Netaji Subhas University, Jamshedpur

MASTER OF SCIENCE IN CHEMISTRY

(SEMESTER PATTERN)

CHOICE BASED CREDIT SYSTEM SYLLABUS

TWO YEARS FULL TIME PROGRAMME

(As per U.G.C. Model Syllabus)

Effective from Academic Session 2018 onwards

Syllabus

Semester - 1

Course No	Course Name	L-T-P-C
CH 410	Transition and Non-transition Metal Chemistry	3-1-0-8
CH 415	Inorganic Chemistry Laboratory	0-0-9-9
CH 420	Principles of Organic Chemistry	3-1-0-8
CH 430	Quantum Chemistry	3-1-0-8
CH 431	Group Theory and Spectroscopy	3-1-0-8
	Total Credits:	12-4-9-41

Semester - 2

Course No	Course Name	L-T-P-C
CH 411	Inorganic Reaction Mechanism and Organometallics	3-1-0-8
CH 421	Organic Reactions Mechanisms	3-1-0-8
CH 425	Organic Chemistry Laboratory	0-0-9-9
CH 432	Chemical Dynamics and Electrochemistry	3-1-0-8
CH 433	Applications of Spectroscopy	3-1-0-8
	Total Credits:	12-4-9-41

Semester - 3

Course No	Course Name	L-T-P-C
CH 500	Graduate Seminar	0-0-2-2
CH 511	Principles of Bioinorganic Chemistry	3-1-0-8
CH 520	Concepts in Organic Synthesis	3-1-0-8
CH 521	Modern Techniques and Scope of Chemical Biology	3-1-0-8
CH 530	Classical and Statistical Thermodynamics	3-1-0-8
CH 535	Physical Chemistry Laboratory	1-0-8-10
	Total Credits:	13-4-10-44

Semester 4

Course No	Course Name	L-T-P-C
CH 501	Computer in Chemistry	2-0-1-5
CH 600	Project	0-0-18-18
CH 6xx	Elective I	3-1-0-8
CH 6xx	Elective II	3-1-0-8
	Total Credits:	8-2-19-39

List of Elective Courses

CH 640 Principle and Applications of Luminoscence Spectroscopy
CH 615 Advanced Organometallic Chemistry
CH 637 Advanced Quantum Chemistry
CH 616 Bioinorganic Chemistry
CH 625 Art in Organic Synthesis
CH 626 Modern Reagents in Organic Synthesis
CH 637 Advance Quantum Chemistry
CH 628 Advances in Nucleic Acid and Lipid Chemistry

Syllabus

CH-410 : Transition and Non-transition Metal Chemistry 3 1 0 8

Non-transition Metal Chemistry: Synthesis, Properties, Structure and Bonding of: Nitrogen, Phosphorous, Sulfur, Pseudohalogen, Interhalogen and Xenon Compounds; Boranes, Carboranes, Metallocarboranes, Borazines, Phosphazenes, Sulfur-Nitrogen compounds, silicates, silicones. Iso- and Hetero-poly anions. Redox Reactions: Latimer diagram, Electrochemical Series. Acids and Bases: Lewis acids and bases; HSAB concept. Transition Metal Chemistry: Nomenclature, Isomerism, Chelate effect, Macrocyclic ligands. Bonding in Coordination Complexes: Crystal-Field theory, d-orbital Splitting in Octahedral, Tetrahedral, Square Planar geometries; Molecular Orbital Theory, p-bonding; Jahn-Teller effect, Spectrochemical series, nephelauxetic series. Electronic Spectra: d-d transitions, Orgel and Tanabe-Sugano diagrams, charge-transfer spectra. Magnetism: Types, determination of magnetic susceptibility, spin-only formula, spin-orbit coupling, spin crossover.

Text Books:

1. Inorganic Chemistry: Principles of Structure and Reactivity by J. E. Huheey, E. A. Keiter and R. L. Keiter, 4th ed. Harper Collins 1993
2. Concepts and Models of Inorganic Chemistry by B. E. Douglas, D. H. McDaniel and J. J. Alexander, John Wiley, 1993, 3rd ed.

References:

1. Physical Inorganic Chemistry: A Coordination Chemistry Approach by S. F. A. Kettle, Spektrum, 1996
2. Chemistry of the Elements by N. N. Greenwood and A. Earnshaw, Pergamon, 1985.
3. Advanced Inorganic Chemistry by F. A. Cotton, G. W. Wilkinson, 5th edition, John-Wiley & Sons, 1988.
4. Physical Methods in Chemistry by R. S. Drago, Saunders, 1992
5. Inorganic Electronic Spectroscopy by A. B. P. Lever, Elsevier, 1984, 2nd Ed.
6. Introduction to Magnetochemistry by A. Ernshaw, Academic press, 1968.

CH-415: Inorganic Chemistry Laboratory 0 0 9 9

Synthesis and characterization of inorganic compound including co-ordination complexes, assemblies.
Synthetic methods: solution chemistry, solid state synthesis, sol-gel methods, multi step synthesis, preparation of isomers, synthesis under inert atmosphere, electrosynthesis.
Characterization: quantitative and qualitative determination of ligand and metal, use of spectral techniques (UV - visible, IR, NMR, ESR, magnetic moment,

analytical methods (conductance, TG, DSC, cyclic voltametry, coulometry).

Text Books:

1. Synthesis and Technique in Inorganic Chemistry: A Laboratory Manual, Gregory S. Girolami, Thomas B. Rauchfuss and Robert J. Angelici. University Science Books.
2. Synthetic methods of organometallic and inorganic chemistry ed. by Wolfgang A. Herrmann, Georg Thieme Verlag, New York, 1997, Vol 7 and 8
3. Vogel's qualitative inorganic analysis, by Svehla, G. Publisher: Harlow : Longman, 1996.
4. Vogel's textbook of quantitative inorganic analysis: including elementary instrumental analysis. By: Arthur Israel Vogel; John Bassett Publisher: London; New York: Longman, 1978.

CH-420 : Principles of Organic Chemistry 3 1 0 8

Structure and Bonding: Review of basic principles of structure and bonding, application of acid base concepts, HSAB theory, aromaticity and antiaromaticity, Hückel's rule, anti-aromaticity, y-aromaticity, homo-aromaticity n-annulenes, heteroannulene, fullerenes, C-60, cryptates, Bonds weaker than covalent; addition compounds, inclusion compounds, crown ethers, cyclodextrins, catenanes and rotaxanes. Stereochemistry: Conformational analysis of cycloalkanes, effect of conformation on reactivity. Elements of symmetry, chirality, molecules with more than one chiral center, projection formulae (i) Fischer (ii) Sawhorse (iii) Newman (iv) Flying Wedge; threo and erythro isomers, methods of resolution, optical purity, enantiotopic and diastereotopic atoms, groups and faces, stereospecific and stereoselective synthesis. Asymmetric synthesis. Optical activity in the absence of chiral carbon. Reaction mechanism: Structure and Reactivity: Types of mechanisms, types of reactions, thermodynamic and kinetic requirements, Hammond postulate, Curtin-Hammett principle, transition states and intermediates, methods of determining mechanisms, isotopic effects. Generation, structure, stability and reactivity of carbocations, carbanions, free radicals, carbenes and nitrenes. Effect of structure on reactivity. The Hammett equation and linear free energy relationship (sigma-rho) relationship, Taft equation.
Oxidation: Different oxidative processes. Hydrocarbons, carbonyl compounds, amines, hydrazines and sulphides. Reduction: Different reductive processes. Hydrocarbons, carbonyl compounds, nitro, nitroso, azo and oxime groups. Hydrogenolysis. Rearrangements: General mechanistic considerations, nature of migration, migratory aptitude, nucleophilic, electrophilic and free radical rearragnement. A detailed study of various arrangements reactions.

Text Books:

1. Advanced Organic Chemistry by J. March, John Wiley & Sons, 1992
2. Stereochemistry of Carbon Compounds by E. J. Eliel, McGraw Hill

Reference:

1. Organic Chemistry by S. H. Pine, McGraw Hill, 1987.
2. Stereochemistry of Organic Compounds by D. Nasipuri, Wiley, 1994.

CH-430: Quantum Chemistry 3 1 0 8

Review of essential mathematical concepts. Origin of the quantum theory. Postulates of quantum mechanics and Schrödinger equation; its application on some model systems viz., free-particle and particle in a box, tunneling, the harmonic oscillator, the rigid rotator, and the hydrogen atom. The variation theorem; linear variation principle; perturbation theory; applications of variational methods and perturbation theory to the helium atom. Ordinary angular momentum, generalized angular momentum, eigenfunctions, and eigenvalues of angular momentum operator, Ladder operator, addition of angular momenta. Spin, antisymmetry, Pauli exclusion principle, Slatter determinantal wave functions. Term symbol (RS and jj coupling) and spectroscopic states, term separation energies of pn and dn configurations, magnetic effects: spin-orbit coupling and Zeeman splitting. Virial theorem. Born-Oppenheimer approximation, VB and MO theory, H_2^+, H_2 molecule problem, Hückel molecular orbital theory and its application to ethylene, butadiene and benzene. Hybridisation and valence MOs of H_2O, NH_3 and CH_4. Introduction to the SCF.

Text Books:

1. Elementary Quantum Chemistry by F. L. Pilar, Dover Publications, Inc. NY, 1990. 2nd Ed.
2. Molecular Quantum Mechanics by P. W. Atkins and R. S. Friedman, 3rd Ed., Oxford Univ. Press, 1997.

References:

1. Quantum Chemistry by Ira N. Levine, Prentice Hall,
2. Introduction to Quantum Chemistry by A. K. Chandra, Tata McGraw Hill.

CH-431: Group Theory and Spectroscopy 3 1 0 8

Group Theory: Definition of group, symmetry, point groups, representation of group, orthogonality theorem, irreducible representation, character table, direct sum, direct product, derivation of projection operator. Spectroscopy: Electromagnetic radiation and its interaction with matter. Uncertainty principle: Natural line width and broadening.
Microwave: classification of molecules, rigid rotor model, selection rules, intensity of spectral lines, effect of isotopic substitution. Stark effect. Infrared: Review of harmonic oscillator, selection rules, vibrational energy of diatomic molecules, zero point energy, force constant and bond strength; anharmonicity, Morse potential energy diagram, vibration-rotation spectroscopy, P, Q, R, branches. Breakdown of Born-Oppenheimer approximation, vibration of polyatomic molecules. normal mode of vibration, group frequencies, overtone, hot bands. Raman: Classical and quantum theories of Raman effect, pure rotational, vibrational and vibrational-rotational Raman spectra, selection rules, mutual exclusion principle. Resonance Raman. Molecular Spectroscopy: Energy levels, MO, vibronic transitions, Franck-Condon principle, electronic spectra of polyatomic molecules. Emission spectra, radiative and non-radiative decay, internal conversion. Photoelectron spectroscopy.

Text Books:

1. Chemical Applications of Group Theory by F.A. Cotton, Wiley Interscience, 1990, 3rd Ed.
2. Fundamentals of Molecular Spectroscopy by C. N. Banwell and E. M. McCash, Tata McGraw Hill, 1994.

Reference:

1. Group Theory and Quantum Mechanics by M. Tinkham, McGraw Hill, 1964.
2. Introduction to Molecular Spectroscopy by G. M. Barrow, McGraw Hill
3. Introduction to Atomic Spectra by H. E. White, McGraw Hill, 1934.
4. Modern Molecular Photochemistry by Nicholas J. Turro, University Science Books, 1991.

Semester 2

CH-411: Inorganic Reaction Mechanism and Organometallics
3 1 0 8

Reaction Mechanism: Substitution in octahedral and square planar complexes; lability, trans-effect, Conjugate base mechanism, racemisation, Electron Transfer Reactions: inner sphere and outer sphere mechanism, Marcus theory. Inorganic photochemistry: Photosubstitution and photoredox reactions of chromium, cobalt and ruthenium compounds, Adamson's rules. Lanthanides and Actinides: Spectral and Magnetic Properties, NMR Shift reagents. Organometallic Chemistry: 18-

electron rule, metal carbonyls, nitrosyls, cabonyl hydrides, isolobal analogy, dioxygen and dinitrogen compounds. Metal alkyls, carbenes, carbynes, alkenes, alkynes, and allyl complexes. Hydrides, Metallocenes, Metal arene complexes. Carbonylate anions, agostic interaction, Oxidative addition and reductive elimination, insertion and elimination reactions. Homogeneous and heterogeneous catalysis. Fluxional molecules. Metal-Metal bonding and Metal clusters.

Text Books:

1. Inorganic Chemistry: Principles of Structure and Reactivity by J. E. Huheey, E. A. Keiter and R. L. Keiter, 4th Ed. Harper Collins 1993.
2. Concepts and Models of Inorganic Chemistry by B. E. Douglas, D. H. McDaniel, J. J. Alexander, John Wiley, 1993, 3rd Ed.

References:

1. Reaction Mechanism in Inorganic Chemistry by R. R. Jordan Oxford Univ. Press, 1998. 2nd Ed.
2. Advanced Inorganic Chemistry by F. A. Cotton and G. W. Wilkinson, John-Wiley & Sons, 1988, 5th Ed.
3. Organometallics by Ch. Elschenbroich, A. Salzer, VCH, 1995, 2nd Ed.
4. Organotransition Metal Chemistry: Fundamental Concepts and Applications by A. Yamamoto, John Wiley 1986.
5. Organometallic Chemistry of the Transition Metals by R. H. Crabtree, John Wiley, 1993, 2nd Ed.
6. Inorganic Chemistry by D. F. Shriver and P. W. Atkins, 3rd Ed., Oxford.

CH-421: Organic Reactions and Mechanisms 3 1 0 8

Aliphatic Nucleophilic Substitution: The SN^2, $S\neg N^1$, mixed $S\neg N^1$ and SN^2 and SET mechanisms. The neighbouring group mechanism. Classical and nonclassical carbocations, phenonium ions, norbornyl system, common carbocation rearrangements. The SN^i mechanism. Nucleophilic substitution at an allylic, aliphatic trigonal and a vinyl carbon. Reactivity effects of substrate structure, attaching nucleophile, leaving group and reaction medium. Electrophilic Substitution: Aliphatic: Bimolecular mechanisms: SE^1, SE^2 and SE^i. The SE^1 mechanism, electrophilic substitution accompanied by double bond shifts. Effect of substrates, leaving group and the solvent polarity on the reactivity. Aromatic: The arenium ion mechanism, orientation and reactivity, energy profile diagrams. The ortho/para ratio, ipso attack, orientation in other ring systems. Quantitative treatment of reactivity in substrates and electrophiles. Aromatic Nucleophile Substitution: The SNAr, SN^1, benzyne and SRN^1 mechanisms. Reactivity; effect of substrate structure, leaving group and attacking nucleophile. Free Radical

Reactions: Types of free radical reactions, free radical substitution mechanism, mechanism at an aromatic substrate, neighbouring group assistance. Reactivity for aliphatic and aromatic substrates at a bridgehead. Reactivity in the attaching radicals. The effect of solvents on reactivity. Addition to Carbon-Carbon Multiple Bonds: Mechanistic and stereochemical aspects of addition reactions involving electrophiles, nucleophiles and free radicals, regio- and chemo-selectivity, orientation and reactivity. Addition to cyclopropane ring. Hydroboration. Addition to Carbon-Hetero Multiple Bonds: Mechanism of metal hydride reduction of saturated and unsaturated carbonyl compounds, acids, esters and nitriles. Addition of Grignard reagents, organozinc and organolithium reagents to carbonyl and unsaturated carbonyl compounds. Elimination Reactions: The E^2, E^1 and E1cB mechanisms and their spectrum. Orientation of the double bond. Reactivity; effects of substrate structures, attaching base, the leaving group and the medium.

Text Books:

1. Advanced Organic Chemistry by J. March, John Wiley & Sons, 1992
2. Organic Chemistry by S. H. Pine, McGraw Hill, 1987.

Reference:

1. Modern Synthetic Reactions by H. O. House, W.A. Benjamin, Inc., 1972
2. Understanding Organic Reaction Mechanism by A. Jacobs, Cambridge 1998.
3. Organic Chemistry by J. M. Hornback, Books Coley, 1998.
4. Organic Chemistry by P.Y. Bruice, Prentice Hall, 1998.
5. Organic Reaction and their Mechanism by P.S. Kalsi, New Age, 1996.

CH – 425: Organic Chemistry Laboratory 0 0 9 9

Separation techniques and characterization (t.l.c, column, distillation, crystallization, GC etc.)
Organic synthesis: Representative reaction to be covered
Esterfication and saponification, Oxidation, Reduction, Nucleophilic substitution, Cycloaddition reactions, Grignard reaction, Condensation reactions, Preparation of dyes, Aromatic electrophilic substitution, Heterocyclic synthesis, Solidphase synthesis, Natural product extraction: Solasidine, Caffeine, Nicotine, Peptine, Rosine, Carotenoids, Computational methods of retro-synthetic analysis modeling and calculation

Text Books:

1. Vogel's Text Book of Practical Organic Chemistry, by Brian S. Furniss, ELBS Longman, 5th edition, 1996.
2. techniques and Experiments for Organic Chemistry, by Addison Ault, University Science Book, 6th Edition.
3. Instrumental techniques for Analytical Chemistry by Frank Settle, Printice

Hall, 1997.

CH-432: Chemical Dynamics and Electrochemistry 3 1 0 8

Chemical Dynamics: Methods of determining rate laws, collision theory of reaction rates, steric factor, Arrhenius equation and activated complex theory, kinetic and thermodynamic control of reactions, ionic reactions, kinetic salt effects, steady state kinetics, unimolecular reactions and their treatments (Lindemann-Hinshelwood and Rice-Ramsperger-Kassel-Marcus [RRKM] theory), Complex reactions (chain reactions, and oscillatory reactions), photochemical reactions, homogeneous catalysis, enzyme kinetics, studies of fast reactions by flow method, relaxation method, flash photolysis and NMR. Dynamics of molecular reactions, probing the transition state, dynamics of barrierless chemical reactions in solution, dynamics of unimolecular reactions. Electrochemistry: Electrochemical cells, Nernst equation and applications of Debye-Huckel-theory, Electrolytic conductivity and the Debye-Hückel-Onsangar treatment, electrified interfaces, overpotential, corrosion.

Text Books:

1. Chemical Kinetics by Keith Laidler, Harper and Row, 1995.
2. Chemical Kinetics: The study of reaction rates in solution by Kenneth A. Connors, VCH, 1990
3. Electrochemistry by Carl H. Hamann, Andrew Hamnett and Wolf Vielstich, Wiley VCH, 1998.

References:

1. Reaction Kinetics by M. J. Pilling and P. W. Seakins, Oxford Press, 1997
2. Modern Electrochemistry 1. Volume 1 and 2, by J. O'M. Bockris and A. K. N. Reddy, Kluwer Academic, 2000.
3. Electrochemical Methods, by A. J. Bard and L. R. Faulkner, John Willey, 1980

CH-433: Applications of Spectroscopy 3 1 0 8

Vibrational: Symmetry and shapes of AB_2, AB_3, AB_4, AB_5 and AB_6, modes of bonding in ambidentate ligands, application of resonance Raman spectroscopy particularly for the study of active sites of metalloproteins. Electron Spin Resonance: Hyperfine coupling, spin polarization for atoms and transition metal

ions, spin-orbit coupling and significance of g-tensor, application of transition metal complexes having one unpaired electron including biological systems and to inorganic free radicals such as PH_4, F_2^- and $[BH_3]^-$.

Nuclear Magnetic Resonance: The contact and pseudo contact shifts, factors affecting nuclear relaxation, some applications including biological systems, an overview of NMR of metal nuclides. Chemical shift, spin-spin interaction, shielding mechanism, complex spin-spin interaction, virtual coupling stereochemistry, hindered rotation, Karplus curve, variation of coupling constant with dihedral angle, nuclear magnetic double resonance, simplification of complex spectra, shift reagent, spin tickling, nuclear overhauser effect (NOE), resonance of other nuclei. 13C NMR: Chemical shift, 13C coupling constants, two-dimensional NMR spectroscopy, NOISY, DEPT, INEPT terminology.

Mössbauer: Basic principles, spectral parameters and spectrum display. Application to the studies of (1) bonding and structures of Fe^{2+} and Fe^{3+} compounds including those of intermediate spin, (2) Sn^{2+} and Sn^{4+} compounds – nature of M-L bond, coordination number, structure and (3) detection of oxidation state and inequivalent MB atoms. Electrochemical techniques: CV, polarography, coulometry, amperometry. Thermal Methods: TGA, DSC and DTA

UV-Vis: Woodward rule for conjugated dienes and carbonyl compounds. IR: Characteristic vibrational frequencies of different functional groups, effect of hydrogen bonding and solvent effect on vibrational frequencies, overtones, combination and Fermi resonance bands.

Mass: Instrumentation, Mass spectral fragmentation of organic compounds, McLafferty rearrangement, examples of mass spectral fragmentation of organic compounds with respect to their structure determination.

ORD & CD: Definition, deduction of absolute configuration, octant rule for ketones.

Data Analysis: Uncertainties, errors, mean, standard deviation, least square fit, testing the fit (C2 test, residual etc.). Signal to noise ratio.

Text Books:

1. Physical Methods in Chemistry by R. S. Drago, Saunders, 1992
2. Inorganic Electronic Spectroscopy by A. B. P. Lever, Elsevier, 1984, 2nd Ed.
3. Spectrometric Identifications of Organic Compounds by R. M. Silverstein, John Wiley, 1991.
4. Introduction to Spectroscopy by D.L. Pavia, G. M. Lampman, G. S. Kriz, Harcourt College Publisher, NY, 2001

References:

1. Organic Spectroscopy by William Kemp, ELBS 3rd Ed. 1994.

Semester 3

CH 511: Principles of Bioinorganic Chemistry 3 – 1 - 0 - 8

Role of alkali and alkaline earth metal ions in biology; Na^{+}-K^{+} Pump, ionophores and crown ethers. Metal site structure, function. Metal ion transport and storage: Ferritin, Transferrin, Siderophores and metallothionein. Electron Transfer: Cytochromes, Iron-Sulfur Proteins and Copper Proteins. Oxygen transport and storage: Hemoglobin, myoglobin, hemerythrin, hemocyanin Oxygen activation: Cytochrome P450, Cytochrome c oxidase. Other metal containing enzymes: Catalase, peroxidase, superoxide dismutase, alcohol dehydrogenase, carbonic anhydrase, carboxypeptidase, xanthine oxidase, nitrogenase, vitamin B12 coenzyme, photosystem I and II, oxygen evolving center. Various spectroscopic methods used in bioinorganic chemistry: electronic spectra, EPR (emphasis on first row transition metal ions and their spectra), brief description of CD / MCD and multinuclear NMR. Applications of newer methods like EXAFS, XANES and ENDOR in characterization of biological molecules. Use of coordination complexes as models for various enzymes, metalloproteins. Role of hazardous materials such as nitric oxide, cyanide and methyl isocyanate etc. in biological systems.

Text Books:

1. S. J. Lippard and J. M. Berg, *Principle of Bioinorganic Chemistry* , University Science Books (1994).
2. Lawrence Que, Jr, *Physical Methods in Bioinorganic Chemistry: Spectroscopy and Magnetism,* University Science Books (2000).

References:

1. F. A. Cotton and G. W. Wilkinson, *Advanced Inorganic Chemistry*, 5th Ed. , John-Wiley & Sons, (1988).

2 D. Banerjea, *Coordination Chemistry*, 2nd Ed, Asian Books Pvt. Ltd. (2007).

3. J. E. Huheey, E. A. Keiter and R. L. Keiter, *Inorganic Chemistry: Principles of Structure and Reactivity* , 4th Ed. Harper Collins (1993).

CH 520: Concepts in Organic Synthesis 3 1 0 8

Pericyclic Reactions: Molecular orbital symmetry, Frontier orbitals of ethylene, 1,3-butadiene, 1,3,5-hexatriene and allyl system. Classification of pericyclic reactions. Woodward-Hoffmann correlation diagrams. FMO and PMO approach. Electrocyclic reaction; conrotatory and disrotatory motions 4n, 4n+2 and allyl systems. Cycloaddition; antrafacial and suprafacial addition, 4n and 4n+2 systems, 2+2 addition of ketenes, 1,3 dipolar cycloadditions and cheleotropic reactions. Sigmatropic Rearrangements; suprafacial and antrafacial shifts of H, sigmatropic shifts involving carbon moieties, 3,3- and 5,5- sigmatropic rearrangements, Claisen, Cope and Aza-Cope rearrangements. Ene reaction. Photochemistry: Quantum yields, intersystem crossing, photosensitization and energy transfer reactions. Photochemistry of olefins and carbonyl compounds, photo oxygenation and photo fragmentation, Photochemistry of aromatic compounds: isomerisation, additions and substitutions. Singlet molecular oxygen reactions. Patterno-Buchi reaction, Di-pimethane rearrangement, Bartons reaction and Photo-Fries

rearrangement. Reagents in Organic Synthesis: Use of the following reagents in organic synthesis and functional group transformations; complex metal hydrides, Gilman's reagent, lithium dimethylcuprate, lithium diisopropylamide (LDA), dicyclohexylcarbodiimide, 1,3-dithiane (reactivity Umpoloung), trimethylsilyl iodide, tri-n-butyltin hydride, Woodward and pervost hydroxylation, osmium tetroxide, DDQ, selenium dioxide, Phase transfer catalysts, crown ethers and Merrifield resin, Peterson's synthesis, Wilkinson's catalyst, Baker yeast. Heterocyclic Chemistry: Synthesis and reactivity of furan, thiophene, pyrrole, pyridine, quinoline, isoquinoline and indole; Skraup synthesis, Fisher indole synthesis. Chemistry of Natural Products: Structure elucidation and biosynthesis of Alkaliods, Terpenoids, Steroids.

Text Books:

1. Frontier Orbital and Organic Chemical Reactions by I. Fleming, John Wiley, 1976.
2. Some modern Methods of Organic Synthesis by W. Carruthers, Cambridge University Press, 1990.
3. Protective Groups in Organic Synthesis by T.W. Greene, Wiley-VCH, 1999.

Reference:

1. Modern Heterocyclic Chemistry by L. A. Paquette, W.A. Benjamin, Inc.,1968.
2. Organic Chemistry by I. L. Finar, Vol II, ELBS, 1968.
3. Heterocyclic Chemistry by T. R. Gilchrist, Longman,1989.
4. Selectivity in Organic Synthesis by Ward, Wiley-VCH, 1999.

CH 521: Modern Techniques and Scope of Chemical Biology 3 1 0 8

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

Text Books:

1. Chemical Biology: A practical course, edited by H. Waldmann and P. Janning. Wiley – VCH Verlag GmbH & Co. 2004
2. Foundations of Chemical biology, by C.M. Dobson, J.A. Gerrard and A.J. Pratt. Oxford Univ. Press. 2002
3. Biochemistry by J. M. Berg, J. L. Tymoczko and L. Stryer. W. H. Freeman and Company, New York

References:

1.Chemical Biology: from small molecules to systems biology and drug design, Vol.-1, edited by S. L. Schreiber, T. Kapoor and G. Wess. Wiley – VCH Verlag GmbH & Co. 2007

2. Chemical Biology: Application and Techniques, edited by Banafshe Larijani, Colin A. Rosser and Rudiger Woscholski, John Wiley & Sons Ltd. England, 2006

3. Principles of Biochemistry by Lehninger, Nelson and Cox, CBS Publishers, 1993.

CH-530: Classical and Statistical Thermodynamics 3 1 0 8

Classical Thermodynamics: Review of the laws of thermodynamics, free energy, chemical potential and entropies. Partial molar quantities and their significances. Determination of these quantities, concept and determination of fugacity. Non-ideal systems: Excess function for non-ideal solutions. Activity, activity coefficient, Debye-Hückel theory for activity coefficient of electrolytic solutions; determination of activity and activity coefficients; ionic strength. Application of phase rule to three component systems; second order phase transitions. Statistical Thermodynamics: Statistical concepts and examples. Simple random walk problem in one dimension. General discussion of mean values and its use for the random walk problem. Specification of the state. Statistical ensembles. Basic postulates. Probability calculations. Behaviour of the density of states. Exact and inexact differentials. Equilibrium conditions and constraints. Reversible and irreversible processes. Distribution of energy between systems in equilibrium. Isolated system. System in contact with heat reservoir. Canonical distribution and its simple applications. Ensembles used as approximation. Calculation of thermodynamic quantities, Gibbs paradox, Validity of the classical approximation, Equipartition theorem and its applications: Specific heats of solids, Maxwell velocity distribution. Quantum Statistics of ideal gases. Identical particles and symmetry requirements. Quantum distribution functions. Maxwell-Boltzman, Photon, Bose-Einstein, and Fermi-Dirac statistics. Quantum statistics in the classical limit. Electromagnetic radiation in thermal equilibrium inside an enclosure. Consequences of Fermi-Dirac equation. Lattice vibration and normal modes. Debye approximation.

Text Books:

1. Physical Chemistry by R. S. Berry, S. A. Rice and J. Ross, Oxford University Press, 2nd Ed. 2000.
2. Fundamental of Statistical and Thermal Physics by F. Reif, McGraw Hill, International edition 1985.

Reference:
1. Physical Chemistry: A Molecular Approach by D. A. McQuarrie and J. D. Simon, University Science Books, 3rd Ed. 2001.
2. Statistical Mechanics by R. K. Pathria, Butterworth-Heinemann, 2nd Ed. 1999.

CH-535: Physical Chemistry Laboratory 1 0 8 10

Introduction to Computers and Computing: Basic structure and functioning of computers with a PC as an illustrative example. Memory, I/O devices. Secondary storage. Computer languages. Operating systems with DOS as an example. Introduction to UNIX and WINDOWS. Data processing, principles of programming. Algorithms and flow-charts.
Experiments based on
UV - Visible spectroscopy with application
Fluorescence Spectroscopy with application
Infrared Spectroscopy
Solvents effects in spectra
Differential Scanning Calorimetry
High Pressure Liquid Chromatography
Spectroscopy Instrumentation
Cyclic voltametry
Temperature dependence of reaction rates
Enzymetic reaction
LB films / Liposomes
Ion selective electrodes
Semiconductor materials
Optical materials

Text Books:

1. A Handbook of Instrumental techniques for analytical chemistry, Ed F. A Settle, 1997, Prentice hall PTR
2. Introduction to Instrumental Analysis by R. D. Braun, 1987, McGraw-Hill Int. Ed.
3. Journal of Chemical Education, ACS: some selected readings and experiments will be offered from this journal.

Semester 4

CH 640 Principles and Applications of Luminescence Spectroscopy 3 1 0 8

Luminescence, a brief history, different kinds of luminescence, electronic transition, transition probability, fluorescence and other de-excitation process, phosphorescence versus non-radiative de-excitation, delayed fluorescence, basic instrumentation of steady-state and time-resolved fluorometer, characteristics of

fluorescence emission, solvent and environmental effects, red-edge effects, effects of intermolecular photophysical processes on emission, static and dynamic quenching, Stern-Volmer kinetics, emission anisotropy, intrinsic and extrinsic probes, chemical sensing probes, probes of analyte recognition, electron transfer probes, energy transfer, energy transfer to multiple acceptor, biochemical applications, pH and CO_2 sensors, protein fluorescence and protein sensors, glucose sensors, novel fluorophores: semiconductor nano particles, lanthanides, metal-ligand complexes, long-wavelenth and long-lifetime fluorophores, advanced techniques in fluorescence spectroscopy.

Text Books:

1.J. R. Lakowicz, Principles of Fluorescence Spectroscopy, Springer, 3rd Ed. 2006.
2.B. Valuer, Molecular Fluorescence, Wiley-VCH, 2002.
3.N. J. Turro, Modern Molecular Photochemistry, University Science Books, 1991.

References:

1. J. R. Lakowicz, Topics in Fluorescence Spectroscopy, Vol. 1: Techniques, Plenum Press, 1991.
2. J. R. Lakowicz, Topics in Fluorescence Spectroscopy, Vol. 4: Probe Design and Chemical Sensing, Kluwer Academic Press, 1994.
3.B. Valuer and J. C. Brochon, New Trends in Fluorescence Spectroscopy: Applications to Chemical and Life Sciences, Springer, 2001.

CH 501: Computers in Chemistry 2 0 1 5

Computer programming in FORTRAN. Computer application in Chemistry: Development of small computer codes involving simple formulae in chemistry, such as van der Waals equation, pH titration, kinetics, radioactive decay. Evaluation of lattice energy and ionic radii from experimental data. Linear simultaneous equations to solve secular equations within the Hückel theory. Elementary structural features such as bond lengths, bond angles, dihedral angles etc., of molecules extracted from a database such as Cambridge database.

Use of computer programmes: Execution of linear regression, X-Y plot, numerical integration and differentiation as well as differential equation solution programmes. Monte Carlo and Molecular dynamics. Programmes with data preferably from physical chemistry laboratory.

Text Books:

1. Computational Chemistry by A. C. Norris, John Wiley
2. Numerical Recipes in FORTRAN/C by W. H. Press, S. A. Teukolsky, W. T. Vetterling and B. P. Flannery, Cambridge University Press, 2nd Ed. 1996.
3. Fortran 77 and Numerical Methods by C. Xavier, New Age International, 2002

Reference:

1. Inside the IBM PC by Peter Norton

CH 615 Advanced Organometallic Chemistry 3-0-1-8

Definition, classifications and bonding in organometallic compounds. Isolobal analogies. Structural methods of Organometallics. Preparative methods.

Spectroscopic techniques in Organometallic chemistry. Electronic and magnetic properties of Organometallic compounds. Stoichiometric and catalytic reactions. Fundamental processes in reactions of organo-transition metal complexes. Applications of transition metal complexes to catalysis, organometallics directed towards organicsynthesis.

Bio-organometallics, Organometallics in environmental chemistry. Metal clusters and models for heterogeneous catalysis. Application of Organometallics in Industry.

Text Books:

1. Organotransition metal chemistry, Fundamental concept and applications, A. Yamamoto, John Wiley, 1986.

2. The organometallic Chemistry of transition metals, R.H. Crabtree, John Wiley, 1994.

CH 637: Advance Quantum Chemistry 3 1 0 8

Introduction: Vector Interpretation of Wavefunction, Hermitian Operator, The Generalized Uncertainty principle, The quantum Mechanical Virial Theorem, Solution of harmonic oscillator (Operator approach), Second quantization (Boson and Fermion), Quantum theory of angular momentum, One electorn Atom, Spin angular momentum.

Approximate solutions to the Schroedinger equation: The Variation method (Time independent and Time Dependent), Time independent perturbation theory (non – degenerate and degenetrate), Time dependent perturbation theory.

Electron Spin and Many - Electron Systems: The Antisymmetry Principle, Spin angular momenta and their Operators, The Orbital Approximation (Slater-determinant, Pauli exclusion principle), Two electron wavefunctions.

The Hartree-Fock Self-Consistent Field Method: The generation of Optimized orbitals, Koopman's Theorem (The Physical Significance of Orbital Energies), The electron correlation energy, Density matrix analysis of the Hartree-Fock

Approximation, Natural orbitals, The matrix solution of the Hartree- Fock Equations (Roothaan's equations).

Introduction to Molecular Structure: The Born - Oppenheimer Approximation, Solution of the Nuclear Equation, Molecular Hartree- Fock Calculations.

Electronic Structure of Linear Molecule: The MO - LCAO Approximation, The Hydrogen Molecule Ion, H_2^+, The Hydrogen molecule, Molecular Configuration - Interactions, The Valence Bond Method, Molecular Perturbation Calculations.

Electronic Structure of Non-linear Molecule: The AH_n molecule: Methane, Ammonia and Water, Hybrid Orbitals: The Ethylene and Benzene Molecules.

Semiempirical Molecular Orbital Methods I - PI Electron Systems: The H¨uckel Approximation for Conjugated Hydrocarbons, The Pariser-Parr-Pople Method.Semiempirical Molecular Orbital Methods II - All valence - Electron systems: The Extended H¨uckel Method, The CNDO Method.

Text Books:

1. Elementary Quantum Chemistry by Frank L. Pilar, 2nd Edition, McGraw - Hill Publishing Company, 1990.
2. Molecular Quantum Mechanics by P. W. Atkins and R. S. Friedman, 3rd Edition, Oxford Univ. Press, 1997.

References:

1. Quantum Chemistry by D. A. McQuarrie, Oxford Univ. Press, 1983.
2. Quantum Chemistry by I. N. Levine, Allyn and Bacon Inc., 3rd Edition.

CH 628 Advances in Nucleic Acid and Lipid Chemistry 3 1 0 8

Nucleic acids: Definition, structure and properties, base pairing, double helices, DNA replication, genetic information storage, transmission and gene expression, chemical synthesis of oligonucleotides, hybridization with synthetic oligonucleotides, characterization and purification techniques, nucleic acids as molecular probes. DNA damages, mutations and repair. Modified nucleic acids: Peptide nucleic acids (PNAs),LNAs, synthesis of PNAs, doubly labeled PNAs as probes for the detection of point mutations. Lipids, fatty acids, bilayer, liposome, lipidation of proteins and peptides, farnesylation of the Ras protein. Synthesis of lipids. Role of lipids in drug delivery and gene delivery. Lipid probes. Biophysical properties of lipid-protein, lipid-peptide interactions. Transport across membranes. Lipidated proteins and peptides in model membranes. Basic concepts of fluorescence and lipid markers. synthesis of fluorescence quencher and lipidated peptides.

Text books:

1. C.M. Dobson, J.A. Gerrard and A.J. Pratt., *Foundations of Chemical biology*, Oxford University Press. 2002.
2. A. Miller and J. Tanner, *Essentials of Chemical Biology*, Willey & Sons Ltd. 2008.

References:
1. S. L. Schreiber, T. Kapoor and G. Wess, *Chemical Biology: from small molecules to systems biology and drug design*, Wiley – VCH Verlag GmbH & Co. 2007.