Sino	Proposed Course Code	Course Name	L-T-P-C
SEMESTER- I			
01	CH-421	Quantum Chemistry	3-0-0-6
02	CH-423	Principles of Organic Chemistry	3-0-0-6
03	CH-42S	Chemistry of s- and p-block elements	3-0-0-6
04	CH-427	Symmetry and Group Theory for Chemists	3-0-0-6
OS	CH-429	Biochemistry	3-0-0-6
06	CH-430	Organic Chemistry Lab	0-0-6-6
07	HS-S13	Technical Communication	2-0-0-4
		Total Credits	**40**
SEMESTER- II			
01	CH-422	Thermodynamics for Chemists	3-0-0-6
02	CH-424	Reagents and tools in Organic Chemistry	3-0-0-6
03	CH-426	Chemistry of Transition Metals	3-0-0-6
04	CH-428	Principle of Molecular Spectroscopy	3-0-0-6
OS	CH-432	Modern Methods of Analysis	3-0-0-6
06	CH-434	Computer in Chemistry	2-0-0-4
07	CH-440	Inorganic Chemistry Lab	0-0-6-6
		Total Credits	**40**
SEMESTER- III			
01	CH-S21	Chemical Kinetics	3-0-0-6
02	CH-S23	Concepts in Organic Chemistry_	3-0-0-6
03	*CH-525*	Organometallic and Bioinorganic Chemistry of Transition Metals	3-0-0-6
04	CH-S30	Physical Chemistry Lab	0-0-6-6
OS	CH-6XX	Elective **I**	3-0-0-6
06	CH-591	Project	0-0-6-6
07	CH-527	Seminar	0-0-0-2
		Total Credits	**38**
SEMESTER- IV			
01	CH-6XX	Elective II	3-0-0-6
02	CH-6XX	Elective III	3-0-0-6
03	CH-522	Comprehensive Viva Voce	0-0-0-2
04	CH-592	Project	0-0-20-20
		Total Credits	**34**

Total credits: 40 + 40 + 38 + 34 = 152

SEMESTER I

Principles of Quantum Mechanics. Review of vectors and vector spaces, matrices and determinants, eigenvalues and eigenvectors, similarity transformations, ordinary differential equations- first and second order. Solution of differential equations by power series method: solutions of Hermite equation in detai 1. Orthogonal ity properties and recurrence relations. Introduction to the solutions of Legendre and Laguerre differential equations, Spherical Harmonics. Introduction to Fourier series and Fourier transforms, convolution theorem.

Solution of the Schrodinger equation for exactly solvable problems such as particle-in-a- box, particle-in-a-ring, harmonic oscillator and rigid rotor. Tunneling, one dimensional potential barriers and wells. Postulates of quantum mechanics, wave functions and probabilities, operators, matrix representations, commutation relationships. Hermitian operators, Commutators and results of measurements in Quantum Mechanics. Eigenfunctions and eigenvalues of operators and superposition principle. States as probability distributions and expectation values. The expansion of arbitrary states in terms of complete set.

Angular momentum, commutation relationships, basis functions and representation of angular momentum operators, Coupling (addition) of angular momenta, Clebsch-Gordan coefficients and Wigner-Eckart theorem.

Solution of the Schrodinger equation for the hydrogen atom, radial and angular probability distributions, atomic orbitals and electron spin, Pauli's exclusion principle and Aufbau principle. RS/jj coupling & Zeeman effect.

The time dependent Schrodinger equation. Co-ordinate and momentum space representation of operators and eigenstates; Properties of eigenstates - single-valuedness, double differentiability, continuity, bounded ness / square integrability. Discrete and continuous distributions; Unitary evolution and reversibility. Schrodinger and Heisenberg representations. Projections and irreversibi Ity.

Time-independent perturbation theory, degenerate states, variational method, Hellmann-Feynman theorem, Spectra and structure of helium atom, term symbols for atoms.

Text Books:

I. E. Kreyszig, Advanced Engineering Mathemaics, S'' Edition, Wi ley Easten, 2014.

2. G. Arfken and Hans J. Weber, Mathematical methods for physicists, Prism Indian Edition, 2003.
3. D. A. McQuarrie, Quantum Chemistry, University Science Books, 2008.
4. P. W. Atkins, Molecular Quantum Mechanics, 2nd Edition, Oxford University Press, 2003.
5. 1. N. Levine, Quantum Chemistry, 3rd edition, Allyn and Bacon 2013.
6. D. J. Griffiths, Introduction to Quantum Mechanics, Pearson Education, *2005.*
7. H. Kuhn, H.-D. Forsterling, and D.H. Waldeck, Principles of Physical Chemistry, 2nd Edition., Wiley, 2009.
8. J. P. Lowe, Quantum Chemistry, K. A. Peterson, 3rd Edition, Academic Press, 2006.

CH 423 PRINCIPLES OF ORGANIC CHEMISTRY 3-0-0-6

Structure and Bonding: Review of basic principles of structure and bonding, application of acid base concepts, HSAB theory, aromaticity and antiaromaticity, Huckel's rule, anti-arornaticity, y-aromaticity, homo-aromaticity n-annulenes, heteroannulene, fullerenes. Reactive intermediates: Carbocations, carbanions, carbenes. electrophiles and nucleophiles. Reactivity, kinetics, and mechanisms. Energy surfaces and transition states. Hammond Postulate. Isotope effects. Harnrnet plot. Steric and polar effects. Empirical scales of solvent effect. pH and Bronsted relationship. Mechanism and catalysis of proton transfer. 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.

Text Books:

1. F. A. Carey and R. A. Sundberg, Advanced Organic Chemistry, Part A: Structure and Mechanisms ,5th Edition, Springer, New York, 2007
2. F. A. Carey and R. A. Sundberg, Advanced Organic Chemistry: Part B: Reaction and Synthesis S" Edition, Springer, New York, 2007
3. T. H. Lowry and K. S. Richardson, Mechanism and theory in organic chemistry, 3rd Ed ilion Harper & Row, New York, J998.

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4. N. S. Isaacs, ELBS, Longman, Physical Organic Chemistry, UK, 1987.
5. D. Nasipuri, Stereochemistry of Organic Compounds. Principles and Applications, 4th Edition, New Academic Science Ltd, 20 I I.
6. D. G. Morris, Stereochemistry, RSC Tutorial Chemistry Text 1,200 I
7. E. L. Eliel and S. H. Wilen, Stereochemistry of Organic Compounds, John Wiley & Sons, New York, 2008.

CH 425 CHEMISTRY OF s- AND p-BLOCK ELEMENTS 3-0-0-6

Chemistry of s- and p- block elements: Alkali and alkaline earth metals: The metals and their halides, oxides and hydroxides, Aqueous solution chemistry including macrocyclic complexes and non-aqueous coordination chemistry.

p-block elements: halides, oxides, oxoaacids and oxoanions, boranes, carboranes, metallocarboranes, nitrides, phosphides, and arsenides, phosphazenes, sulfides and selenides, Interhalogen compounds and polyhalogen ions, compounds of xenon, krypton and radon

Organometallic compounds of s- and p-block elements.

Text Books:

I. J. D. Lee, Concise Inorganic Chemistry, Wiley-Blackwell; 5th edition 1999.
2. C. Housecroft and Alan G. Sharpe, Inorganic Chemistry by; Pearson; 4th Edition 2012.

Reference Books:

1. N. N. Greenwood, A. Earnshaw, Chemistry ofthe Elements, Butterworth-Heinemann; 2nd Edition (December 9, 1997)
2. F. Albert Cotton, Geoffrey Wilkinson, Carlos A. Murillo, Manfred Bochmann; Advanced Inorganic Chemistry by Wiley-Interscience; 6th Edition (April 13, 1999)
I. D Banerjea ,Coordination Chemistry, Asian Books 3rd edition 2009.

CH 427 SYMMETRY AND GROUP THEOTY FOR CHEM.IST 3-0-0-6

The concept of groups, symmetry operations and symmetry elements in molecules, matrix representations of symmetry operations, point groups, irreducible representations and character tables. Great orthogonality theorem and its proof.

Application of group theory to atomic orbitals ın ligand fields, molecular orbitals, hybridization. Classification of normal vibrational modes, selection rules in vibrational and electronic spectroscopy.

Text Books:

1. F. A. Cotton, Chemical Applications of Group Theory, Wiley, 3rd Edition 2008.
2. D. M. Bishop, Group theory and Chemistry, Dover, 1993.
3. R. L. Carter, Molecular Symmetry and Group Theory, 2009.

·CR 429 BIOtiiEt\iisTR\ 3-0-0·6

Chemistry of Biomolecules : Proteins, lipids & membranes, carbohydrates, nucleic acids, vitamins and coenzymes.

Molecular mechanisms offUlldamental processes: Metabolism of proteins, lipids and carbohydrates, electron transport and phosphorylation; Biosynthesis of carbohydrates, lipids, amino acids & nucleic acids.

Biochemistry of Enzymes : Physical organic chemistry of enzymatic catalysis, Analysis of enzyme kinetics and receptor-ligand interactions, Enzymatic reaction mechanisms

Fundamentals of genetics and evolution: Central dogma of life, Introductory genetics, Regulation of gene expression, mutation and genetic diseases

Biochemistry of viruses and virus infection: Fundamentals of virus properties, virus multiplication, disease mechanisms, prevention and intervention of infection, threats to human and animal health through emergence and evolution.

Biochemical and molecular analysis of selected human diseases: Lipid metabolism and atherosclerosis, cell cycle regulation and oncogene function in cancer, human immunodeficiency virus (HIV), acquired immunodeficiency disease syndrome (AI DS), autoimmune diseases

Biochemical techıı iques: Different analytical techniques to intercept proteins, DNA, RNA; recombinant DNA techniques, fingerprinting technology and PCR.

Text Books:

I. David Lee Nelson, Albert L. Lehninger, Michael M. Cox, Principles of Biochemistry, 2008, 5th Edition W H Freeman Limited.

Reference Books:

I. Jeremy M. Berg, John L. Tymoczko, Lubert Stryer, Biochemistry, 5th Edition, 2002 W H Freeman Limited

2. Colin Ratledge and Bjorn Kristiansen, Basic Biotechnology 2nd Edition 2001 , Cambridge University Press.

3. M. L. Srivastava, Bioanalytical Techniques, Narosa Publishers 2008.

CH 430 ' -: , ORGANIC CHEMISTRY LAB- . . . 3-0-0-6. :.~

Separation of two-component mixtures of organic compounds. Synthesis and isolation of organic compounds with an emphasis on different techniques of reaction set-up (air-sensitive, moisture-sensitive etc.), separation / purification (extraction, Soxhlet extraction, recrystallization, distillation, column chromatography) and monitoring of reaction by TLC. Structure determination of the isolated pure compounds by NMR spectroscopy, IR Spectroscopy and Mass spectrometry.

Text Books:

I. A.1. Vogel A.R. Tatchell B.S. Furnis ,Vogel's Text Book of Practical Organic Chernistry.S'" Edition, 2003.

2. A. Ault, Techniques and Experiments for Organic Chemistry, University Science Book, 6th Edition] 998

3. J. Leonard, B. Lygo and G. Procter, Advanced Practical Organic Chemistry.B" Edition CRC Press 2013.

HS 513 ' TECHNICAL COMMUNICATION 2-0-0-4 :

SEMESTER II

CH 422 THERMODYNAMICS FOR CHEMIST 3-0-0-6

Classical Thermodynamics: Concept of entropy, reversible and irreversible processes, Clausius inequality, Free energies, Criteria of spontaneity. Fundamental equations for open systems, Partial molar quantities and chemical potential, Gibbs-Duhem equation, Real gases and fugacity.

Thermodynamics of ideal and non-ideal solutions: Liquid-liquid solutions, liquid-solid solutions, multicomponent systems and excess thermodynamic properties, Activity of ideal, regular and ionic solutions. Thermodynamic equation of state.

Phase behaviour of one and two component systems, Ehrenfest classification of phase transitions.

Statistical Thermodynamics: Concept of ensembles, Canonical ensemble; Boltzmann distribution, Thermodynamic quantities and canonical partition function. Grand canonical ensemble, Fermi-Dirac and Bose-Einstein distributions. Molecular partition functions, translational, rotational and vibrational partition functions. Ideal monoatomic and diatomic gases, classical partition functions, thermodynamic properties, Equipartition theorem, Chemical equilibrium.

Real gases, intermolecular potential and virial coefficients. Debye and Einstein theory of heat capacity of solids. Structure and thermal properties of liquids, Pair correlation functions.

Linear response theory, Irreversible processes, Onsager's law, Entropy production, Non-equilibrium stationary states.

Text Books:

1. P. Atkins and J. Paula, Physical Chemistry, 8th Edition, Oxford University Press, Oxford 2006.
2. D. A. McQuarrie and J. D. Simon, Molecular Thermodynamics, University Science Books, California 2011.
3. D. A. McQuarrie, Statistical Mechanics, University Science Books, California 2005.
4. B. Widom, Statistical Mechanics - A Concise Introduction for Chemists, Cambridge University Press 2012.
5. D. Chandler, Introduction to Modern Statistical Mechanics, Oxford University Press 1987.

CH 424 REAGENTS AND TOOLS IN ORGANIC CHEMISTRY 3-0-0-6

Oxidation: Oxidation involving organosulfur (such as Swern) and organoselenium compounds; Dess-Martin, IBX and related hypervalent iodine based oxidations, Ag2CO)celite Prevost, photosensitised oxidation, dimethyldioxirane, Ru04, 2-sulfonyl oxaziridne, transition metal catalysed oxidation, oxidation at unfunctionalised carbons, Flerning-Tamao oxidation, and microbial oxidations.

Reduction: Using silanes, AI and B based reagents (e.g. DIBAL, L-selectride, K-selectride, Red-AI etc.), low valent Ti species, microbial reductions (NADH model etc.)

Asymmetric Synthesis: Sharpless epoxidation and dihydroxylation, Jacobsen's epoxidation, Corey's oxazaborolidine catalyzed reduction, Noyoris BINAP reduction, SAMP, RAMP, Evans oxazoline and Oppolzer sultarns, Aldol reaction (in brief: only principles using models).

C-C Bond Formation:

a) via anions to electron withdrawing groups (carbonyl group, esters, -$N0_2$, -S02Ph, -CN etc.)
b) via Band Si enolates
c) via imines
d) Michael additions (cuprates etc.)
e) Via allyl boron, allyl tin, allyl and vinyl silanes
f) Metal catalyzed Cyclopropanation reactions (including Simmons Smith reaction)
g) Ring-closing, ring-opening and cross metathesis

C-H activation by using metal and organocatalysis

Text Books:

1. W. Carruthers, I. Coldham, Some Modern Methods of Organic Synthesis, Cambridge University Press 2008.
2. M. B.Smith, Organic Synthesis, 3rd Edition. 20 II.
3. Carreira, E. M.; Kvaerno, Classics in stereoselective synthesis, Wiely -VCH L 2009
4. J. Tsuji, Transition metal reagents and catalysts, Wiely -VCH 2000
5. Li, Ji-Jack, C-H Bond Activation in Organic Synthesis, CRC Press, 2015
6. M. B. Smith, March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure, ih Edition, Wiley, 2013
7. Clayden, N. Greeves, S. Warren and P. Wothers, Organic Chemistry, Oxford University Press, 2nd Edition 2012.

CH 426 CHEMISTRY OF TRANSITION METALS 3-0-0-6

Chemistry of Transition Metals: Transition Metal Chemistry: Introduction (Periodic trends and Electronic configurations), Bonding in Coordination Complexes: Crystal-Field theory and Ligand Field theory, Molecular Orbital Theory, Jahn-Teller effect, Spectrochemical series, nephelauxetic series. Electronic Spectra: d-d transitions, Orgel and Tanabe-Sugano diagrams, charge-transfer spectra. Aqueous chemistry of 3d ions (Frost diagram and Irving-Williams series), Magnetic properties.

Reaction mechanisms of d-Block metal complexes: Aspects of Ligand substitutions in square planar and octahedral complexes; Electron-transfer processes: inner sphere and outer sphere mechanism;

Inner transition metals: Introduction (f-orbitals and oxidation states, atomic and ionic sizes), spectroscopic and magnetic properties, Inorganic/organometallic compounds and coordination complexes.

Text Books:

1. J. D. Lee, Concise Inorganic Chemistry; Wiley-Blackwell; S" edition 2008.
2. Catherine Housecroft and Alan G. Sharpe, Inorganic Chemistry; Pearson; 4th edition 2012.

Reference Books:

2. N. N. Greenwood, A. Earnshaw; Butterworth-Heinemann .Chernistry of the Elements; 2nd Edition 1997.
3. F. Albert Cotton, Geoffrey Wilkinson, Carlos A. Murillo, Manfred Bochrnann, Advanced Inorganic Chemistry, Wiley-Interscience; 6th Edition 1999.

CD 428 PRINCIPLE'OF MOLECULAR SPECTROSCOPY 3-0-0-6

Introduction: Interaction of radiation with matter, Einstein coefficients, time dependent perturbation theory, transition probability, transition dipole moments and selection rules, factors that control spectral linewidth and lineshape. Beer-Lambert law and absorbance.

Molecular Spectroscopy: The rigid diatomic rotor, energy eigenvalues and eigenstates, selection rules, intensity of rotational transitions, the role of rotational level degeneracy, the role of nuclear spin in determining allowed rotational energy levels. Classification of polyatornic rotors and the non-rigid rotor.

Vibrational spectroscopy, harmonic and anharmonic oscillators, Morse potential, mechanical and electrical anharrnonicity, selection rules. The determination of anharrnoncity constant and equilibrium vibrational frequency from fundamental and overtones. Normal modes of vibration, G and F matrices, internal and symmetry coordinates.

Electronic transitions, Franck-Condon principle. Vertical transitions. Selection rules, parity, symmetry and spin selection rules. Polarization of transitions. Fluorescence and phosphorescence.

Raman spectroscopy, polarizability and selection rules for rotation and vibrational Raman spectra.

Nuclear Magnetic Resonance Spectroscopy: Introduction. General principles, Chemical shift, spin-spin splitting, area of peak, shift reagents.

Text Books:

I. P. W. Atkins, Molecular Quantum Mechanics, 2nd edition, Oxford University Press, S" ed ition 2012.

2. P. F. Bernath, Spectra of Atoms and Molecules, 2nd Edition, Oxford University Press, *2005.*

3. E. B. Wilson, Jr., J. C. Decius and P. C. Cross, Molecular Vibrations: The Theory of Infrared and Raman Spectra, Dover Publ ications, 2001.

4. C. N. Banwell, Fundamentals of Molecular Spectroscopy, Slh Edition, 2013.

CM 432 MODERN METHOD OF ANALYSIS 3-0-0-6

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, simpl ification of complex spectra, shift reagent, spin tickl ing, nuclear overhauser effect (NOE), resonance of other nuclei. 13C NMR: Chemical shift, 13C coupling constants, two-dimensional NMR spectroscopy, NOISY, DEPT, INEPT terminology.

Cyclic Voltarnmetry: Basic principles, instrumentations and applications;

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, Mcl.afferty 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.

Text Books:

I. R. S. Drago, Physical Methods in Chemistry, Saunders, 1992

2. A. B. P. Lever, Inorganic Electronic Spectroscopy, Elsevier, 1984, 2nd Ed.

3. R. M. Silverstein, Spectrometric Identifications of Organic Compounds, John Wiley, 1991.

4. D.L. Pavia, G. M. Lampman, G. S. Kriz ,Introduction to Spectroscopy, Harcourt College Publisher, NY, S'' Edition *2015.*

Reference Book:

1. W. Kemp, Organic Spectroscopy, ELBS 3rd Ed. 2008.

CH 434 COMPUTER IN CHEMISTRY 3-0-0-6

Numerical methods with basic understanding of theoretical and computational chemistry, methodologies and terminology using C or FORTRAN or Python programming.

Detailed C or FORTRAN or Python programming:

Numerical interpolation, Polynomial and cubic spline interpolation, extrapolation of data.

Numerical first and second derivatives, error analysis and Richardson's method.

Non-linear equations and roots of polynomials, Newton-Raphson method, secant method and Bairstow method.

Numerical integration: Gaussian quadrature-Gauss-Hermite and Gauss-Legendre intervals; applications form quantum chemistry with Gaussian orbitals

Linear algebra: Householder reduction and LU decompositions, matrix mversion, determinant evaluation and eigenvalues and eigenvectors of hermitian (complex) and symmetric (real) matrices.

Iterative methods for large-scale eigen value problems - Lanczos recursion, Arnoldi algorithm and Davidson's method. Or Fast Fourier transform, Fourier transform of real data in two and three dimensions.

Introduction to finite basis representation and discrete variable. Simple applications from computational chemistry and spectroscopy.

Text Books:

I. Press, W.H., Teukolsky, S.A., Vetterling W.T.and Flannery, B.P., Numerical Recipes; The Art of scientific Computing, Cambridge University Press, New York, 2007.
2. C. Lanczos, Applied Analysis, Dover New York, 2010.
3. S.E. Koonin, and D.C. Meredith, Computational Physics, Fortran Version, Westview Press, U.S.A., 1998
4. B. W. Kerninghan and D.M. Ritchie, The C Programming Language, Prentice Hall, New Jersey, 2nd Edition 1990.
5. Computational Methods 111 Physics and Engineering S. S. M. Wong. An Introduction to Computational Physics by Tao Pang.

CH 440 INORGANIC CHEMISTRY LAB 3-0-0-6

Synthesis and characterization of inorganic compound including coordination complexes, assemblies. Synthetic methods: solution chemistry, solid state synthesis, sol-gel methods, multi step synthesis, preparation of isomers, synthesis under inert atmosphere. Characterization: quantitative and qualitative determination of ligand and metal, use of spectral techniques (UV - Visible, IR, NMR, analytical methods (conductance, TG, DSC, cyclic voltametry).

Text Books:

I. G. S. Girolami, T. B. Rauchfuss and R. J. Angelici, Synthesis and Technique in Inorganic Chemistry: A Laboratory Manual, University Science Books. 3rd Edition 1999.

2. Synthetic methods of organometallic and inorganic chemistry ed. by Wolfgang A. Herrmann, Georg Thieme Verlag, New York, 1997, Vol 7 and 8.

3. G. Svehla, Vogel's qualitative inorganic analysis, Publisher: Harlow: Longman, 7th Edition 2002

4. A.lsrael Vogel, J. Bassett, Vogel's textbook of quantitative inorganic analysis: including elementary instrumental analysis. Publ isher: London; New York: Longman, 1978.

SEMESTER III

CH 521 . CHEMICAL KINETICS 3-0~O-6.r'--,<'

Theories of Reaction Rates: Potential energy surfaces-adiabatic and non-adiabatic curve crossing Processes- transition state theory- activation/thermodynarn ic parameters, Various theories of Unirnolecular reactions. Elementary Reactions in Solutions: Influence of solvent properties on rate. Different types of molecular interactions in solution. Diffusion and activation controlled reactions.

Kinetics in the Excited State: Jablonski diagram. Kinetics of unimolecular and bimolecular photophysical and photochemical processes. Resonance energy transfer rates-Fluorescence quenching kinetics in solution and gas phase.

Fast Reaction Kinetics: Relaxation methods, Stopped flow method, Laser Flash Photolysis, flow tube methods.

Electrode Kinetics: Metal/solution interface- Dependence of electrochemical reaction rate on overpotential-current density for single step and multi-step processes-Influence of electrical double layer on rate constants. Activation and diffusion controlled processes- Marcus kinetics and quadratic dependence of Gibbs free energies-electron transfer processes involving organic and inorganic

compounds. Different types of overpotentials. Experimental methods for elucidation of reaction mechanism.

Text Books:

l. 1. I Steinfeld, J. S. Francisco and William L. Hase, Chemical Kinetics and Dynamics; Prentice Hall, 2nd Edition, 1998.
2. K. J. Laidler,; "Chemical Kinetics", 3rd Edition 1997 , Benjamin-Cummings. Indian reprint Pearson 2009.
3. K. K. Rohatgi - Mukkerjee, "Fundamentals of Photochemistry", Wiley Eastern Ltd., 3rd edition 2014.
4. W.J.Albery; Electrode kinetics Clarendon Press, Oxford J975.
5. C.H. Banford and R.G. Compton (ed) Comprehensive chemical kinetics, Vol26 Electrode kinetics - principles and methodology, Elsevier science publishers 1986.

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, sigrnatropic shifts involving carbon moieties, 3,3- and 5,5- sigrnatropic 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-pirnethane rearrangement, Bartons reaction and Photo-Fries rearrangement. 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.]. L. Finar, Organic Chemistry, Vol II, ELBS, 1968.
2. T. R. Gilchrist, Longman, Heterocyclic Chemistry 1989.
3. Ward, Selectivity in Organic Synthesis, Wiley- VCH, 1999.
4. Ґ. Fleming, Molecular Orbitals and Organic Chemical Reactions, Student Edition Wiley, 2009.
5. T.W. Greene, Protective Groups in Organic Synthesis ,Wiley-VCH, 1999.
6. L. A. Paquette, W.A. Benjamin, Modern Heterocyclic Chemistry, Inc.1968.
7. S. Sankararaman, Pericyclic reaction, Wiley VCH, 2005.
8. J. M. Coxan and B. Halton ,Organic Photochemistry, Cambridge University Press, 1987.

CH 525 ORGANOMETALLIC A.~D BIOINORGANIC CHEMISTRY OF TRANSITION METALS 3-0-0-6

Organometallic Chemistry: Introduction: 18- electron rule and their limitations, electron counting.; Transition Metal hydrides, alkyls, aryls, carbonyls, nitrosyls, phosphines and related ligands, Mechanism of Substitution reactions.;

Organometallic complexes of n-bound ligands (Alkene, Alkyne, Allyl, Diene, Cyclopentadienyl, Arenes and other Alicyclic Ligands);

Mechanism and application of Oxidative Addition and Reductive Elimination reaction, Insertion and Elimination, Nucleophilic and Electrophilic Addition and Abstraction.

Transition metal organometallic complexes containing multiple metal-ligand bonds: Carbenes, Carbynes, N-Heterocyclic Carbenes

Introduction to application of organometallic reactions 111 Homogeneous Catalysis: Alkene Isomerization, Alkene Hydrogenation, Alkene Hydroformylation, Hydrocyanation of Butadiene, Alkene Hydrosilation and Hydroboration, cross-Coupling Reactions, and alkene metathesis.

Bioinorganic Chemistry: Biological Significance of Iron, Zinc, Copper, Molybdenum, Cobalt, Chromium, Vanadium, and Nickel and their storage and transport; Biomineralization of Iron.

Oxygen transport and storage: Hemoglobin, myoglobin, hemerythrin, hemocyanin.

Oxygen activation: Cytochrome P450, Cytochrome c oxidase.

Electron Transfer: Cytochromes, Iron-Sulfur Proteins and Copper Proteins.

Other metal containing enzymes: Catalase, peroxidase, superoxide dismutase, alcohol dehydrogenase, carbonic anhydrase, carboxypeptidase, xanthine oxidase, nitrogenase, vitamin B 12 coenzyme, photosystem I and II.

Text Books:

l. BD Gupta, Anil 1. Elias, Basic Organometallic Chemistry: Concepts, Syntheses and Applications Paperback, Universities Press; 2nd Edition (May 30, 2013).

2. Robert H. Crabtree, The Organometallic Chemistry of the Transition Metals,; Wiley; 6th Edition (April 21, 2014).

3. C. Housecroft , Alan G. Sharpe, Inorganic Chemistry, Pearson; 41h Edition (September 4, 2012).

4. Harry B. Gray, Edward l. Stiefel, Joan Selverstone Valentine, Ivano Bertini, Biological Inorganic Chemistry: Structure and Reactivity, University Science Book; Isl Edition (October 30,2006).

Reference Books:

I. N. N. Greenwood, A. Earnshaw; Butterworth-Heinemann; Chemistry of the Elements, 2nd edition 1997.

2. f. Albert Cotton, Geoffrey Wilkinson, Carlos A. Murillo, Manfred Bochmann; Advanced Inorganic Chemistry Wiley-Interscience; 6th Edition 1999.

CH 530 PHYSICAL CHEMISTRY LAB 0-0--6

Experiments on thermodynamics, kinetics, catalysis, electrochemistry, spectroscopy, photochemistry and rnacrorno lecules.

Text Books:

I. B. Viswanathan, P. S. Raghavan, Practical Physical Chemistry, Viva Books, 20 IO.

2. A. M. Halpern, G. C. McBane, Experimental Physical Chemistry: A Laboratory Text Book, 3rd Edition.; W. H. Freeman, 2006.

CH 6XX - ELECTIVE J 3-0-0-6

CH 591' PROJECT 0-0-6-6

CH 527 SEMINAR 0-0-0-2

SEMESTER IV

CH 6XX	**ELECTl VE II**	**3-0-0-6**
CH 6XX	**ELECTIVE IJ1;**	**3-0-0-6**
CH 522	**COMPREHENSIVE VIVA VOCE**	**0-0-0-2**