation of minimum and maximum, limits & continuity. Partial differentiations. Exact and inexact differentials. Numerical differentiation. The gamma and delta functions.

Integral Calculus: Indefinite and definite integrals, improper integrals. Methods of integration. Surface and volume integrals. Numerical integrations.

Differential Equations: Ordinary first- and second-order differential equations. Partial differential equations. Solution of inexact differential equations by the method of integrating factors. Power series and extended power series solutions. Numerical solutions.

Special functions: Hermite, Legendre and Laguerre polynomials, recursion relations.

Matrices and Determinants. Eigenvalues and eigenvectors. Orthogonal transformation. Rank & inverse of matrix.

Solution of Linear Systems: Gaussian elimination, Cramer's rule. Gauss-Jordan elimination. Gauss-Seidel and Jacobi methods.

Solution of non-Linear Systems: Newton-Raphson method.

Curve fittings.

Probability and Statistics: Permutation & Combination. Probability. Stirling's approximation. Lagrange multipliers.

Suggested reading:

1. Molecular Symmetry and Group Theory. Allan Vincent, John Wiley & Sons, LTD.
2. Symmetry: An introduction to group theory and its applications. R. McWeeny, Dover Publications, Inc.
3. Chemical Applications of Group Theory. F. A. Cotton, John Wiley & Sons, Inc.
4. Symmetry and Structure. S. F. A. Kettle, Wiley.
5. Mathematics for Physical Chemistry. R. G. Mortimer, Academic Press.
6. Advanced Engineering Mathematics. E. Kreyszig, Wiley.
6. Mathematics for Chemistry and Physics. G. Turrell, Academic Press.
7.Numerical Analysis: A Practical Approach. Melvin J. Maron, Macmillan Publishinh Co., Inc. NY & Collier Macmillan Publishers, London.

CY- 401: Basic Concepts and Coordination Chemistry (3 credits)

Shapes of Small Molecules: VSEPR theory - Coordination polyhedra - Enumeration of geometrical and optical isomers. (3 h)

Theory of Acids and Bases: Bronsted and Lewis acids and bases - Gas phase versus solution acidity - Solvent leveling effects - Hardness and softness - Surface acidity. (5 h)

Oxidation and Reduction: Use of redox potential data - Nernst equation - Influence of complex formation, precipitation, change of pH and concentration on redox potentials - Analysis of redox cycles - Redox stability in water - Disproportionation/Comproportionation - Frost, Latimer and Pourbaix diagrams. (6 h)

Coordination Chemistry: d-orbital splitting in various fields – Spectroscopic states and term symbols - Hole formalism - Tanabe-Sugano and Orgel diagrams - Derivation of Ligand field parameters (Dq. B) from electronic spectra - Magnetic moments - Orbital contribution, spin-orbit coupling and covalency - Molecular orbitals and energy level diagrams for common symmetries - Bonding involving pi-donor ligands - Back-bonding - f-orbital splitting - Spectral and magnetic properties of f-block elements. (18 h)

Inorganic Reaction Mechanisms: Substitution reactions - Dissociative and associative interchange - *trans*-effect - Linear free energy relations - Rearrangements - Berry pseudo rotation - Electron transfer reactions - Photo-dissociation, -substitution and -redox reactions, Fluxional molecules. (8 h)

Suggested reading:

(1) P. Atkins, T. Overton, J. Rourke, M. Weller, F. Armstrong: Shriver and Atkins' Inorganic Chemistry, Fifth Edition, 2009, OUP or D. F. Shriver and P. W. Atkins, ‘’Inorganic Chemistry’’, 3rd Edn, OUP, 1999.

(2) C. Housecroft, A. G. Sharpe, ‘’Inorganic Chemistry’’, 3rd Edn, (or 4th Edn in 2012) Prentice Hall/Pearson, 2008.

(3) F. A. Cotton, G. Wilkinson, Advanced Inorganic Chemistry, 5th Edn, John Wiley, 1988 (or F. A. Cotton, C. A. Murillo, M. Bochmann and R. N. Grimes, ‘’Advanced Inorganic Chemistry’’, 6th Edn Wiley, 1999).

(4) J. E. Huheey, E. A. Keiter, R. L. Keiter, ‘’Inorganic Chemistry: Principles of Structure and Reactivity’’, 4th Edn, Prentice Hall, 1997 (or a previous edition).

(5) G. L. Miessler, D. A. Tarr, ‘’Inorganic Chemistry’’, 3rd Edn, Pearson Education, 2004.

(6) G. Wulfsberg, ‘’Inorganic Chemistry’’, University Science Books, 2000.

CY-402: Physical Organic Chemistry (3 credits)

Structure and bonding: Description of molecular structure using valence bond concept (Hybridization, bond lengths and angles). (2 h)

M.O. and V.B. methods (Huckel's MO Method, pictorial representation of MOs for molecules, qualitative application of MO theory to reactivity). (5 h)

Inductive, resonance, hyperconjugation and field effects, hydrogen bonding. (2 h)

Aromaticity and Huckel's rule (energy, structural, electronic criteria for aromaticity and relationship among them, aromaticity for annulenes, charged rings, homoaromaticity, fused rings, heteroaromaticiy). (4 h)

Thermodynamics and kinetics: Acids and bases, HSAB principle, bond energies and thermochemistry, kinetic parameters, Hammond's postulate, Kinetic isotope effects, kinetic and thermodynamic control (general relationship between thermodynamic stability and reaction rate). (7 h)

Linear free energy relationships for substituent effects (numerical expression and application to characterization of reaction mechanisms). (4 h)

Stereochemistry: Chirality and isomerism in organic systems, resolution and asymmetric synthesis, conformational analysis of acyclic and cyclic systems, Curtin-Hammett principle. Effect of conformation on reactivity: stereoelectronic effects. (10 h)

Supramolecular chemistry: Host-guest systems, crowns, cryptands, clathrates and inclusion complexes. (2 h)

Suggested reading:

1. F. A. Carey, R. J. Sundberg, Advanced Organic Chemistry, Structure and Mechanisms, Part A, 5th Edition, Springer, 2007.
2. E. V. Anslyn, D. A. Dougherty, Modern Physical Organic Chemistry Illustrated Edition, University Science, 2005.
3. M. B. Smith and J. March, March Advanced Organic Chemistry, 6th edition, Wiley, 2007.
4. A. J. Kirby, Stereoelectronic Effects, Oxford University Press, 1996.
5. Peter Sykes, A Guide Book to Mechanism in Organic Chemistry, 6th edition, Pearson Education.
6. Ian Fleming, Molecular Orbitals and Organic Chemical Reactions-Student Edition, Wiley, London, 2009.
7. E. L. Eliel and S. H. Wilen, Stereochemistry of Organic Compounds Wiley Student Edition, 2008.

CY-403: Quantum Chemistry (3 credits)

Review of classical mechanics. Wave-particle duality and Uncertainty principle.

Postulates of quantum mechanics. Operator algebra. Properties of hermitian operators. Eigenvalue problem. Commutators and Uncertainty Principle.

Elementary applications of quantum mechanics- unbound motion in one dimension. Tunneling. Bound motion – particle-in-a-box (1D & 3D), harmonic oscillator and rigid rotor. Angular momentum algebra- Hydrogen atom.

Methods of obtaining approximate solution to the time independent Schrödinger equation – perturbation theory and variational method. Application.

Many electron atoms. Spin and Pauli exclusion principle. Hund's rule. Slater determinants. Electronic term symbols.

Suggested reading:

1. Quantum Chemistry, H. Eyring, J. Walter and G. E. Kimball, John Wiley & Sons.
2. Quantum Chemistry, D. A. McQuarrie, University Science Books.
3. Quantum Chemistry. I. N. Levine, PHI Learning Private Ltd.
4. Quantum Mechanics, L. Pauling and E. B. Wilson,McGraw Hill International Ed.
5. Quantum Mechanics, N. Zettili, John Wiley and Sons.
6. Molecular Quantum Mechanics. P. W. Atkins and R. S. Friedman, Oxford University Press.
7. The Chemical Bond, J. N. Murrell, S. F. A. Kettle and J. M. Tedder, John Wiley and Sons.
8. Modern Quantum Chemistry. A. Szabo and N. S. Ostlund.

CY-404: Inorganic Chemistry Lab: Quantitative and Qualitative Analysis (3 credits)

Quantitative Analysis

Statistical analysis of data sampling methods.

Redox titrations (permanganometry, dichromatometry, iodometry).

Complexometric titrations using EDTA (estimation of some metal ions, hardness of water).

Precipitation titration (estimation of Ag).

Quantitative separation of metal ions from a binary mixture (e.g. Cu^{2+}/Fe^{3+}).

Gravimetric analysis (e.g. estimation of Ni^{2+}).

Analysis of ores and minerals (e. g. Iron ore, Potassium alum).

Ion exchange separation of metal ions (e.g. Zn^{2+}/Mg^{2+}).

Ion exchange separation of oxidation states (e.g. VO_3^-/VO^{2+}).

Qualitative Analysis

Reactions of some less common metal ions (Tl, W, Mo, V, Zr, Th, U).

Simple reactions to illustrate the aqueous chemistry of some typical transition metal ions - several oxidation states of V, Cr, Mn - oxoions - Peroxo ions; complex formation of Co^{2+} - H_2O-HCl reaction.

Group separation of cations (mostly trace elements).

Suggested reading:

(1) Vogel's Textbook of Quantitative Chemical Analysis, 5th Edn, Orient Longman, 1989.

(2) Vogel's Textbook of Macro and Semimicro Qualitative Inorganic Analysis, 5th Edn, Orient Longman, 1982.

CY-405: Organic Chemistry Lab-Techniques (3 credits)

Different laboratory techniques-melting point, distillation, TLC, column chromatography, crystallization.

Separation and analysis of organic compounds.

Suggested Reading:

1. A.I. Vogel, Textbook of Practical Organic Chemistry, 4th edition.

2. Laboratory manual.

CY-451: Main Group and Inner Transition Elements (3 credits)

Perspectives, periodicity & periodic anomalies – Relativistic effects on chemical properties (2 h)

Hydrogen and its compounds: H-bond and its influence on the structure and properties of crystals- Hydrides→classification: electron deficient, electron precise and electron rich hydrides (2 h)

Alkali and alkaline earth metals: Solutions in liquid ammonia - Synthesis, properties, uses and structures of crown ether complexes, cryptands and organometallic compounds (2 h)

Group 13 elements: Borides, borates, boron halides, boranes, carboranes and metallocarboranes, BN compounds, transition-metal stabilized borylene and boryllithium, organoaluminum compounds, Lewis Base adducts of AlR_3 compounds, Subvalent organo-Al compounds, Organo-gallium, -indium, and –thallium compounds (8 h)

Group 14 elements: Allotropes of Carbon- C_{60} and its compounds (fullerenes) - carbon nanotubes: synthesis and properties -Intercalation compounds of graphite - Pure Silicon, silica and silicates, Silicones - Low coordinated and hypervalent Silicon compounds - Brief survey of Ge, Sn, and Pb chemistry- Organo-germanium, -tin, and -lead compounds (6 h)

Group 15 elements: P(V) compounds (structure, bonding, reactivity) - P(III) compounds: diphosphenes, phosphaalkenes, iminophosphanes - P-containing ring systems (phosphabenzene, phosphole), phosphazenes, P-S compounds (7 h)

Group 16 elements: Sulfur - polycationic and anionic species - SN compounds.(3 h)

Group 17 elements: Charge-transfer complexes of halogens, interhalogen compounds, halogen oxides and oxygen fluorides, pseudohalogens. (3 h)

Group 18 elements: Noble gas clathrates and compounds. (3 h)

Inner transition elements: Chemistry of f-block elements - Binary compounds - Organometallic compounds - Relation to p-block and d-block chemistry - Transactinides (super-heavy elements). (4 h)

Suggested reading:

(1) A. G. Massey, “Main group chemistry”, Wiley, 2000.
(2) N. N. Greenwood and A. Earnshaw, “Chemistry of the Elements”, Pergamon Press, 1989.
(3) P. Atkins, T. Overton, J. Rourke, M. Weller, F. Armstrong: Shriver and Atkins' Inorganic Chemistry, Fifth Edition, 2009, OUP or D. F. Shriver and P. W. Atkins, ‘’Inorganic Chemistry’’, 3rd Edn, OUP, 1999.
(4) C. Housecroft, A. G. Sharpe, ‘’Inorganic Chemistry’’, 3rd Edn, (or 4th Edn in 2012) Prentice Hall/Pearson, 2008.
(5) F. A. Cotton, G. Wilkinson, Advanced Inorganic Chemistry, 5th Edn, John Wiley, 1988 (or F. A. Cotton , C. A. Murillo, M. Bochmann and R. N. Grimes, ‘’Advanced Inorganic Chemistry’’, 6th Edn Wiley, 1999).
(6) J. E. Huheey, E. A. Keiter, R. L. Keiter, ‘’Inorganic Chemistry: Principles of Structure and Reactivity’’, 4th Edn, Prentice Hall, 1997 (or a previous edition).

CY-452: Organic Reactions and Mechanisms (3 credits)

Methods of formation, structure determination and reactions of the following reactive intermediates: carbocations, carbanions, free radicals, carbenes and nitrenes, arynes and related species. (5 h)

Detailed reaction mechanisms and effect of different parameters in the regio-, stereo-, chemo-selective outcome of addition, substitution, elimination, oxidation, reduction, rearrangement and pericyclic reactions. (22 h)

Baldwin ring closure rules, formation of 3,4,5 and 6 membered rings (2 h)

Reactions of aromatic heterocycles: Synthesis and properties. (4 h)

Organic photochemical reactions. (3 h)

Suggested reading:

1. M. B. Smith and J. March, March Advanced Organic Chemistry, 6th edition, Wiley, 2007.
2. F. A. Carey, R. J. Sundberg, Advanced Organic Chemistry, Structure and Mechanisms, Part A, 5th Edition, Springer, 2007.
3. J. Clayden, N. Greeves, S. Warren and P. Wothers, Organic Chemistry, 1st edition, Oxford University Press, 2001.
4. K. Peter C. Vollhardt and N. E. Schore, Organic Chemistry, W. H. Freeman and Company, 1999.
5. Peter Sykes, A Guide Book to Mechanism in Organic Chemistry, 6th edition, Pearson Education.
6. Ian Fleming, Molecular Orbitals and Organic Chemical Reactions-Student Edition, Wiley, London, 2009.
7. J. D. Coyle, Introduction to Organic Photochemistry, Wiley, 1991.
8. B. Halton, J. M. Coxon, Organic Photochemistry, Cambridge University Press, 2011.
9. S. Sankararaman, Pericyclic Reactions: A Textbook: Reactions, Applications and Theory, Wiley-VCH, 2005.

CY-453: Molecular Spectroscopy (3 credits)

Interaction of radiation with matter, semiclassical treatment. Time-dependent perturbation theory and transition rates. Electric dipole, quadrupole and magnetic dipole transitions. Selection rules. Line width and line shapes.

Rotational, vibrational and ro-vibrational spectroscopy of di-atomic molecules. Selection rules. Rotational energy levels of polyatomic molecules. Classification of rotors and selection rules. Applications. Polyatomic molecular vibrations. Local and normal modes. Infrared spectroscopy, selection rules. Rotational and vibrational Raman Spectroscopy and selection rules.

Franck-Condon principle. Electronic spectroscopy. Selection rules. Resonance Raman transitions and application. Radiative and nonradiative decay- internal conversion and intersystem crossing. Principles of Laser.

Electron Spectroscopy- PES, XPS and ESCA.

NMR spectroscopy-origin of chemical shift and spin-spin coupling. AX, AX2 and AXn systems. Paramagnetic shifts and their applications. Introduction to relaxation processes in solution.

EPR spectroscopy-relaxation processes. Origin of g-shifts and hyperfine coupling. Negative spin densities. Experimental determination of g, A and D tensors-their interpretation with examples.

Principles of Mossbauer spectroscopy. Origin of isomer shifts, quadrupole splitting and h. f. s.

Suggested reading:

1. Molecular Spectroscopy. I. N. Levine, Wiley –Interscience Publication.
2. Molecular Spectroscopy. J. D. Graybeal,McGraw Hill.
3. Modern Spectroscopy. J. M. Hollas, John Wiley & Sons.
4. High Resolution Spectroscopy. J. M. Hollas, Butterworths.
5. Fundamentals of Molecular Spectroscopy. C. N. Banwell and E. M. McCash, Tata McGraw-Hill publishing.
6. Principles of Ultraviolet Photoelectron Spectroscopy, J. W. Rabalais, John Wiley & Sons.
7. Molecular Spectra & Molecular Structure. G. Herzberg, Van Nostrand Reinhold Company.

CY-454: Chemical and Statistical Thermodynamics (3 credits)

Review of classical thermodynamics. Mathematical apparatus.

Concepts of statistical thermodynamics. Micro canonical, canonical and grand canonical ensembles. Ensemble averages. Most probable distribution. Undetermined multipliers. Fluctuations.

Boltzmann statistics, Fermi-Dirac statistics and Bose-Einstein statistics.

Ideal monatomic, diatomic and polyatomic gas. Partition functions.

Equilibrium constant in terms of partition functions, Debye-Hückel theory. Statistical mechanics of ionic solutions. Flory-Higgins theory of polymer solutions. Specific heats of solids- Einstein and Debye models.

Virial equation of state and virial coefficients. The law of corresponding states. Elementary kinetic theory of transport in gases.

Suggested reading:

1. Physical Chemistry. P. W. Atkins and J. de Paula, Oxford University Press.
2. Physical Chemistry. I. N. Levine, McGraw Hill.
3. Physical Chemistry. R. G. Mortimer, Academic Press.
4. Statistical Mechanics. D. A. McQuarrie, University Science Books.

CY-455: Biological Chemistry (3 credits)

Cell Structure and Function: Structure of prokaryotic and eukaryotic cells, intracellular organelles and their function, comparison of plant and animal cells.

Introduction of biomolecules: Examples of biomolecules and building blocks of biopolymers. Types of reactions occurring in cells, structure of ice and liquid water, hydrogen bonding and hydrophobic interactions, buffers and the Henderson-Hasselbalch equation.

Nucleotides and nucleic acids: Ribonucleotides and deoxyribonucleotides, RNA and DNA. Base pairing, double helical structure of DNA and forces stabilizing nucleic acid structure. Methods used in nucleic acid separation and characterization, nucleic acid sequencing.

Transcription and translation: Messenger RNA, RNA polymerase and protein synthesis. Control of transcription and protein-DNA interactions. The genetic code, tRNA structure and codon-anticodon interactions. Ribosomes and their structure. Gene cloning and site-directed mutagenesis.

Amino acids, peptides and proteins: Primary structure of proteins, end group determination, amino acid analysis and the Edman degradation (protein sequencing), Ramachandran plot and the secondary structure of proteins α-helix, β-pleated sheet, β-bend and collagen triple helix. Tertiary structure and structural motifs - protein folding and domain structure of proteins. Oligomeric proteins. Purification and characterization of proteins, functions of proteins.

Enzymes and catalysis: Substrate specificity of enzymes, requirement of coenzymes, regulation of enzyme activity and allosteric effect, enzyme nomenclature, enzyme kinetics and the Michaelis-Menten equation, various types of enzyme inhibition. application of enzymes in chemical synthesis, enzyme models and their applications.

Carbohydrates: Monosaccharides, oligosaccharides and polysaccharides, carbohydrates of glycolipids and glycoproteins, role of sugars in biological recognition, blood group substances.

Lipids and membranes: Common classes of lipids - glycerolipids, phospholipids, sphingolipids and glycolipids. Self-association of lipids - formation of micelles, reverse micelles and membranes, gel and liquid-crystalline phases. Lipid phase polymorphism - bilayer, hexagonal and cubic phases. Liposomes and their properties and applications. Biological membranes and the fluid mosaic model, current models of biological membranes, membrane proteins and their functions, membrane asymmetry.

Introduction to metabolism: Overview of metabolism, catabolic and anabolic processes, glycolysis, citric acid cycle and oxidative phosphorylation.

Suggested reading:

1. Biochemistry by *D. Voet & J. G. Voet*, 4th Edition (2010) John Wiley
2. Lehninger Principles of Biochemistry by *D. L Nelson & M. M. Cox*, 5th Edition (2008) W. H. Freeman and CBS Publishers, New Delhi
3. Biochemistry by *J. M. Berg, J. L. Tymoczko & L. Stryer*, 5th Edition (2002) W. H. Freeman

CY-456: Inorganic Chemistry Lab: Synthesis (3 credits)

Prerequisite: None

Synthesis of a variety of Inorganic Compounds/Complexes of 3d metal ions, main group elements and rare earths by using common experimental techniques.

Introduction to various physical measurements (IR, UV-vis, mass, NMR, magnetic susceptibility, EPR and X-ray diffraction) for characterization of the compounds.

Analysis and interpretation of the physical data of the compounds to determine their structures.

Study of the related literature.

Preparation of Scientific Reports.

CY-457: Physical Chemistry Lab (3 credits)

1. Kinetics of iodine clock reaction
2. Study of an oscillating reaction
3. Determination of dipole moment change on electronic excitation
4. Adsorption of acetic acid on charcoal
5. Estimation of CMC of a micelle using fluorescence
6. Spectrophotometric determination of pK_a
7. Estimation of CMC of a micelle using conductance
8. Conductometric titration of a charge transfer complex
9. Phase diagram of a 3-component system
10. Determination of excited state acidity constant
11. Kinetics of an enzyme-catalyzed reaction
12. Potentiometric titration of a redox reaction
13. Differential scanning calorimetric study
14. Determination of the unit cell of a crystal

FN-206: Chemistry for All (3 credits)

Prerequisites: High School Chemistry / Physical Science

Foundation: Elements, Atoms, Subatomic particles, Discovery, Periodic Table, Radioactive Elements, Stability and reactivity, Molecules, Characterization, Properties and Chemical Reactions. Chemical compounds and functional groups (for students with non-chemistry background). Solids, liquids and gases; properties.

Environment and Impact on Daily Life: Sun (nuclear fusion), Liquid water – Importance of H–bond (potable, hard and soft), Importance of trees and plants, Photosynthesis – oxygen supply to air and water. Greenhouse effect, Atmospheric chemical pollution and its impact. Nuclear waste, Industrial chemical pollution, Pesticides – fertilizers, organic farming etc. Chemistry in the Living Beings, Healthy food pyramid, Essential chemical components (Fe, Ca, Na K, Vitamins, Proteins, Fat) – in relation to eye, blood, bones, brain, heart etc. Chemistry of food and food products.

Medicines: Common drugs and their function inside the body, Side effect of Drugs.

Petroleum Products: Polymers, Types – From commodity to engineering plastics, Structure, Applications – from buckets to rocket nose cones.

Suggested Reading:

Suggested by Instructor

CY-501: Spectroscopic Methods for Structure Elucidation (3 credits)

NMR Spectroscopy: ^{1}H NMR, Zeeman splitting, effect of magnetic field strength on sensitivity and resolution, chemical shift d, inductive and anisotropic effects on d, chemical structure correlations of d, chemical and magnetic equivalence of spins, spin-spin coupling, structural correlation to coupling constant J, first order patterns. Second order effects, examples of AB, AX and ABX systems, simplification of second order spectrum, selective decoupling, use of chemical shift reagents for stereochemical assignments. ^{13}C NMR, introduction to FT technique, relaxation phenomena, NOE effects, ^{1}H and ^{13}C chemical shifts to structure correlations. Study of dynamic processes by VT NMR, restricted rotation (DMF, DMA, biphenyls, annulenes), cyclohexane ring inversion, degenerate rearrangements (bullvalene and related systems). 2D NMR spectroscopy. Multinuclear NMR. (16 h)

Electronic spectroscopy: Basic principle, electronic transitions and application to structure elucidation. (3 h)

Polarimetry: Optical rotatory dispersion and circular dichroism. (1 h)

Infrared Spectroscopy: organic functional group identification through IR spectroscopy. (5 h)

Mass spectrometry: Basic principles, ionization techniques, isotope abundance, molecular ion, fragmentation processes of organic molecules, deduction of structure through mass spectral fragmentation, high resolution MS, soft ionization methods, ESI-MS and MALDI-MS, illustrative examples from macromolecules and supramolecules. (6 h)

Structure elucidation problems using the above spectroscopic techniques. (6 h)

Suggested reading:

1. R. M. Silverstein, F. X. Webster, D. J. Kiemle, Spectrometric identification of organic compounds, 7th edition, John Wiley, 2005.
2. Organic Spectroscopy, W. Kemp, 3rd edition, Macmillan, 2011.
3. D. H. Williams and I. Fleming, *Spectroscopic Methods in Organic Chemistry*, McGraw Hill, 6th edition 2007.
4. D. L. Pavia and G. M. Lampman Spectroscopy 4th Edition, Brooks Cole, 2012.
5. P. S. Kalsi, Spectroscopy of Organic Compounds, 6th edition, New age international, 2004.

CY-502: Advanced Organic Synthesis (3 credits)

Synthetic analysis and Planning: Retrosynthetic analysis, synthetic equivalent, control of stereochemistry, linear, convergent and divergent syntheses. (4 h)

Use of protecting groups in multi-step synthesis: Different protection and deprotection methods. (3 h)

Modern synthetic methods involving various oxidizing, reducing agents, C-C bond forming reactions by alkylation, acylation, organometallic, radical, pericyclic reactions and rerrangements. Discussion of selected syntheses of natural products/bioactive molecules/organic materials. (24 h)

Organocataytic transformations and C-H activation reactions-selected examples. Solid phase organic synthesis. (3 h)

Atom economy, step economy and green chemistry and environmental aspects. (2 h)

Suggested reading:

1. G. S. Zweifel and M. H. Nantz, *Modern Organic Synthesis-An Introduction*, W. H. Freeman and Company, 2006.
2. A. Carey and and R. J. Sundberg, *Advanced Organic Chemistry,* Part B, Fifth Edition, 2007
3. E. J. Corey and X. M. Cheng*, The Logics of Chemical Synthesis,* Wiley, 1989*.*
4. K. C. Nicolaou, *Classics in Total Synthesis*, Vol 1, 2 and 3.
5. S. Warren and P. Wyatt, Organic Synthesis: The *Disconnection Approach,* 2nd edition, Wiley, 2008.
6. J. H. Fuhrhop, G. Li, *Organic Synthesis: Concepts and Methods, 3rd edition,* VCH, 1994.
7. W. Carruthers, *Some Methods of Organic Synthesis*, Cambridge University Press.
8. H. O. House, Modern Synthetic Reactions, Benjamin-Cummings Publishing Co. 1972.

CY-503: Chemical Dynamics (3 credits)

Review of basic concepts in kinetics

Fast reactions: experimental techniques

Theories of reaction rates

Unimolecular reactions

Reactions in solution: reactions between ions, diffusion-controlled reactions, electron transfer reactions

Composite reactions including photochemical reactions

Homogeneous and heterogeneous catalysis

Kinetic isotope effect

Molecular reaction dynamics

Transport properties: Diffusion, viscosity, thermal conductivity, ion transport, dynamic electrochemistry

Suggested reading:

1. Physical Chemistry: A Molecular Approach. D. A. McQuarrie and J. D. Simon, University Science books
2. Physical Chemistry. P. W. Atkins and J. de Paula, Oxford University Press.
3. Physical Chemistry. I. N. Levine, McGraw Hill.
4. Chemical Kinetics. K.J. Laidler, Pearson.
5. Chemical Kinetics and Reaction Dynamics, P.L. Houston, Dover Publications, 2006

CY-504: Chemical Binding (3 credits)

The Born-Oppenheimer approximation. Electronic structure theory: MO and VB theories, application to H2+ and H2. MO and VB wavefunctions of polyatomic systems. Hückel pi-electron theory. Walsh diagram and molecular geometry.

Hartree-Fock theory, Brillouin conditation, Non-orthogonal basis and Roothaan equation, SCF method. Koopmann's theorem.

Post Hartree-Fock methods. Electron correlation. Basis sets.

Density functional theory and application.

Suggested reading:

1. Quantum Chemistry, H. Eyring, J. Walter and G. E. Kimball, John Wiley & Sons.
2. Quantum Chemistry, D. A. McQuarrie, University Science Books.
3. Quantum Chemistry. I. N. Levine, PHI Learning Private Ltd.
4. Molecular Quantum Mechanics. P. W. Atkins and R. S. Friedman, Oxford University Press.
5. The Chemical Bond, J. N. Murrell, S. F. A. Kettle and J. M. Tedder, John Wiley and Sons.
6. Modern Quantum Chemistry. A. Szabo and N. S. Ostlund.

CY-505: Advanced Inorganic Chemistry (3 credits)

Recent Advances in Main Group Chemistry: Low and hypervalent compounds – p(pi)-p(pi) bonding in heavier main group chemistry. (3 h)

Organometallic Chemistry: Complexes with pi-acceptor and sigma-donor ligands - 16 electron and 18 electron rules – Stability and Reactivity - Isolobal analogy - Structure and bonding - Agostic interaction. (8 h)

Homogeneous and Heterogeneous Catalysis: Hydrogenation, carbonylation, polymerization, Wacker oxidation and other reactions catalyzed by transition metal complexes. (5 h)

Metal Cluster Compounds: Metal-metal bond - Carbonyl and non-carbonyl clusters - Structure and bonding - Low-dimensional solids - Clusters in catalysis. (4 h)

Bioinorganic Chemistry: Biochemistry of iron– its storage, transport and function; Transport and storage of dioxygen– structure and function of haemoglobin, myoglobin, hemocyanin and hemerythrin; Electron transport proteins– cytochromes and Fe-S proteins; Copper containing enzymes– blue and non-blue copper enzymes, ascorbate oxidase, tyrosynase, galactose oxidase, superoxide dismutase; Zinc containing enzymes– carboxy peptidase A, carbonic anhydrase, alcohol dehydrogenase; Iron containing enzymes– catalase, peroxidase and cytochrome P-450; Photosynthesis; Nitrogen fixation; Bioinorganic chemistry of alkali and alkaline earth metal cations; Toxicity of metals. (16 h)

Inorganic Photochemistry: Ligand field photochemistry of d^n complexes - Photochemistry of carbonyl compounds - Energy conversion (solar) and photodecomposition of water. (4 h)

Suggested reading:

(1) Textbooks suggested for CY-401.

(2) B. D. Gupta, A. J. Elias, “Basic Organometallic Chemistry”, University Press, 2010.

(3) I. Bertini, H. B. Gray, S. J. Lippard, J.S. Valentine, “Bioinorganic Chemistry”, VLSE with Univ. Sci. Books, 1998.

CY-506: Organic Chemistry Lab: Synthesis (3 credits)

Multistep organic synthesis involving oxidation, reduction, electrophilic substitution, organometallic reagents, cycloaddition, photochemical, rearrangements, radical and enzymatic reactions.

Resolution of racemic organic compounds.

Characterization of the synthesized compounds using different analytical techniques.

Suggested reading:

1. A.I. Vogel, Textbook of Practical Organic Chemistry, 4th edition.
2. Laboratory manual.

CY-507: Instrumentation and Computer Applications Lab (3 credits)

Instrumentation (electronics)

E1 - Measuring instruments- Introduction to tools and kits; electronic components, mutimeter, potentiometer, decade boxes, power supply, CRO. Simple measurements and cross checks (e.g., resistance read from color codes vs measurement using multimeter)

E2 - (a) Capacitor as charge storage device. Introduction to circuit; kinetics of charging and discharging for several capacitors (b) Measurement of dielectric constant of a solvent (e.g., methanol) by the use of a variable capacitor

E3 - RC, LR, LCR circuits. Concept of filter circuits; determination of cut-off frequency by the use of circuits; frequency selection by the use of LCR circuit; tuning and matching frequencies in NMR and EPR spectrometers by the use of LCR

E4 - Diode characteristics and rectifier circuits. Thermionic emission and VI curve of diodes; measurement of VI curves of diodes including Zener; AC to DC conversion by half-wave and full-wave rectifier circuits; bridge rectification circuit; use of capacitor filters; ripple factor

E5 - Transistor amplifier circuits. Base, emitter and collector in the transistor; forward and reverse bias; soldering the amplifier circuit; voltage amplification by the use of different resistors in the amplifier circuit

E6 - Inverting and non-inverting amplifiers; simple integration and differentiation using operational amplifier

E7 - RS 232 cable and port; computer-instrument interfacing

Computational

C1 - Study of normal modes- optimization of molecular geometry, computation of normal modes and frequencies, analysis of the symmetries of the normal modes, effect of molecular symmetry on the degeneracies, impact of mass on the frequencies

C2 - Determination of equilibrium constants- optimization of molecular geometry of reactant and product, computation of the rotational constants, vibrational frequencies etc., calculation of partition functions, calculation of equilibrium constant at different temperatures

C3 - Determination of rate constants- optimization of molecular geometry of reactant and product, calculation of transition state, computation of the rotational constants, vibrational frequencies etc. for the reactant and transition state, calculation of partition functions, calculation of rates at different temperatures

C4 - Franck-Condon spectral calculations- optimization of the geometry of the ground, excited and ionized excited states, calculation of the vibrational frequencies of these states, calculation of the transition energies and oscillator strengths for the photo-electron spectra

C5 - Construction of Walsh diagram- computation of the MO energies at different geometries of a molecule (eg. H_2O, Li_2O), examination of the molecular orbitals and their symmetries, plot of the MO energies versus the geometric parameter reactant, qualitative analysis of the trends in the orbital energy variations

C6 - Woodward – Hoffman correlation diagrams- optimization of the geometries of cyclobutene and butadiene, computation of the molecular orbitals and their energies as a function of ring opening of cyclobutene under con- and dis-rotatory modes, plot of the frontier MO energies *vs* the ring opening coordinate (maintenance of symmetry), analysis of the plots and discussion about thermal / photochemical processes

C7 - Molecular modeling- H-bonded complexes – geometry optimization, analysis of energetics; exciton coupling in chromophore aggregates; effects of solvation

Alternative experiments- Intrinsic reaction coordinate, Natural bond orbital analysis

CY-551: Chemistry of Materials (3 credits)

Solid State Structure: Order - spatial, orientational; Types of solids; Symmetry in crystals - primitive lattice vector – Wigner-Seitz cell - crystal systems - Bravais lattices - crystallographic point groups and space groups; X-ray diffraction - reciprocal lattice - Ewald construction - structure factor - crystal structure solution and refinement - common crystal structure motifs; Quasicrystals. (6 h)

Defects and Nonstoichiometery: Point, line and plane defects; Intrinsic and extrinsic defects - vacancies, Schottky and Frenkel defects - charge compensation; Nonstoichiometry and defects - thermodynamic and structural aspects; Color centres. (3 h)

Thermal Properties: Lattice vibrations - phonon spectrum; Lattice heat capacity; Thermal expansion; Thermal conductivity. (4 h)

Electrical Properties: Free electron theory - electrical conductivity and Ohm's law - Hall effect; Band theory - band gap - metals and semiconductors - intrinsic and extrinsic semiconductors; Hopping semiconductors; Semiconductor/metal transition; p-n junctions; Superconductors - Meissner effect - type I and II superconductors - isotope effect - basic concepts of BCS theory - manifestations of the energy gap - Josephson devices. (10 h)

Magnetic Properties: Classification of magnetic materials; Langevin diamagnetism; Quantum theory of paramagnetism; Cooperative phenomena - ferro, antiferro and ferrimagnetism - magnetic domains and hysteresis; Superparamagnetism. (4 h)

Optical Properties: Optical reflectance - plasmon frequency; Raman scattering in crystals; Photoconduction; Photo and electroluminescence; Lasers; Photovoltaic and photoelectrochemical effects. (3 h)

General Concepts in Materials Synthesis: Phase diagrams; Preparation of pure materials; Nucleation and crystal growth; Crystal growth techniques; Zone refining. (2 h)

Brief Introduction to Different Classes of Materials: High T_C superconductors, Ionic conductors, Polymers, Liquid crystals, Molecular materials, Nanomaterials (8 h)

Suggested reading:

1. H. V. Keer, Principles of the Solid State (541.0421 K25P)
2. L. E. Smart and E. A. Moore, Solid State Chemistry: an Introduction (541.0421 Sm295)
3. M. T. Weller, Inorganic Materials Chemistry (546 W45I)
4. K. J. Klabunde, Nanoscale Materials in Chemistry (660 K66N)
5. W. D. Callister, Materials Science and Engineering, An Introduction (620.11 C13M)
6. C. Kittel, Introduction to Solid State Physics (530.41 K65I)
7. Journals like Chemistry of Materials, Journal of Materials Chemistry, Advanced Materials etc..

Web resource: http://chemistry.uohyd.ernet.in/~cy551/

CY-552: Seminar Course (3 credits)

The main objectives of this course are (i) to train the students to read and understand the journal literature and (ii) to improve their communication skills. Each student has to give a seminar (power-point presentation) on a topic based on a review in a chemistry journal that should have appeared during the previous 10 years. Each seminar will be of 30 minutes [20 min (presentation) + 10 min (Q & A)] duration. Students are expected to be active during all the seminars. Each student has to submit an essay based on the topic he/she has chosen which should be consistent with his/her talk. A final written examination based on the seminars presented by the students will be conducted at the end of the course.

Evaluation is done on the basis of oral presentation [60 marks including Q & A], essay [20 marks] and final written examination [20 marks].

CY-553: Project (3 credits)

Each student is assigned to a faculty supervisor to carry out a research project. They will be trained in searching research literature as well as experimental and computational work specific to the chosen research problem. At the end of the project, they will submit a report of the work done and make a presentation.

CY-571: Organometallic Chemistry (Elective, 2 credits)

Prerequisite: None

Organometallic Chemsitry of Main Group and Transition metals for applications in organic transformations. (4 h)

Carbanionic Organometallics: Organolithium, magnesium, zinc , copper and titanium reagents. (4 h)

Chemistry of Organoboron, aluminium, silicon and tin compounds. (4 h)

Organomercurials and organothalium compounds. (1 h)

Chemistry of Metal carbonyls: chromium, iron and cobalt carbonyl reagents. (2 h)

Metal carbon multiple bonds: carbenes, carbynes, and N-heterocyclic carbenes. (2 h)

Chemistry of Metallocenes: Ferrocene and related compounds. (2 h)

Organometallic Chemistry of the Noble Metal: Pd, Rh, Ru and Au catalyzed reactions, involving metal catalyzed coupling, CH activation and metathesis reactions. (5 h)

Suggested reading:

1. D. Astruc, Organometallic Chemistry and Catalysis, Springer, 2007.
2. J. F. Hartwig, Organotransition metal chemistry, University Science Books, 2010.
3. R. H. Crabtree, The Organometallic Chemistry of the Transition Metals, 4th edition, Wiley, 2005.
4. L. S. Hegedus, B. C. G. Södenberg, Transition Metals in the Synthesis of Complex Organic Molecules, University Science Books, 2010.

CY-572: Supramolecular Chemistry (Elective, 2 credits)

Prerequisite: None

Concepts –Definition, Development and Classification.Binding Constants, Supramolecular interactions (3 h)

Supramolecular Chemistry in Life –Ionophores, Porphyrin and other TetrapyrrolicMacrocycles, Coenzymes, Neurotransmitters, DNA and Biochemical Self-assembly. (3 h)

Cation Binding Hosts – Podand, Crown Ether, Cryptand, Spherand.Nomenclature, Selectivity and Solution Behaviour.Alkalides,Electrides, Calixarenes, Siderophores. (6 h)

Anion binding hosts - Challenges and Concepts,Biological Receptors,Conversion of Cation Hosts to Anion Hosts, Neutral Receptors, Metal-Containing Receptors, Cholapods. (3 h)

Ion Pair Receptors - Contact Ion Pairs, Cascade Complexes, Remote Anion and Cation Binding Sites, Symport and Metals Extraction. (2 h)

Hosts for Neutral Receptors -Clathrates, Inclusion Compounds, Zeolites, Intercalates, Coordination Polymers, Guest Binding by Cavitands andCyclodextrins. (6 h)

Crystal Engineering – Concepts, Crystal Nucleation and Growth, Understanding Crystal Structures, Polymorphism, Co-crystals. (3 h)

Suggested reading:

1. "Supramolecular Chemistry"by J. W. Steed & J. L. Atwood, 2nd Edn John Wiley, 2009.
2. "Crystal Engineering. The Design of Organic Solids" by G.R. Desiraju, Elsevier, 1989.
3. Recommended Review Articles in the field of supramolecular chemistry.

CY-573: Stereoselective Organic Synthesis (Elective, 2 credits)

Prerequisite: CY-452, CY-502 (or equivalent)

Brief review of stereochemistry. (1 h)

Chiral pool approach, Acyclic stereoselection: reactions at a-and b-positions of a chiral center. Auxillary econtrolled stereoselection: Evans oxazolidones, Oppolzer sultams, Myers amides, Enders RAMP/SAMP, Shollkopf. (8 h)

Enantioselective alkylation allylation and crotylation reactions. (2 h)

Asymmetric oxidation [epoxidation (Sharpless, Jacobsen, Shi), dihydroxylation (Sharpless)], reduction (Noyori, Corey, Pfaltz) (3 h)

Organocatalyzed asymmetric synthesis. (2 h)

Desymmetrization, Kinetic resolution reactions. (3 h)

Application of the above methods in synthesis of selected biologically relevant molecules. (5 h)

Suggested reading:

1. M. Nogrady, Stereoselective Synthesis: A Practical Approach, Wiley, 2008.
2. E. M. Carreira, L. Kvaerno Classics in Stereoselective Synthesis, Wiley-VCH: Weinheim, Germany, 2009.
3. K. C. Nicolaou, E. J. Sorenson, Classics in Total Synthesis, Wiley-VCH.
4. K. C. Nicolaou, S. A. Snyder, Classics in Total Synthesis II, Wiley-VCH.

CY-574: Advanced Magnetic Resonance (Elective, 2 credits)

Prerequisite: CY-403, CY-453 (or equivalent)

Objective: The course centrally discusses the limitations of the classical Bloch equation, and then takes one through reduced density operator (matrix) formalism in isomorphous spaces to calculate the final states of interacting spins in pulsed Fourier Transformed magnetic resonance. Students will be able to understand and design new experiments to achieve desired objectives.

Syllabus:

Review of electron and nuclear spins - angular momentum and magnetic moment: classical and quantum descriptions

Larmor precession, energy levels, and Bloch equation

Angular momentum operators of single and coupled spins: density matrix, unitary transformation, spin angular momentum product operators, spin Hamiltonians, transformations under the influence of rf and microwave pulses, coherence transfer

Spin Relaxation

Scalar and Dipolar interactions, Fermi contact and hyperfine interactions

Chemical shift, *g*-value, anisotropy

Effect of distortion of structure and symmetry on *g*-value

Molecular structure determination from *J*-coupling and NOE constraints

Magnetic field gradients, molecular diffusion, NMR and EPR imaging

Suggested reading:

R R Ernst, G Bodenhausen, A Wokaun “Principles of Nuclear Magnetic Resonance in One and Two Dimensions” (Oxford Science)

CY 575: Density Functional Theory (Elective, 2 credits)

Prerequisite: CY-403 (or equivalent)

Many-electron wave functions; electron distributions and densities.

The Thomas-Fermi and Hartree-Fock Model. Slater Exchange Approximation.

The Hohenberg–Kohn theorems and the Kohn–Sham (KS) approach.

The Exchange-Correlation Functional. The Local Density Approximation (LDA).

The Generalized Gradient Approximation (GGA).

Hybrid functionals and the meta-GGA approaches.The Random Phase Approximation (RPA).

Implementations of density functional theory.

CY-576: Advanced Chemical Dynamics (Elective, 2 credits)

Prerequisite: CY-403, CY-404, CY-453, CY-454, CY-503 (or equivalent)

Gas Phase Dynamics: Molecular beam scattering, Review of potential energy surface.

Dynamics of Molecular Collisions: Quasi-classical and quantum dynamics, cross section and rate constant. Microscopic mechanism of selected chemical reactions. Roming atom mechanism.

Microscopic interpretation of Arrhenius parameters.

Introduction to condensed phase dynamics, Krammer's theory and solvent effects.

Microscopic reversibility and detailed balance.

Marcus theory of electron transfer.

Femtochemistry- spectroscopic probing of transition state and control of chemical reactivity.

Suggested reading:

1. Theories of Molecular Reaction Dynamics, N. E. Henriksen and F. Y. Hansen, Oxford University Press.
2. Molecular Reaction Dynamics, R. D. Levine, Cambridge University Press.
3. Molecular Reaction Dynamics and Chemical Reactivity, R. D. Levine and R. B. Bernstein, Oxford University Press.
4. Tutorials in Molecular Reaction Dynamics, Eds. M. Brouard and C. Vallance, RSC Publishing.

CY-577: Computational Chemistry (Elective, 2 credits)

Prerequisite: CY-403 (or equivalent)

One hour lecture + two hours laboratory per week

Review of Electronic Structure Theory: Hartree-Fock, MP2, DFT and configuration interaction. Basis sets, convergence.

Geometry optimization, frequency calculation, location of transition state, intrinsic reaction coordinates, population analysis, natural bond orbital analysis, calculation of thermodynamic parameters.
Calculation of molecular excited electronic states.
Representative examples.

Suggested reading:

1. Quantum Chemistry, I. N. Levine, PHI Learning Private Limited.
2. Essentials of Computational Chemistry- Theories and Models, C. J. Cramer, John Wiley and Sons, Ltd.
3. Introduction to Computational Chemistry, F. Jensen, John Wiley and Sons, Ltd.
4. Computational Chemistry- a Practical Guide for Applying Techniques to Real-World Problems, D. C. Young, John Wiley and Sons, Ltd.

CY-578: Physical Methods for Inorganic Chemistry (Elective, 2 credits)

Prerequisite: CY-453 (or equivalent)

Electronic and Photoelectron Spectroscopy: Excitation and ejection of electrons- Core level and valence- electron level photoelectron spectroscopy- Valence excitation spectroscopy- - Electronic spectra of transition metal complexes (3 h)

Vibrational Spectroscopy: Applications to Inorganic systems- Raman Spectra (1.5 h)

NMR Spectroscopy- Time scale- Multinuclear and Organometallic NMR spectroscopy -More common spin-1/2 nuclei, ^{19}F, ^{31}P, ^{29}Si, ^{119}Sn, ^{195}Pt - Quadrupolar nuclei, e.g. ^{6}Li, ^{11}B, ^{14}N, ^{17}O and their characteristics and applications- Relaxation - Fluxional Processes- NMR spectroscopy of paramagnetic compounds- Lanthanide shift reagents, Shiftless reagents- Multiple resonance (3 h)

ESR Spectroscopy – Hamiltonian, Zeeman interaction, g-tensor, g–spread, g-value anisotropy, hyperfine coupling, and hyperfine anisotropy - dipolar contributions spin densities; exchange coupling, zero-field splitting- magnetic anisotropy - liquid, powder and single crystal studies - Variable temperature techniques- Examples from bioinorganic, coordination compounds and clusters (4.5 h)

Magnetism- Overview - Curie and Curie-Weiss law – Super exchange mechanism, Heisenberg-Dirac-van Vleck (HDvV) operator – Bleaney Bowers model- Spin ladder - Magnetic Measurements, Mechanisms of magnetic coupling - coupling in dimers - Single molecule magnets – Quantum tunneling - magneto structural correlations- Examples: Cu dimers, Spin clusters of Mn, Fe, and Cr, Mixed valence species (3 h)

Mössbauer Spectroscopy- Principles- ^{57}Fe - Isomer shift, quadrupole splitting, magnetic hyperfine splitting, selected applications in Fe^{n+} systems, Fe-S systems- Bioinorganic systems, Carbonyl compounds (1.5 h)

Diffraction methods: Distinction among X-ray, neutron and electron diffraction techniques- Single crystals and interpretation of results from X-ray crystallography (1.5 h)

Suggested reading:

(1) E. A. V. Ebsworth, D. W. H. Rankin and S. Cradock, Structural methods in Inorganic Chemistry, ELBS, (Blackwell), 1987.

(2) R. S. Drago, Physical Methods in Chemistry (Saunders publishing)

(3) R. A. Scott and C. M. Lukehart (Editors) Applications of Physical Methods to Inorganic and Bioinorganic Chemistry, 2007 [also available as *Encyclopedia of Inorganic Chemistry, 5 Volume Set*]

CY- 579: Polymer Chemistry (Elective, 2 credits)

Prerequisite: None

Definition: Polymer, monomer, repeat unit, polymerization- Classification: Polymers based on source and polymerizations-polymer composition and structure- Nomenclature- IUPAC, Non-IUPAC, structure-based, and trade names- Types of polymers based on their molecular structure (linear, branched, cross-linked, block) and stereochemistry of repeating units (Tacticity in polymers)- Effect of Polymer structure on their properties (3 h)

Polymer Synthesis: Step, chain and miscellaneous polymerizations- Kinetics of polymerization- Anionic, Cationic, ATRP, ROMP, RAFT, Free radical polymerization- Polymerization of cyclic organic compounds - Reactions of synthetic polymers - Biological polymers - Inorganic elements in polymers- State of Polymerization: Emulsion, Dispersion, Solution, Solid-state etc. (6 h)

Polymer characterization - Chemical analysis of polymers, spectroscopic methods-IR, NMR, ESR, X-Ray Diffraction analysis- Microscopy- light Microscopy, Electron Microscopy and Electron Diffraction, Scanning electron microscopy- Thermal analysis- DSC, TGA, DMA, Rheology, Physical testing; stress-strain properties in tension (4.5 h)

Molecular Weights and Sizes: Solubility parameters, Thermodynamics of mixing, Flory-Huggins Theory for polymer solution, Flory-Huggins parameter, Polymer shape and size, measurement techniques-viscosity, colligative properties, chromatography, light scattering (Zimm plot) (3 h)

Physical State and Morphology: Crystalline and Amorphous state- Thermal transitions- Glass-Rubber transition - Mechanical properties− stress-strain behaviour - Elastomer, Fibers and Plastics (3 h)

Polymer Blend and Nanocomposites: Preparation, Types of blends, types of nanofillers, Thermodynamical considerations, Property enhancements, Uses (1.5 h)

Application of Synthetic Polymers: Materials and Biological importance and uses. Nanomaterials, Conducting polymers, Polymers for Energy applications. Physical aspects of polymers (1.5 h)

Suggested reading:

1. L. H. Sperling, Introduction to Physical Polymer Science, Wiley (1986)
2. H.R. Allcock and F.W. Lampe, Contemporary Polymer Chemistry, Prentice Hall (1990)
3. George Odian, Principles of Polymerization, 4th Edn, John Wiley (2004)
4. M. P. Stevens, Polymer Chemistry: An Introduction (2nd Edn), Oxford University Press (1990)
5. F.W. Billmeyer, Jr., Textbook of Polymer Science (1984), paperback
6. Relevant topics from modern literature

CY-580: Natural Products and Medicinal Chemistry (Elective, 2 credits)

Prerequisite: None

Biosynthesis, total synthesis, structure elucidation and biological significance of selected natural products. (12 h)

Introduction to drug discovery: Sources of drugs-natural products, drugs from organic synthesis, drug discovery and development (2 h)

Drug structure and biological activity-pharmaceutically important functional groups physicochemical properties of drugs, electronic effects, spatial properties of drugs Fate of drugs in the body-absorption, distribution, metabolism, and excretion. Chemistry of drug metabolism, modifications to decrease metabolism, prodrugs Molecular mechanism of drug action-drug targets, receptors, enzymes, nucleic acids, non-receptor targets (5 h)

Chemistry of selected drug classes-pharmacodynamic, chemotherapeutic, antibacterial, antiviral, antineoplastic, cardio-vascular, CNS, antihistamine, diabetic, analgesic and anti-inflammatory drugs. (5 h)

Suggested reading:

1. K. C. Nicolaou, *Classics in Total Synthesis*, Vol 1, 2 and 3.
2. J. H. Fuhrhop, G. Li, *Organic Synthesis: Concepts and Methods, 3rd edition,* VCH, 1994.
3. J. Mann, Chemical Aspects of Biosynthesis, Oxford University Press, 1994.
4. R. B. Silverman, The Organic Chemistry of Drug Design and Action, 2nd edition, Elsevier, New York, 2004.
5. G. L. Patrick, An Introduction to Medicinal Chemistry-5, Oxford University Press, 2013.

CY-581 Introduction to High Energy Materials (Elective, 2 credits)

Prerequisite: None

Brief review of thermodynamics: Laws of thermodynamics, Definition of heat, energy, internal energy, enthalpy, free energy and entropy. Relationship between ΔE and ΔH, C_p and C_v. (2 h)

Thermo chemistry: Standard enthalpy of formation, enthalpy changes in reactions, thermo chemical equations, heat of combustion, Hess Law, calculations of enthalpies for various types of reactions. (2 h)

Requirement for High Energy Materials (HEM): Explanation for energy release using bond energy calculations, energy release with respect to heats of formation, heat of explosion, Density factor, oxygen balance. (5 h)

Volume of gas and heat releases in an explosion, Pressure and temperature rise in an explosion reaction, explosive power and power index. (3 h)

Decomposition products from explosion reactions: Kistiakowesky-Wilkinson rule, modified K-W rule, Springer-Robert rule, water-gas equilibrium, determination of composition of decomposition products using equilibrium chemistry. (4 h)

Bomb calorimeter, Use of TG-DTA and DSC for determination of various energetic parameters of HEM. (2 h)

Clssification of HEM: classification based on chemical groups present, Activation energy required for initiation of HEM, Classification based on explosive power and energy required for initiation of HEM. (3 h)

Burning of HEM, detonation and deflagration processes, propellant and pyrotechnics. Propellant composition, fuel, oxidizers, binders, plasticizers, thermite mixture, and other ingradients. (2 h)

Synthesis of representative examples of HEM. (2 h)

CY-582: Molecules and Materials for Electricity Production and Storage (Elective, 2 credits)

Prerequisite: None

Molecules and Materials for Electricity Storage Devices: Primary and secondary batteries and their working principles, electrode reactions, Inorganic and Organic Materials for anodes, cathodes and for transport of electrons and ions. Liquid and solid electrolytes used in the batteries.

Molecules and Materials for Renewable Electricity Harvesting Devices: Photovoltaic effect. Various types of solar cells and their operating principles. Inorganic and Organic Semiconductors, electron transport and hole transport in solar cells, efficiency of the solar cells and energy payback time.

CY-583: C–H Functionalization (Elective, 2 credits)

1) Origin and earlier reports: Concept and classification of C-H functionalization, C-H functionalization of acidic C-H bonds, C-H functionalization of less acidic C-H bonds (2h)

2) Friedel-Crafts reaction, intramolecular Friedel-Crafts reaction, asymmetric intramolecular Friedel-Crafts reaction, application to synthesis of natural products and bioactive compounds (3h)

3) Free radical mediated C-H functionalization reactions, Breslow remote functionalization and applications, other reactions (3h)

4) Fujiwara–Moritani reaction, Heck reaction including asymmetric Heck reaction, intramolecular Heck reaction, asymmetric intramolecular Heck reaction, application to synthesis of natural products and bioactive compounds, Catellani reaction (5h)

5) Baylis-Hillman reaction, asymmetric Baylis-Hillman reaction, intramolecular Baylis-Hillman reaction, asymmetric intramolecular Baylis-Hillman reaction, application to synthesis of natural products and bioactive compounds (5h)

6) C-H functionalization *via* C-H activation, origin of C-H bond activation and earlier reports, development of concept of C-H functionalization *via* C-H activation, asymmetric C-H functionalization *via* C-H activation, intramolecular version, asymmetric intramolecular version, application to synthesis of natural products and bioactive compounds (5h)

7) Miscellaneous reactions (1h)

References

Books: (1) Smith, M. B. March, J. J*. March's Advanced Organic Chemistry: Reactions, Mechanisms and Structure*, 7th ed.; Wiley: New York, 2013**.** (2) Carey, F. A.; Sundberg, R. J. *Advanced Organic Chemistry*; *Part A & B*, 5th ed.; Springer: New York, 2007. (3) Mundy, B. P ; Ellerd, M. G. ; Favaloro, F. G. *Name Reactions and Reagents in Organic synthesis* (2005) second edition John-Wiley and Sons Inc. New Jersey

Reviews: (1) *Beilstein J. Org. Chem.* **2010**, *6*, 6. doi:10.3762/bjoc.6.6. (2) *Acc. Chem. Res.* **1980***, 13*, 170-177. (3) *Chem. Soc. Rev.* **2011,** *40*, 5122–5150. (4) *Chem. Rev.* **2000**, *100*, 3009-3066. (5) *Chem. Soc. Rev.* **2012**, *41*, 68-78. (6) *Chem. Rev.* **2010**, *110,* 5447–5674. (7) *Chem. Rev.* **2019**, *119,* 2192–2452. (8) *Chem. Soc. Rev.* **2018***, 47,* 8925−8967. (9) *Nat. Chem.* **2013**, *5,* 369 –375.

CY-584: Flow Chemistry and Process Intensification (2.0 credits)

Prerequisite: MSc courses up to 3rd year of Integrated 5 year MSc / BSc degree courses for 2 year MSc

Contents:

Introduction to flow chemistry and its advantages (2)

Recapitulate basic concepts of physical chemistry and reaction kinetics (2)

Principles and equations of flow chemistry (3)

Heterogeneous catalysis in flow chemistry reactions (4)

Pharmaceutical synthesis in flow reactors (5)

Different types of flow reactors (2)

Hazardous batch reactions done with ease in flow (3)

Handling of solids, liquids and gases reactants in flow (2)

Manufacture of Entresto/ commercial drugs in flow chemistry process (2)

Crystallization of polymorphs, cocrystals and salts in flow mode (4)

Important safety aspects essential in flow chemistry (2)

Video illustration of flow reactions (1)

Lectures by eminent academics covering recent research (3)

Brainstorming on design / development of batch to flow reactions by students (2)

Suggested Reading:

1. Masuda et al. Flow fine synthesis with heterogeneous catalysts. Tetrahedron 2018, 74, 1705-1730.
2. Domokos et al. Integrated Continuous Pharmaceutical Technologies-A Review. Org. Process Res. Dev. 2021, 25, 721-739.
3. Mascia et al. End-to-End Continuous Manufacturing of Pharmaceuticals: Integrated Synthesis, Purification, and Final Dosage Formation. Angew. Chem. Int. Ed. 2013, 52, 12359-12363.

4. Bedard et al. Science, 2018, 361, 1220-1225.

5. Plutschack et al. The Hitchhiker's Guide to Flow Chemistry. Chem. Rev. 2017, 117, 11796-11893.

6. Cole et al. Kilogram-scale prexasertib monolactate monohydrate synthesisvunder continuous-flow CGMP conditions. Science, 356, 2017, 1144-1150.

7. Drahl, C&EN, March 12, 2018, p. 12.

8. Thaisrovings et al. Development of an Organometallic Flow Chemistry Reaction at Pilot-Plant Scale for the Manufacture of Verubecestat. Org. Process Res. Devp. 2018, 22, 403-408.

9. Akwi & Watts, Continuous flow chemistry: where are we now? Recent applications, challenges and limitations. Chem. Commun. 2018,54, 13894-13928.

10. Kleinbeck et al. Application of Transition-Metal Catalysis, Biocatalysis, and Flow Chemistry as State-of-the-Art Technologies in the Synthesis of LCZ696. J. Org. Chem. 2020, 85, 11, 6844–6853.

11. Narala et al. Pharmaceutical Co-crystals, Salts, and Co-amorphous Systems: A novel opportunity of hot-melt extrusion. Journal of Drug Delivery Science and Technology, 2021, 61, 102209.

12. Gerardy & Monbaliu. Multistep Continuous-Flow Processes for the Preparation of Heterocyclic Active Pharmaceutical Ingredients. Top. Heterocycl. Chem. DOI: 10.1007/7081_2018_21.

13. Hartman, McMullen, Jensen. Deciding Whether To Go with the Flow: Evaluating the Merits of Flow Reactors for Synthesis. Angewandte Chemie International Edition, 2011, 50, 33, 7502-7519.

14. Gutmann, Cantillo, Oliver Kappe. Continuous-Flow Technology—A Tool for the Safe Manufacturing of Active Pharmaceutical Ingredients. Angewandte Chemie International Edition, 2015, 54, 23, 6688-6728.

15. Norbert Kockmann et al. Safety assessment in development and operation of modular continuous-flow processes. React. Chem. Eng., 2017, 2, 258-280.

Web resource: http://chemistry.uohyd.ac.in/~CY584/