CURRICULUM AND SYLLABUS

M.Sc. Chemistry

DEPARTMENT OF CHEMISTRY

KALASALINGAM UNIVERSITY

(Kalasalingam Academy of Research and Education)
ANAND NAGAR, KRISHNANKOIL - 626 126

(July 2017)

COURSE STRUCTURE OF M.Sc. CHEMISTRY (2- YEARS) PROGRAMME

FIRST YEAR

Semester-I

Code No.	Subject	L	T	P	C
CHY4001	Inorganic Chemistry-I	5	1	0	4
CHY4002	Organic Chemistry-I	5	1	0	4
CHY4003	Physical Chemistry-I	5	1	0	4
CHY4004	Analytical Techniques	5	1	0	4
CHY4081	Inorganic Chemistry Laboratory	0	0	6	4
	Total	20	4	6	20

Semester-II

Code No.	Subject	L	T	P	C
CHY4007	Inorganic Chemistry-II	5	1	0	4
CHY4008	Organic Chemistry-II	5	1	0	4
CHY4009	Physical Chemistry-II	5	1	0	4
CHY4010	Spectroscopy	5	1	0	4
CHY4082	Organic Chemistry Laboratory	0	0	6	4
	Total	20	4	6	20

SECOND YEAR

Semester-III

Code No.	Subject	L	T	P	C
CHY5001	Synthetic Strategies in Natural Product Chemistry	5	1	0	4
CHY5002	Electrochemistry and Photochemistry	5	1	0	4
CHY5003	Statistical Thermodynamics	5	1	0	4
CHY****	Elective - I	5	1	0	4
CHY5081	Physical Chemistry Laboratory	0	0	6	4
	Total	20	4	6	20

Semester-IV

Code No.	Subject	L	T	P	C
CHY5004	Polymeric Materials	5	1	0	4
CHY****	Elective -II	5	1	0	4
CHY 5099	Project Work	0	0	0	12
	Total	10	2	0	20

Elective Papers

Code No.	Subject	L	T	P	C
CHY5011	Corrosion Science	5	1	0	4
CHY5012	Modern Methodologies in Organic Synthesis	5	1	0	4
CHY 5013	Nanomaterials	5	1	0	4
CHY 5014	Green Chemistry	5	1	0	4
CHY 5015	Environmental Chemistry	5	1	0	4

Total Credits (from I to IV Semester) = 80

SEMESTER-I

CHY4001	Inorganic Chemistry-I	L	T	P	C
		5	1	0	4

Unit – I: Chemistry of Coordination Compounds:

General Characteristics of transition elements, Basic concepts of coordination chemistry, types of ligands, nomenclature of coordination complexes, chelate effect, geometry and isomerism, Theories of coordination compounds, Werner, Sidgwick's theory. Crystal field theory, crystal field splitting application of d-orbital splittings to explain magnetic properties, low spin (L-S) and high spin (H-S) complexes, crystal field stabilization energy, spectrochemical series, weak and strong field complexes, thermodynamic and related aspects of crystal fields, ionic radii, heats of ligation, lattice energy, site preference energy and spinels.

Unit – II: Electronic Structure and Bonding Reactivity of Transition Metal Complexes:

VB and MO theory of complexes (quantitative principles involved in complexes with pi and without pi bonding) and ligand field theories and molecular symmetry, angular overlap model, Jahn Teller effects, electronic spectra of transition metal complexes, Orbital angular momentum, spin angular momentum, Term symbols, J-J coupling, L-S coupling, Selection rule, Orgel and Tanabe –Sugano diagrams, charge transfer and d-d transitions, nephelauxetic series

Unit – III: Chemistry of Non-Transition Elements-I:

Brief discussion on the properties of the non-transition elements like C, B and Si: special feature of individual elements; synthesis, properties and structure of their halides and oxides, polymorphism of carbon, properties and structure of boranes (small boranes and their anions B_1-B_4), boron nitride, borazines, metallocarboranes, silicates, silicones, diamond, graphite, Zeolites

Unit – IV: Chemistry Of Non-Transition Elements-II:

Nitrogen, Phosphorous, sulphur and noble gas compounds, Hydrides, Oxides and oxy acids of nitrogen, phosphorous, sulphur and halogens, phosphazenes, sulphur-nitrogen compounds, inter halogen compounds, pseudohalogens, noble gas compounds:

Unit – V: Chemistry of Lanthanides and Actinides:

Magnetism: dia, para, ferro and antiferromagnetism, magnetic susceptibility measurements - Gouy method – quenching of orbital angular moment - spin orbit coupling- orbital contribution to magnetic moments-application of magnetic measurements to structure elucidation - Spin cross over phenomena in coordination complexes. Chemistry of lanthanides and actinides, lanthanide contraction, oxidation states, spectral and magnetic properties, use of lanthanide compounds as shift reagents.

Reference Books:

1. F.A.Cotton and G.Wilkinson, Advanced Inorganic Chemistry, 6th ed., John Wiley & Sons, Inc., New York, 2004.
2. J.E.Huheey, Inorganic Chemistry, Principles, Structure and Reactivity, Harper and Row, 3rd Edn, 1983.

3. Wahid.U.Malik, G.D.Tuli and R.D.Madhan, Selected Topics in Inorganic Chemistry, S.Chand & Company Ltd, New Delhi, 2004.
4. Morris Sylvin, Bioinorganic Chemistry, Sarup & Sons, New Delhi, 2003.
5. Banerjea, Coordination Chemistry, Tata McGraw-Hill Publishing Co. Ltd., New Delhi, 1997.
6. W.L. Jolly, Modern Inorganic Chemistry, 2nd Edn., McGraw-Hill, 1991.
7. B.Douglas, D.McDaniel, J.Alexander, Concepts and Models of Inorganic Chemistry, 3rd Edn., John Wiley, 2001.
8. N.N.Greenwood, A. Earnshaw, Chemistry of the Elements, 2nd Edn, Pergamon Press, 1989
9. S.F.A.Kettle, Coordination chemistry ECBS (1973).
10. R.Gopalan and V.Ramalingam, Concise Coordination Chemistry, Vikas publishing House (P) Ltd, New Delhi, 2003.

CHY4002	Organic Chemistry–I	L	T	P	C
		5	1	0	4

Unit – I: Structure, Bonding, and polar bonds and their consequences:

Atomic structure – Orbitals, electron configuration; Development of chemical bonding theory – Valence bond theory and molecular orbital theory; Hybridization – sp^3, sp^2 and sp, hybridization of other atoms (nitrogen and oxygen); Polar covalent bonds – Electronegativity and dipole moment; Resonance - Rules for resonance forms and technique for drawing resonance forms; Acids and bases – The Bronsted-Lowry and Lewis definition, acid base strength, predicting acid base reactions from *p*Ka, organic acids and bases.

Unit – II: Stereochemistry and conformational analysis:

Enantiomers and tetrahedral carbon, Pasteur's discovery of enantiomers, optical activity, specific rotation, sequence rules, diastereomers, meso compounds; Molecules with more than two chiral centres; Racemic mixtures and their resolution; Isomerism – A brief review; Fischer projections – assigning R, S configurations; Chirality – Atoms other than carbon; Chirality in nature; Stereochemistry of alkanes and cycloalkanes – Conformations of ethane, propane, butane; Conformation and stability of cycloalkanes – The Baeyer-Strain theory; Cyclopropane – an orbital view, conformations of cyclobutane, cyclopentane and cyclohexane; conformational mobility of cyclohexane; Conformational analysis of mono and disubstituted cyclohexanes.

Unit – III: Nucleophilic Substitution Reactions, Elimination Reactions and Addition to Carbon-Carbon Multiple Bonds

Nucleophilic substitution reactions - S_N1, S_N2, and S_Ni reactions, mechanisms and stereochemistry. Parameters influencing reaction rates; Neighbouring group participation by π and σ bonds, Synthetic applications of nucleophilic substitution reactions involving alcohols, thiols, amines and hydrides: Elimination reactions – E1 and E2 reactions, Mechanism and stereochemistry; Effects of substrate structure, attacking base, leaving group and medium; Formation of other double bonds (C=N, C=O) and triple bonds by elimination reactions; Mechanism and orientation in pyrolytic elimination. Addition reactions – Mechanism and stereochemistry of addition reactions involving electrophiles, nucleophiles and free radicals.

Unit–IV: Aromaticity, Aromatic Electrophilic and Nucleophilic Substitution Reactions:
Aromaticity – Criteria, Huckel's rule, Aromatic hydrocarbons, Aromatic heterocyclic compounds, Chemical consequences of aromaticity; Antiaromaticity; Molecular orbital description of aromaticity and antiaromaticity, Aromaticity of compounds with morethan 10π electrons –a few representative examples including fullerenes, annulenes, and hetero annulenes. General mechanism for aromatic electrophilic substitution reactions - Orientation-Reactivity-mechanism of nitration, halogenation-Friedel-Crafts reaction, sulphonation and Gattermann-Koch Formylation-Aromatic nucleophilic substitution – Addition-elimination and elimination-addition strategies.

Unit – V: Free Radicals and Application to Green Chemistry:

Free radicals –Aspects, Types, Reaction styles, Orientation in radical additions, Reactivity in radical additions, Reaction patterns of radicals, Generation of radicals; Familiar and close radicals in our life; Stable free radicals; Physical and chemical characteristics of free radicals – Orbital interactions

between radicals and olefins, Baldwin's rule; Functional group conversion – Radical coupling reaction, Radical reduction, Conversion to hydroxy and other functional groups; Free radicals for green chemistry – Design of free radical precursors, Application to environmentally benign synthesis.

Reference Books:

1. R. T. Morrison and R. N. Boyd, " Organic Chemistry", 6th ed., Prentice-Hall of India (P) Ltd., New Delhi, 1995.
2. P. S. Kalsi, Stereochemistry-Conformation and Mechanism, New Age International (P) Ltd, VI Edn., New Delhi, 2005.
3. Jerry March, Advanced organic chemistry-reactions mechanisms and structure, McGraw-Hill, 1968.
4. P.Y.Bruice, Organic Chemistry, 6th Edition, 2011.
5. F.A.Carey and R.J.Sundberg: Advanced Organic Chemistry, Third Edition Plenum Press, 1990.
6. John Mc Murry, Fundamentals of Organic Chemistry (Fifth Edition), Brooks/Cole, Thomson-Brooks/Cole, 2003.
7. I.L. Finar, Organic Chemistry, Vol I & II, Pearson, Education Singapore, 2004.
8. H. Togo, Advanced Free Radical Reactions for Organic Synthesis, Elsevier, 2004.

CHY4003	Physical Chemistry–I	L	T	P	C
		5	1	0	4

Unit – I: Equilibrium Thermodynamics:

Concept of entropy, second and third law of thermodynamics, residual entropy. Free energy, chemical potential, fugacity, liquids and solutions: ideal and non-ideal solutions, chemical equilibrium Non-equilibrium thermodynamics Entropy of irreversible processes – Clausius inequality; entropy production (heat flow, chemical reactions, electrochemical reactions) and entropy flow; Entropy production in open systems; Rate of entropy production – generalized forces and fluxes; Phenomenological equations, Onsager reciprocity relation; Stationary non-equilibrium states - states of minimum entropy production.

Unit – II: Statistical Thermodynamics:

MB statistics and distribution, ensembles, partition functions and molecular partition function, Vibrational, rotational, electronic partition functions-thermodynamic functions in terms of partition functions. Mean energy BE, FD statistics, Comparison between MB, BE and FD. Residual entropy, heat capacity of mono and diatomic gases, chemical equilibrium, Einstein and Debye theories of heat capacity of solids

Unit – III: Chemical Kinetics:

Molecularity, order and rate of reactions, Arrehenius theory, Collision and activated complex theory comparison of results with Eyring and Arrhenius equation-reactive collisions, molecular beam experiments, introduction to potential energy surface-–ionic reactions: salt effect Complex reactions: reversible, pre-equilibrium, consecutive, chain and photochemical, oscillatory reactions, enzyme kinetics-Lindenmann's theory of uni-molecular reactions Molecular reaction dynamics. Fast reaction kinetics Flow method, Flash photolysis

Unit – IV: Solid State Chemistry:

Types of solids, covalent, ionic, molecular and metallic solids, lattice energy, cohesive energy and Madelung constants, Vander Waals forces, hydrogen bonding, unit cell, crystal lattice, structure of simple ionic compounds (AX, AX_2, ABX_3), z radius ratio and closed packed structures. Imperfection and related phenomena-defects in solids: point defects, line defects and plane defects. Thermal properties-Heat capacities of solids: Dulong –Petit law, thermal conductivity of insulators and thermal expansion coefficient. Electrical conductivity origin of band gap. Fermy energy, density of states, thermal conductivity of metals, semiconductors and superconductivity.

Unit – V: Electrochemistry:

Activities in electrolytic solutions mean activity coefficient, Debye-Huckel treatment of dilute electrolyte solutions, origin of electrode potential, half cell potential, electrochemical cell, Nernst equation, thermodynamics of electrochemical cell: Electrical double layer-electrode kinetics; rate of charge transfer, current density, Butler–Volmer equation- Different approximations to it. Mechanism determination of electrodic reactions-H_2 evolution.

Reference Books:

1. F.W.Sears, "An Introductions to Thermodynamics, Kinetic Theory of Gases and Statistical Mechanics" Addision Wesley Pub. Cambridge, 1969.
2. F.C.Andrews, "Equilibrium to Statistical Mechanics" John Wiley, 2nd Edition, 1975.
3. Malcolm Dole, "Introduction to Statistical Thermodynmics" Prentice Hall, 1954.
4. L.K.Nash,"Statistical Thermodynamics" Addison Wesley, 2nd Edition, Addison-Wesley Pub. Co., 1974.
5. Joseph Kestin and J.R. Dorfman, "A course in statistical thermodynamics", Academic press, 1971.
6. IIya Prigogine, Introduction to thermodynamic irreversible processes, 3rd Edition, Interscience Publishers,1968.
7. H. V. Keer, Principles of Solid State, Wiley Eastern Limited, 1993.
8. W.R.West, Solid State Chemistry and its Application, John Wiley and Sons, New York, 1984.
9. J. O'M. Bockris and A.K.N. Reddy, Modern Electrochemistry, 2nd Ed., Vols 1, 2A, 2B, Kluwer/Plenum, 1998 (Vol 1), 2001 (Vols 2A, 2B),(1st ed.Vols. 1, 2, Plenum 1973 QD 553 B6).
10. P. W. Atkins Physical Chemistry, 6th Edition Oxford, 1998.
11. Y. V. C. Rao, An introduction to Thermodynamics, Wiley Eastern, 1993.
12. M. Ladd, Introduction to Physical Chemistry, Cambridge, 1998.
13. D.A.McQuarrie and J.D.Simon Physical Chemistry, A molecular Approach, Viva 1998.
14. F.W.Sears & G.L.Salinger, Thermodynamics, Kinetic theory & Statistical thermodynamics, Narosa, 1986.
15. J.Rajaram and J.C. Kuriacose, Thermodynamics, Shoban Lal Chand & Nagin Lal (P) Ltd, 1999.
16. K. J. Laidler "Chemical Kinetics, 3rd Ed., Pearson Education Inc., New Delhi, 2004.

CHY4004	Analytical Techniques	L	T	P	C
		5	1	0	4

Unit – I: Chromatographic Methods:

Introduction to Chromatography and types of techniques: ion exchange chromatography, Column Chromatography, Paper Chromatography, Thin Layer Chromatography (TLC), Gas Chromatography (GC), High Pressure Liquid Chromatography, Ion Chromatography, Gel Permeation Chromatography– Applications.

Unit – II: Electroanalytical Methods:

Electron transfer-mass transport (diffusion, convection, migration) Ilkovic equation-Polarograpic analysis-sampled current voltammetry: Potentiometry and Amperometric analytical methods - Chronoamperometry, chronocoulometry-Polarography- pulse polarographic methods: Tast pulse, normal pulse, and differential pulse – Applications.

Unit – III: Voltammetry Methods

Voltammetry- Cyclic votammetry- reversible, totally irreversible, quasi-reversible processes-applications. Controlled Potential methods: current –time behaviour, Electrogravimetry, Electroseparation- Coulometric measurements: controlled current methods: Stripping voltammetry and Hydrodynamic electrochemical methods of analysis.

Unit – IV: Imaging Methods:

Basic Studies and Principles of SEM, TEM, AFM, Scanning Tunnelling Microscope (STM) – Applications.

Unit – V: Thermoanalytical Methods:

Thermal methods of analysis: Principles and instrumentations of TG and DTA. Complementary nature of TG and DTA. Differential scanning calorimeter (DSC). Applications of thermal methods in analytical chemistry and in the study of minerals and polymers.

Reference Books:

1. C.N.R.Rao, A.Muller, A.K.Cheetham, Chemistry of Nanomaterials (Vol. 1&2), Wiley-VCH Verlag GmbH & Co. KGaA, Germany, 2004.
2. Charles P. Poole Jr and Frank J. Owens, Introduction to Nanotechnology Willey Student Edition, Singapore, 2003.
3. A.J.Bard and L.R.Faulkner, Electrochemical Methods, Fundamentals and applications, John Wiley, 1980.
4. P. Kissinger and W. R. Heinman, Laboratory Techniques in Electroanalytical Chemistry, Taylor & Francis, Inc., 1996.
5. P.H.Reiger, Electrochemistry, Prientice, Hall, 1987.
6. James A. Plan Beck, Electroanalytical Chemistry-Basic Principles and Applications, John Wiley & Sons, 1982.

7. B. H. Vassos and G. W. Ewing Electroanalytical Chemistry, John Wiley and Sons, Inc., 1983.
8. D. A. Skoog, D. M. West, F. J. Holler, S. R. Crouch, Fundamental of Analytical Chemistry, 7th Ed., Saunders College Publishing Co., New York, 1999.
9. A.I.Vogel, A.R.Tatchell, B.S.Furnis, A.J.Hannaford, P.W.G.Smith, Vogel's Textbook of Practical Organic Chemistry (5th Edition), Longman, 1989.
10. F.W. Fifield and D. Kealey, Principles and Practice of Analytical Chemistry, 2nd Edition, International Book Company, London, 1983.

CHY4081	Inorganic Chemistry Laboratory	L	T	P	C
		0	0	6	4

1. Preparation of any five coordination complexes.
2. Interpretation of the electronic spectrum and calculation of D_q values in respect of Ni (II) complex.
3. Semimicro qualitative analysis: Analysis of common and rare cations in a mixture
4. Estimation of metal ions by complexometric and Cerimetric titrations.
5. Spectrocolorimetric analysis.
6. Training to use software: Excel, Origin, Mercury, Powerpoint.

Reference Books:

1. Vogel's Text Book of Inorganic Qualitative Analysis, 4th edition, ELBS, London, 1974.
2. V.V.Ramanujam, Inorganic Semi Micro Qualitative Analysis, 3rd edition, The National Publishing Company, Chennai, 1974.

SEMESTER-II

CHY4007	Inorganic Chemistry-II	L	T	P	C
		5	1	0	4

Unit – I: Inorganic Reaction Mechanism:

Isomerism and nomenclature of coordination compounds, Formation of complexes, stability constants Inert and labile compounds, substitution reactions of octahedral complexes, dissociative, associative, anation, aquation, conjugate base mechanism; substitution reactions of square planar complexes, trans effect, trans effect series, theories of trans effect; electron transfer reactions. Concept of hard and soft acids and bases. Stabilisation of unusual oxidation states-stereochemistry of coordination compounds

Unit – II: Organometallic Chemistry-I:

Compounds with transition metal to carbon bonds: classification of ligands nomenclature, eighteen electron rule; transition metal carbonyls: range of compounds and structure, bonding vibrational spectra, preparation, reactions; transition metal organometallics: square planar complexes, metal alkyls, metal alkylidenes and metal alkylidynes; structure and bonding: metal-olefin bond and arene metal bond. Compounds with ligands having extended pi systems: bis(cyclopentadienyl) compounds, cyclopentadienyl carbonyl compounds, bis(arene) compounds, arene carbonyl compounds-fluxional molecules.

Unit – III: Organometallic Chemistry-II:

Organometallic reactions and catalysis: oxidative addition, reductive elimination, insertion, hydride elimination, abstraction; olefin hydrogenation, hydroformylation, Wacker process, Ziegler-Natta polymerization, Olefin metathesis, Monsanto acetic acid synthesis, Fisher-Tropsch process, Hydroxylation.

Unit – IV: Bioinorganic Chemistry:

Metal ions in biological systems; heme proteins, haemoglobin, myoglobin, hemerythrin, hemocyanin, ferritin, transferring, cytochromes and vitamin B_{12}; Iron-Sulphur Proteins: rubrdoxin, ferredoxin and model systems. Metalloenzymes: active sites, carboxy peptidase, carbonic anhydrase, superoxide dismutase, xanthine oxidase, peroxidase and catalase; photosynthesis, water oxidation, nitrogen fixation, nitrogenase; ion pump, metallodrugs.

Unit – V: Inorganic Photochemistry:

Basic Principles, Basic photochemical processes, Kashia's rule, Thexi state, Photo substitution reactions, Adamson's rules, Photo substitution reactions of Cr(III)-Polypyridyls, Rh(III) Ammine Complexes, Ru-Polypyridyl complexes, Ligand photo reactions, photoredox reactions, comparison of Fe(II) and Ru(II) complexes, Photo reactions and Solar energy conversions , Photo synthesis in plants and Bacterio chlorophyll photosynthesis, photolysis of water using Inorganic precursors.

Reference Books:

1. J. D. Lee, A New Concise Inorganic Chemistry, 3rd Edn., ELBS, 1987.
2. P. Powell, Principles of Organometallic Chemistry, 2nd Edn., ELBS, 1991.
3. M. F. Purcell, J.C.Kotz, Inorganic Chemistry, Saunder, 1977.
4. R. W. Hay, Bio Inorganic Chemistry, Ellis, Horwood, 1987.
5. R. M. Roat-Malone, BioInorganic Chemistry, John Wiley, 2002.
6. T. M. Loehr, Iron carriers and Iron proteins, VCH, 1989.
7. S. L. Lippord, Progress in In organic Chemistry, John, Wiley, Vol.30, 1983.
8. J. E. Huheey, Inorganic Chemistry, Principles, Structure and Reactivity, Harper and Row, 3rd Edn, 1983.
9. Inorganic Photochemistry, J. Chem. Educ., vol. 60, no. 10, 1983.
10. Elements of Inorganic Photochemistry, G. J. Ferraudi, John Wiley & Sons, 1988.
11. K. K. Rohatgi-Mukherjee, *Fundamentals of Photochemistry*, Wiley, New York, 3rd Edition, 2002.
12. Turro, N. J., "Modern Molecular Photochemistry", Benjamin-Cummings, NY, 1978.

CHY4008	Organic Chemistry-II	L	T	P	C
		5	1	0	4

Unit – I: Reagents in Organic Synthesis:

Palladium on Carbon, Lithium tri-tert-butoxyaluminium hydride, Diazomethane, Sodium Periodate, Grignard Reagents, Dicyclohexylcarbodiimide (DCC), Pyridinium chlorochromate, *Di*-isobutyl aluminum hydride (DIBAL), Lithium *di*-isopropyl Amide (LDA), Sodium amide, Aluminum chloride, Osmium tetroxide, N-Bromo succinimide, Wilkinson's catalyst, Phase-transfer catalysts, Introductory treatment to the application of palladium, ruthenium and indium reagents in organic synthesis.

Unit – II: Ring Constructions and Rearrangements:

Construction of ring systems - Darzens condensation, Simmons–Smith reactions, Staudinger reaction (β - lactams synthesis), Reaction of isocyanates with alkenes, Borsche–Drechsel cyclization, Paal-Knorr pyrrole syntheses, Pechmann coumarin synthesis, Bischler–Napieralski synthesis, Corey–Nicolaou macrolactonization. Rearrangements – Baker–Venkataraman, Evans-Mislow, Wagner–Meerwein rearrangements, Beckmann, Overman, Schmidt, Curtius, Wolff rearrangements, Boulton–Katritzky.

Unit – III: Oxidation and Reduction:

Oxidation – Alcohols to carbonyls/acids - Corey–Kim, and Swern oxidations; Aldehyde to phenol - Dakin oxidation; Alkenes to epoxides - Sharpless asymmetric and Jacobsen epoxidations; Alkenes to diols - Prevost reaction; Ketones to esters/lactones - Baeyer–Villiger oxidation; Alkenes to alcohols – Hydroboration, Wacker oxidations, Silanes to alcohols/ketones - Fleming−Kumada and Saegusa oxidations; Halides to aldehydes - Sommelet reaction; Reduction – Imine to amine - Borch reductive amination; Ketones/Esters/thiolesters/alkenes to alcohols/aldehydes/alkanes - Corey-Bakshi-Shibata, Bouveault–Blanc, Fukuyama, Midland, and Wolff–Kishner reductions, Noyori hydrogenation; Acetylenic alcohol to allylic alcohol - Chan alkyne reduction; Alcohols to alkenes - Corey–Winter reductive olefination.

Unit – IV: Organic Photochemistry and Pericyclic Reactions:

Photochemistry – Definitions- Grotthuss-Draper law, Stark-Einstein law, quantum yield; Mechanistic background – Frank-Condon principle, Jablonski diagram, singlet and triplet states, photosensitization, quenching; Photochemical reactions – Alkene isomerisation, carbonyl compounds (background, reactions – Norrish type-I and Type-II reactions, Paterno-Buchi reaction, photoenolization reaction), Enone reactions ([2+2] cycloaddition and the de Mayo reactions), di-π-methane rearrangements, Barton reaction. Molecular orbitals and Pericyclic reactions; Electrocyclic reactions; Stereochemistry of thermal and electrocyclic reactions; photochemical electrocyclic reactions; Cycloaddition reactions, stereochemistry of cycloaddition reactions; Sigmatropic rearrangements with examples; Rules for pericyclic reactions.

Unit – V: Heterocycles and nucleic acids:

Five-membered unsaturated heterocycles; Structure of pyrrole, furan and thiophene; Electrophilic substitution reactions of pyrrole, furan and thiophene; Six membered heterocycle – Pyridine and its electrophilic and nucleophilic substitutions; Fused ring heterocycles; Nucleic acids and nucleotides;

Structure of nucleic acids; Base pairing in DNA – The Watson-Crick model; Nucleic acid and heredity; Replication of DNA; Structure and synthesis of RNA – Transcription; RNA and protein biosynthesis – translation; DNA sequencing; DNA synthesis; polymerase chain reaction.

Reference Books:

1. B.P.Mundy, M.G.Ellerd, F.G.Favaloro, Name Reactions and Reagents in Organic Synthesis, 2nd Edition, 2005
2. Adam Jacobs; Understanding Organic Reaction Mechanism, Cambridge University Press 1997.
3. Jie Jack Li, Name Reactions, 5th Edition (Springer), 2014
4. M.A.Fox and J.K.Whitesell., Organic Chemistry, Jones and Bartlett Publishers 1994.
5. F.A.Carey and R.J.Sundberg (Part A and B) Kluwer Academic/ Plenum Publishers 2000.
6. Clayden et al Advanced organic chemistry 2004.
7. R.J.Simmonds: Chemistry of Biomolecules: An Introduction, RSC
8. John McMurry, Fundamentals of Organic Chemistry (Fifth Edition), Brooks/Cole, Thomson-Brooks/Cole, 2003.

CHY4009	Physical Chemistry-II	L	T	P	C
		5	1	0	4

Unit – I: Quantum Chemistry:

Inadequacy of classical mechanics-Wave particle dualism-Heisenberg's uncertainty principle-Eigen functions-Postulates of quantum mechanics –Application of wave mechanics to simple systems-Particle in one and three dimensional boxes- degeneracy. Application of wave mechanics to one dimensional simple harmonic oscillator-Rigid rotor-Hydrogen atom-Pauli's exclusion principle-Slater determinant-Approximation methods to helium atom.

Unit – II: Group Theory-Concept And Applications:

Symmetry elements and symmetry operations Group-Definition-Group multiplication table--Reducible and irreducible representation–Point groups-Systematic methodology for fixing point groups for simple compounds-Great orthogonality theorem (Non-Mathematical) and its consequences-Construction of character table (C_2V and C_3V groups)-Direct product representation. Application of group theory to vibrational and Raman spectra-ammonia and water molecules-Application of group theory to electronic spectroscopy –formaldehyde and ethylene.

Unit – III: Surface Phenomena:

Adsorption of gases on solids-Physical and chemical adsorption-Solid-gas interface-Langmuir and BET isotherms, Surface area determination –mechanism of uni and bimolecular surface reactions – Langmuir and Hinshelwood and Langmuir-Riedel mechanisms –Gibbs adsorption isotherm.

Unit – IV: Photochemistry:

Photochemical principles – Absorption of light by atoms and molecules-Reaction paths of excited molecules- Jablonski diagram – Fluorescence and Phosphorescence – Photochemical chain reaction – Chemiluminescence, fluorescence quenching: concentration quenching, quenching by excimer and exciplex emission, fluorescence resonance energy transfer between photexcited donor and acceptor systems. Stern-Volmer relation, critical energy transfer distances, energy transfer efficiency, examples and analytical significance, bimolecular collisional V quenching and Stern-Volmer equation.

Unit – V: Nuclear Chemistry:

Properties of nucleus – different types of nuclear forces –liquid drop model, shell model nucleus. Nuclear reactions induced by charged particles. Q value- nuclear reactions cross sections, significance and determination. Types of reactions-radioactive decay and equilibrium-chemical effects of nuclear transformation-fission and fusion, fission products and fission yields. Production of feed materials for nuclear reactors, radioactive techniques-tracer techniques, neutron activation analysis, counting techniques such as G.M. ionisation and proportional counter. Application of radioisotopes.

Reference Books:

1. S.N.Datta: Lectures on Chemical bonding and quantum chemistry, 1998.
2. P.W.Atkins: Molecular Quantum Mechanics, Clarendon Press, Oxford, 1983.
3. F.A.Cotton; Chemical Applications of Group Theory, Willey Eastern, 1985.
4. Kaplus and Porter Atoms and Molecule 1973.
5. R.K.Prasad:Quantum Chemistry, New Age International Publishers, Revised edition, 2006.
6. A.K.Chandra, Introductory Quantum Chemistry, 4th Edition,Tata McGraw-Hill Education, 1994.
7. K.V.Raman, Group theory and its application to Chemistry, Tata McGraw Hill Publishing Co.,1990.
8. K.K.Rohatgi Mukherjee "Fundamental of Photochemistry", New Age International (P) Ltd, Publisher, New Delhi, 2003.
9. H.J.Arinikar, Essential of nuclear Chemistry, 4th ed., New Age International (P) Ltd., New Delhi, 1997.
10. A.K.Chandra, "Introductory Quantum Chemistry", 4th Ed., Tata McGraw Hill, New Delhi, 1994.

CHY4010	Spectroscopy	L	T	P	C
		5	1	0	4

Unit – I: UV-Visible Spectroscopy:

Electromagnetic radiation, energy and electromagnetic spectrum, units, absorption of energy by organic compounds. UV-Visible spectroscopy: Basic principles, theory, instrumentation and applications of UV-Visible spectroscopy. Application of UV-Visible spectroscopy to structure elucidation of organic compounds. Woodward- Fisher rules for calculating absorption maximum in Dienes, α, β-unsaturated carbonyl compounds. Octant rules, Application of ORD-CD to stereo chemical assignments.

Unit – II: IR and Raman Spectroscopy:

IR-Spectroscopy-Basic Principles, theory, Molecular vibrations, vibrational frequency, factors influencing vibrational frequency, instrumentation, infrared spectrum, finger print region and characteristic frequencies of common functional groups. Application of IR spectroscopy to structure elucidation of organic compounds. Basic Principles of Raman Spectroscopy and its application.

Unit – III: NMR Spectroscopy:

Basic principles-introduction to NPR technique-CW and FT NMR techniques, 1H NMR spectral parameters-Intensity, chemical shift, multiplicity, coupling constant factors affecting. Analysis of first order and second–order spectra, structure determination of organic compounds by ^{1}HNMR spectra. ^{13}C NMR Proton coupled, off-resonance decoupled, proton noise decoupled ^{13}C NMR spectra, Assignment of chemical shifts of common organic compounds and functional groups: Introduction to multinuclear NMR of common hetero atoms present in organic compounds (N, F, O, P, S & D).
^{2}D NMR techniques ^{1}H-^{1}H COSY, ^{1}H-^{13}C COSY-NOSEY spectra.

Unit – IV: Mass Spectroscopy:

Basic principles, techniques of ion production and ion and daughter ions, molecular ion and isotope abundance, nitrogen rule-energetics of fragmentation. Metastable ions, common fragmentation pathways-fragmentation of common chemical classes. Mc Lafferty rearrangement. Structural elucidation.
Applications of IR, NMR and Mass spectroscopy for structure elucidation of organic compounds.

Unit – V: ESR, NQR and Mossbauer Spectroscopy:

Electron spin resonance: g value, hyperfine structure, esr of hydrogen atom, free radicals, esr of simple free radicals in solutions, Spin densities, spin polarisation, anisotropy of Zeeman and Hyperfine interactions. ESR of spin transition Metal ions: s = 1/2 systems, g and A anisotropy. Effect of spin orbit interaction. d^{1} system in a tetragonal field. Covalency effects. EPR spectra of transition ion (s = 1/2), S > 1/2 systems, Zero field splittings, EPR of Metallo enzymes.
NQR and Mossbauer Spectroscopy: Principles, isomer shift, quadrupole effect of magnetic field, applications to iron and tin compounds.

Reference Books:

1. William Kemp, Organic Spectroscopy, Third Edition, MacMillon (1994).
2. D.H.William and lan Fleming, Spectroscopic methods in organic chemistry, Tata McGraw Hill (1998).
3. R.M.Silverstein and F.X.Webster, Spectrometric identification of organic compounds; John Wiley and Sons, Inc., Sixth edition (1997).
4. A.B.P. Lever, Inorganic Electronic Spectroscopy, 1986.
5. J. Pilbrow; Transition ion EPR (Oxford) 1968.
6. C.N.Banwell: Fundamentals of Molecular Spectroscopy, 4th edn.Tata McGraw Hill,1996.
7. A.E.Derome: Modern NMR Techniques for Chemical Research, Pergamon Press, 1987.
8. R.S.Drago: Physical Methods for Chemists, Second Edition, Saunders College Publication, 1992.
9. D.H.Williams and I.Flemming: Spectroscopic Methods in Organic Chemistry, Fourth Edition, McGraw-Hill, 1966.
10. Norman B.Colthup, Lawrence H. Daly, Stephen E. Wiberley, Introduction to Infrared and Raman Spectroscopy, 3rd edition, Academic Press, 1990.
11. V.R.Dani, Organic Spectroscopy, Tata McGraw Hill Publishing Co. Ltd, New Delhi, 1998.

CHY4082	Organic Chemistry Laboratory	L	T	P	C
		0	0	6	4

1. Introductory experiments on Chromatographic technique –TLC, CC and PC.
2. Separation and identification of organic compounds in a mixture.
3. Preparation of organic compounds illustrating important synthetic reactions.
4. Training to use software: ChemDraw, ISI Draw.

Reference Books:

1. A.I.Vogel, A.R.Tatchell , B.S.Furnis, A.J.Hannaford, P.W.G.Smith, Vogel's Textbook of Practical Organic Chemistry (5th Edition), Longman, 1989.
2. Bansal Raj K, Laboratory Manual of Organic Chemistry, New Age International, 2009.

SEMESTER-III

CHY5001	Synthetic Strategies in Natural Products Chemistry	L	T	P	C
		5	1	0	4

Unit – I: Classification of natural products:

Introduction to natural product chemistry; classification of natural products, isolation techniques and physiochemical data, Structural elucidation of Natural Products based on joint application of UV,IR, PMR, CMR and mass spectroscopy. Alkaloids, peptides and amino acid derivatives, and carbohydrates Present examples of natural products and some simple biosynthetic pathways showing how metabolites are formed in nature.

Unit – II: Retrosynthetic approaches in Natural Products Synthesis

Origin for retrosynthetic analysis –Types of approaches for retrosynthesis; Transform-based approaches - goal guidance, Structure-based and topological approaches - Structure-goal (S-goal) approaches Retrosynthesis of fumagillol: Stereochemical approaches - Stereochemical simplification - Transform stereoselectivity, Stereochemical convolution - Clearable stereocenters, Stereochemical approaches for polycyclic and acyclic systems; retrosynthetic analyses of Longifolene

Unit – III: Total synthesis of Important Natural Products:

Total synthesis of Recifeiolide, Biotin, Humulene, Farnesol, Kahweol, Cafestol, Fumagillin, Longifolene Prostaglandins E_1, $F_{1\alpha}$ and their 11-epimers, (±)-Prostaglandins E_1, $F_{1\alpha}$, $F_{1\beta}$, A_1 and B_1, General synthesis of prostaglandins Lipoxins, Bongkrekic acid

Unit – IV: Biomolecules – Carbohydrates and amino acids:

Classification of carbohydrates, configuration of mono saccarides, D, L sugars, configuration of aldoses, cyclic structure of monosaccarides, monosaccaride anomers, reactions of monosaccarides, stereochemistry of glucose; Disaccarides; polysaccharides and their synthesis; Other important carbohydrates; cell-surface carbohydrates and carbohydrate vaccines; Structure of amino acids, isoelectric points, synthesis of α-amino acids, resolution of R, S amino acids.

Unit – V: Biomolecules – Peptides, proteins and lipids:

Peptides and proteins, covalent bonding in peptides; Structure determination of peptides – amino acid analysis; Sequencing of peptides – The Edman degradation and C-terminal residue determination; Synthesis of peptides; Automated peptide synthesis – The Merrifield solid-phase technique; Classification of proteins; Protein structure; Enzymes – working of enzyme, citrate synthase; Protein denaturation; Lipids – Waxes, fats, oils and soap; Phospholipids; Prostaglandins; Terpenes, biosynthesis of terpenes; Steroids, stereochemistry of steroids; steroid biosynthesis.

Reference Books:

1. S. Warren & P. Wyatt. Organic Synthesis: The Disconnection Approach, John Wiley & Sons (2008).
2. R. Xu, Y. Ye & W. Zhao. Introduction to Natural Products Chemistry, CRC Press (2011).
3. E. J. Corey & Xue-Min Cheng. The Logic of Chemical Synthesis, John Wiley & Sons (1995).
4. D. Goldsmith, M. C. Pirrung & A. T. Morehead. Total Synthesis of Natural Products, John Wiley & Sons (2007).
5. W. H. Pearson. Advances in Heterocyclic Natural Product Synthesis, Jai Press (1996).
6. D. Barton,K. Nakanishi & O. Meth-Cohn. Comprehensive Natural Products Chemistry, Elsevier (1999).
7. I. L. Finar, Organic Chemistry Vol. I & Vol. II- Pearson Education,
8. F. A. Carey and R. J. Sundberg, (Eds) 3rd Edition, Part B. Plenum/Rosetta, 1990.
9. Atta-ur-Rahman, Studies in Natural Products Chemistry, Vol.1 and 2, Elsevier, 1988.
10. John McMurry, Fundamentals of Organic Chemistry (Fifth Edition), Brooks/Cole, Thomson-Brooks/Cole, 2003.
11. R. Krishnaswamy, Chemistry of Natural Products; A Unified Approach, Universities Press.

CHY5002	Electrochemistry and Photochemistry	L	T	P	C
		5	1	0	4

Unit-I: Electrochemistry I:

Mean ionic activity and mean ionic activity coefficient - concept of ionic strength, Debye - Huckel theory of strong electrolytes - activity coefficient of strong electrolytes - determination of activity coefficient by electrochemical method. Debye Huckel limiting law - qualitative and quantitative verification - limitation of Debye Huckel limiting law at appreciable concentrations of electrolytes - Huckel equation - Debye - Huckel - Bronsted equation .

Unit-II: Electrochemistry II:

Electrode - electrolyte interface - adsorption at electrified interface - electrical double layer - electro capillary phenomenon - Lippmann equation - Structure of double layers - Helmholtz - Perrin, Guoy - Chappmann and Stern model of electrical double layers. Diffusion - Fick's law of diffusion - Effect of ionic association on conductance-electrokinetic phenomena-membrane potential.

Unit-III: Electrochemistry III:

Mechanism of electrode reactions - polarization and overpotential - the Butler-Volmer equation for one step and multistep electron transfer reactions - significance of electron exchange current density and symmetry factor - transfer coefficient and its significance - mechanism of the hydrogen and oxygen evolution reactions. Corrosition and passivation of metals - Pourbaix diagram - Evan's diagram - fuell cells - electrodeposition - principle and applications.

Unit-IV: Photochemistry I:

Absorption and emission of radiation - Franck - Condon Principle - decay of electronically excited states - Jablonsky diagram - radiative and non radiative processes - fluorescence and phosphorescence - spin forbidden radiative transition - internal conversion and intersection crossing - energy transfer process - kinetics of unimolecular and bimolecular photophysical processes-excimers and exciplexes - static and dynamic quenching - Stern-Volmer analysis.

Unit-V: Photochemistry II:

Experimental methods - quantum yield and life time measurements - steady state principle - quantum yield and chemical actinometry. kinetics of photochemical reactions : hydrogen and halogen reactions, photoredox, photosubstitution, photoisomerization and photosensitized reactions - photovoltaic and photogalvanic cells, photoelectrochemical cells, photo assisted electrolysis of water, aspects of solar energy conversion. Radiation chemistry - Interaction of high energy radiation with matter - primary and secondary processes - G value - radialysis of water - hydrated electron.

Reference Books:

1. S.Glasstone, Introduction to Electrochemistry, Affiliated East West Press, New Delhi, 1960.
2. D.R.Crow, Principles and Applications to Electrochemistry, Chapman and Hall, 1991.
3. R.Crow, Principles and Applications to Electrochemistry, Chapman and Hall, 1991.

4. P.H.Rieger, Electrochemistry, Chapman and Hall, New York, 1994.
5. M.C.Gupta, Statistical Theromdynamics, Wiley Easter, New Delhi, 1990.
6. R.Hasee, Thermodynamics Of Irreversible Process, Addition Wesley, Reading, Mass, 1969.
7. N.J.Turro, Modern Molecular Photochemistry, Benjamin, Cumming, Menlo Park, California, 1978.
8. K.K.Rohatgi Mukherjee, Fundamentals Of Photochemistry, Wiley Eastern Ltd., 1978.
9. S.Glasstone, Text Book Of Physical Chemistry

CHY5003	Statistical Thermodynamics	L	T	P	C
		5	1	0	4

Unit I - Introduction:

Objectives of statistical thermodynamics – concept of thermodynamics and mathematical probabilities- distribution of distinguishable and non-distinguishable particles. Partition function – evaluation of translational, vibrational and rotational partition functions for mono, diatomic ideal gases- thermodynamic functions in terms of partition functions – application of partition function to heat capacity of ideal gases – nuclear partition function – contribution to heat capacity of *ortho* and *para* hydrogen. Heat capacity of solids – Einstein and Debye models.

UNIT – II: Statistical Mechanical Ensembles:

Need for statistical approach- Permutations and combinations – Distribution – probability – Relation between entropy and probability – sterling approximation- Types of particles- Boson, Fermion, Boltzmannons – Microstate – most probable distribution –derivation of Maxwell –Boltzmann distribution law- statistical weight factor (g_i),definition of partition function Q – Relation between thermodynamic functions and Q Molecular partition functions (q) factorization of partition function – derivation of translational Partition function and calculation of entropy and internal energy by translational mode.

UNIT – III: Quantum Statistics:

Introduction to quantum statistics – distribution law for fermions Fermi- Dirac statistics and for bosons Bose – Einstein statistics – comparison with Maxwell – Boltzmann distribution law and their applications – radiation law – electron gas in metals.

UNIT – IV: Classical Statistics of Independent Particles:

Different types of ensembles, ensemble averaging, distribution law (Boltzmann statistics) partition function and thermodynamic parameters, relation between molecular and molar partition functions, translational partition function, rotational partition function or linear and non-linear molecules, vibrational partition function, electronic partition function ,reference state of zero energy for evaluating partition function, equilibrium constant in terms of partition function. Applications of statistical thermodynamics , equipartition theorem, heat capacity behavior of crystals,

Unit – V: Non-equilibrium Thermodynamics:

Entropy of irreversible processes- Clausius inequality, entropy production (heat flow, chemical reactions, electrochemical reactions) and entropy flow , entropy production in open systems, Rte of entropy production – generalized forces fluxes, phenomenological equations, Onsager reciprocity relation, electrokinetic phenomena , stationary non-equilibrium states- states of minimum entropy production.

Text Books:

1. G.S.Rush Brooke, Statistical Mechanics, Oxford University Press
2. T.L.Hill, Introduction to statistical Thermodynamics Addison Wesely
3. M.C.Gupta, Statistical thermodynamics, Wiley Easter, New Delhi,1990
4. R.Hasee, Thermodynamics of irreversible process,Addition Wesely, Reading mass, 1969
5. Elements of statistical Thermodynamics- L.K.Nash, Addison Wesely
6. Statistical thermodynamics by B.J..Mc Celland, Chapman and Hall
7. Thermodynamics of Irreversible Processes by Iila Prigogine.
8. Thermodynamics of steady state by Denbeigh
9. Advanced physical chemistry by S.N.Blinder, The Macmilan Company 1967
10. Thermodynamics by R.C.Srivatsava,S.Saha and A.K.Jain, Prentice –hall, India.

Reference Books:

1. Elements of statistical thermodynamics - L. K. Nash, Addison Wesley
2. Theoretical Chemistry by S. Glasstone.
3. J. Rajaram, J.C. Kuriakose, Thermodynamics, S Chand and Co., 1999.
4. M.C. Gupta, Statistical Thermodynamics, New age international, 2007
5. L.K. Nash, Elements of Classical and Statistical Mechanics, 2nd Edn., Addison Wesley, 1972.
6. C. Kalidas, M.V. Sangaranarayanan, Non-equilibrium Thermodynamics, Macmillan India, 2002.

CHY5081	Physical Chemistry Laboratory	L	T	P	C
		0	0	6	4

1. Molecular weight determination by cryoscopic methods, Formula of complexes.
2. Phase diagrams:
   i. Two component liquid–liquid and solid-liquid systems.
   ii. Three component liquid-liquid systems.
3. Kinetics –Acid hydrolysis of ester – determination of energy of activation (Ea).
4. Kinetics–Acid hydrolysis of ester-Comparison of strength of acids/ Determination of Ea.
5. Kinetics- Saponification of ester –Determination of Ea.
6. Distribution law-study of iodine-iodide equilibrium.
7. Adsorption –Oxalic Acid/Acetic Acid on Charcoal using Freundlich isotherm.
8. Conductometry: Cell constant, conductivity of a weak-acid, solubility of sparingly soluble salt, conductometric titrations.
9. Potentiometer: Measurement of electrode potentials, activity coefficients and potentiometric titrations.

Reference Books:

1. Alexander Findlay, Bryan Philip Levitt, Findlay's Practical Physical Chemistry, 9 th Edition, Wiley, 1972.
2. J.B.Yadav, Advanced Practical Physical Chemistry, Goel Publishing House,.2001.

SEMESTER – IV

CHY5004	Polymeric Materials	L	T	P	C
		5	1	0	4

Unit – I: Basic Concept and Polymeric Materials:

Introduction - classification - polymerization: chain growth - step growth - coordination - copolymerization - ring opening metathesis polymerization (ROMP) - polymerization techniques: bulk - solution - suspension - emulsion. Thermoplastic polymers: Polyvinyl chloride - PTFE - polyacrylonitrile. Thermosetting resins: phenolic resins - epoxy resins - silicones - polyurethane, UF resin, ABS polymer.

Unit – II: Structure and Properties:

Morphology and order in crystalline polymers: configurations of polymer chains - crystal structures of polymers - morphology of crystalline polymers - crystallization and melting. Polymer structure and physical properties: crystalline melting point Tm - melting point of homologous series, effect of chain flexibility and other steric factors - glass transition temperature (T_g) - Factors affecting the Tg - Relationship between Tm and T_g.

Unit – III: Characterization and Testing:

Determination of molecular weight: Number, weight and viscosity average molecular weights - characterization of polymers by IR and NMR - thermal properties by TGA and DSC. Mechanical test: tensile strength - impact strength - Rockwell hardness - abrasion resistance. Test for electrical resistance: dielectric constant - arc resistance - dielectric strength.

Unit – IV: Elastomers Technology:

Compounding and elastomer properties, vulcanization - chemistry of vulcanization, sulphur vulcanization, physical aspects of vulcanization. Reinforcement, types of fillers, carbon black.

Unit – V: Polymer Processing Techniques:

Plastics - elastomerics - fibres - calendaring – die casting - rotational casting - film casting- compression moulding - injection moulding - blow moulding - extrusion moulding - thermoforming - fibre spinning.

Reference Books:

1. Textbook of Polymer Science: F. W. Billmeyer JR. John Wiley & Sons, 3rd Ed., 1984.
2. Polymer Science: V. R.Gowariker, N. V. Viswanathan and J. Sreedhar, New age International Publishers, Reprint 2013.
3. Encyclopedia of Polymer Science and Engineering: H.F.Mark (Ed.), Wiley- Interscience, New York, 1991.
4. Plastic Materials: A. Brydson, 4th Edition, Butterworth – Heimann Ltd., London, 2002.
5. Polymer Chemistry - An Introduction: R.B.Seymour and C.E. Carraher, JR., Marcel Dekker Inc., 2005.

6. Rubber Technology: Maurice Morton, Van Nostrand Reinhold, New York, 2002.
7. Principles of Polymerization: G. Odian, 3rd Ed., Wiley-Interscience, 2009.
8. Polymer Science and Technology, Joel R. Fried, 2nd Ed., PHI Learning Private Limited, 2010.
9. Journal articles from current literature.

ELECTIVE PAPERS

CHY5011	Corrosion Science	L	T	P	C
		5	1	0	4

Unit – I: Introduction:
Corrosion-Definition, Classification, Expressions for corrosion rate, EMF series and Galvanic series-Merits and Demerits, Pourbaix diagram for iron, magnesium and aluminium, High temperature corrosion, Pilling-Bed worth ratio.

Unit – II: Corrosion Principles:

Introduction, Electrochemical reactions, Application of thermodynamics to corrosion, Polarization-Activation polarization and Concentration polarization, Mixed potential theory, Exchange current density, Tafel equation, Passivity-Mechanism of the growth and breakdown of passive film.

Unit – III: Forms of Corrosion:

Uniform corrosion-Atmospheric corrosion, Galvanic corrosion, Crevice corrosion, Pitting corrosion, Intergranular corrosion, Stress corrosion cracking, Dezincification, Erosion corrosion, Corrosion fatigue, Hydrogen damage.

Unit – IV: Corrosion Testing:

Introduction, Classification, Purpose of corrosion testing, Huey test for stainless steel, Streicher test for stainless steel, Stress corrosion test, salt spray test, humidity and porosity tests, Accelerated weathering tests. Electrochemical methods of corrosion rate measurements by Tafel polarization, linear polarization, and impedence spectroscopy-ASTM Standards for corrosion testing.

Unit – V: Corrosion Protection:

Introduction, Material selection, Alteration of environment, Design, Cathodic protection and Anodic protection, Coatings-metallic and other inorganic coatings, Organic coatings, Electroless plating and Anodizing, Corrosion inhibitors, Failure analysis.

Reference Books:

1. Fontana and Greene, Corrosion Engineering, McGraw Hill Book Co, New York, 1983.
2. Raj Narayan, An introduction to metallic corrosion and its prevention, Oxford and IBH, New Delhi, 1983.
3. S.N.Banerjee, "An Introduction to Corrosion Science and Corrosion Inhibition", Oxonian Press P.Ltd, New Delhi, 1985.
4. Denny A. Jones, Principles and Prevention of corrosion, Macmillan Publishing Company, 1991.
5. Zahi Ahmed, Principles of corrosion engineering & corrosion control, Butterworth Heinemann, 2006.
6. Budinski, K.G., Surface Engineering for wear resistance, Prentice Hall Inc, Engelwood Cliff, New Jersey, USA, 1988.
7. Uhlig, H.H., Corrosion and Corrosion control, John Wiley and sons, New York, USA, 1985.

CHY5012	Modern Methodologies in Organic Synthesis	L	T	P	C
		5	1	0	4

Unit – I: Construction of ring systems:

Three membered rings – Blum–Ittah aziridine synthesis, Corey−Chaykovsky and Simmons–Smith reactions, Darzens condensation, Perkin synthesis; Four membered rings – Paternó–Büchi reaction, Cumulenes cycloaddition, Reaction of ketenes with alkenes, Staudinger reaction (β - lactams synthesis), Reaction of isocyanates with alkenes; Five membered rings – Bartoli indole, Erlenmeyer−Plöchl azlactone, Claisen isoxazole, Paal–Knorr furan, Fischer oxazole, Knorr pyrazole, and Paal-Knorr pyrrole syntheses, Borsche–Drechsel cyclization, Thorpe−Ziegler reaction; Six membered rings - Algar−Flynn−Oyamada, Pictet–Spengler, Bischler–Napieralski, and Allan–Robinson reactions, Bergman cyclization, Pechmann coumarin synthesis; Small/macrocyclic rings - Ring-closing metathesis (RCM), Corey–Nicolaou macrolactonization.

Unit – II: Rearrangements:

Baker–Venkataraman, Ireland–Claisen (silyl ketene acetal), Beckmann, Newman−Kwart, Gabriel–Colman, Boulton–Katritzky, Mislow–Evans, Brook, Carroll, Overman, Chapman, Hofmann, Ciamician–Dennsted, Schmidt, Curtius, Demjanov, Favorskii, Lossen, Meyer–Schuster, Pummerer, Neber, Wagner–Meerwein, Payne, Smiles, Rupe, and Wolff rearrangements.

Unit – III: Oxidation and reduction:

Oxidation – Alcohols to carbonyls/acids - Corey–Kim, Dess−Martin periodinane, Jones, Collins–Sarett, and Swern oxidations; Aldehyde to phenol - Dakin oxidation; Alkenes to epoxides - Sharpless asymmetric, Shi, and Jacobsen epoxidations; Alkenes to diols - Sharpless asymmetric dihydroxylation, Prevost reaction; Ketones to esters/lactones - Baeyer–Villiger oxidation; Alkenes to alcohols – Hydroboration, Wacker oxidations, Silanes to alcohols/ketones - Fleming−Kumada, Rubottom, and Saegusa oxidations; Halides to aldehydes - Sommelet reaction; Reduction – Imine to amine - Borch reductive amination, Leuckart–Wallach reaction; Ketones/Esters/thiolesters/alkenes to alcohols/aldehydes/alkanes - Corey-Bakshi-Shibata, Bouveault–Blanc, Fukuyama, Midland, and Wolff–Kishner reductions, Noyori hydrogenation; Acetylenic alcohol to allylic alcohol - Chan alkyne reduction; Alcohols to alkenes - Corey–Winter reductive olefination.

Unit – IV: Catalytic C-C and C-X bond formations:

C-C Bond formation - Baylis–Hillman, Henry, Wittig, Horner–Wadsworth–Emmons, Mukaiyama aldol, and Hosomi–Sakurai reactions, Mukaiyama Michael addition, Cadiot–Chodkiewicz, Glaser, Kumada, Ullmann, Eglinton, Sonogashira, Heck, Stille, Hiyama, McMurry, Suzuki–Miyaura, and Negishi coupling reactions; C-X bond formation - Buchwald–Hartwig amination, Chan–Lam C–X coupling, Miyaura borylation, Tsuji−Trost, Pinner, Diels-Alder, and Ritter reactions.

Unit – V: Multi-component reactions (MCR's):

Mannich, Bucherer–Bergs, Passerini, Biginelli, Gewald, Petasis, Kabachnik-Fields, Ugi, Pauson–Khand, and Asinger reactions, Strecker, Kindler thioamide, Hantzsch dihydropyridine, Radziszewski imidazole, Hantzsch pyrrole, Robinson's tropinone, Bossio's oxazole, and Kobayashi's pyrroloquinoxline syntheses, Palladium catalyzed synthesis of tetrahydrofuran, pyrroles, imidazolines,

oxazolines, Copper catalyzed synthesis of propargyl amides, benzimidazoles, N-fused imidazoles, triazoles, tetrazoles, Iodine catalyzed synthesis of pyrroles, Base catalyzed synthesis of substituted benzenes, Catalyst free synthesis of azepines, Solvent free synthesis of thioamides.

Reference Books:

1. F. A. Cary & R. I. Sundberg, Advanced Organic Chemistry, Part A & B, 5th Edn. Springer (2009).
2. B. P. Mundy, M. G. Ellerd, & F. G. Favaloro. Name Reactions and Reagents in Organic Synthesis, Wiley-Interscience (2005).
3. A. Hassner & I. Namboothiri. Organic Syntheses Based on Name Reactions, Elsevier (2012).
4. W. Carruthers, Modern Methods of Organic Synthesis, Cambridge University Press (1996).
5. L. Kurti & B. Czako. Strategic Applications of Named Reactions in Organic Synthesis, Elsevier (2005).
6. M. Beller & C. Bolm, Transition metals for organic synthesis, Wiley-VCH (2004).
7. J. Tsuji, Palladium Reagents and Catalysts, New Perspectives for the 21st Century, John Wiley & Sons (2003).
8. R. Noyori, Asymmetric Catalysis in Organic Synthesis, John Wiley & Sons (1994).
9. J. Zhu & H. Bienaymé, Multicomponent Reactions, Wiley-VCH (2005).

CHY5013	Nanomaterials	L	T	P	C
		5	1	0	4

Unit – I: Basics of Nanomaterials:

Basics of nanomaterials: Properties of materials & nanomaterials, quantum confinement effect, surface to volume ratio, surface properties of nanoparticles. Classification of the nano materials – zero dimensional, one dimensional, two dimensional and three dimensional nanostructures. Mechanical, optical, electronic, magnetic, thermal and chemical properties of nanomaterials. Size dependent properties-size dependent absorption spectra.

Unit – II: Synthesis of Nanomaterials by Chemical Routes:

Chemical precipitation and coprecipitation, metal nanocrystals by reduction, sol-gel synthesis, microemulsions or reverse micelles, solvothermal synthesis, thermolysis routes, microwave heating synthesis, sonochemical synthesis, electrochemical synthesis, photochemical synthesis, synthesis in supercritical fluids, self-assembly strategies.

Unit – III: Fabrication of Nanomaterials by Physical Methods:

Inert gas condensation, arc discharge, plasma arc technique, RF plasma, MW plasma, ion sputtering, laser ablation, laser pyrolysis, molecular beam epitaxy, chemical vapour deposition method and electro deposition.

Unit – IV: Characterization of Nanomaterials:

X-ray diffraction, Scanning Electron Microscopy (SEM), Scanning Probe Microscopy (SPM), TEM and EDAX analysis, Atomic force Microscopy (AFM); Spectroscopic characterizations: UV-Visible and NMR spectroscopy; Surface Characterization: X-ray Photoelectron Spectroscopy (XPS), Secondary Ion Mass Spectroscopy (SIMS); Thermal Characterization: DTA, TGA, DSC.

Unit – V: Applications of Nanomaterials:

Catalysis on nanoparticles, oxide reactions, semiconductors, sensors, and electronic devices, photochemistry and nanophotonics, applications of CNTs, nanomaterials in biology and medicine.

Reference Books:

1. Charles P. Poole, Frank J. Owens, “Introduction to Nanotechnology”, Wiley Interscience, 2003.
2. C. N. R. Rao, A. Mu¨ller, A. K. Cheetham, “The Chemistry of Nanomaterials: Synthesis, Properties and Applications” WILEY-VCH Verlag GmbH & Co. KGaA, Weinheim, 2004
3. G. Schmidt, “Nanoparticles: From theory to applications”, Wiley, Weinheim 2004.
4. G. B. Sergeev, “Nanochemistry” Kidlington, Oxford OX5 1GB, UK, 2006.
5. C. N. R. Rao, A. Mu¨ller, A. K. Cheetham, “Nanomaterials Chemistry: Recent developments and new directions” WILEY-VCH Verlag GmbH & Co. KGaA, Weinheim, 2007
6. C.N.R. Rao, G.U. Kulkarni, P.J. Thomas, Nanocrystals: Synthesis, Properties and Applications” Springer Series in materials science-95, Springer-Verlag Berlin Heidelberg 2007
7. Znong Lin Wang, “Characterization of nanophase materials” WILEY-VCH Verlag GmbH & Co. KGaA, Weinheim, 2000.

CHY5014	Green Chemistry	L	T	P	C
		5	1	0	4

Unit – I: Basic Concepts of Green Chemistry:

Definition of green chemistry, need of green chemistry and eco-efficiency, Environmental protection laws, challenges and green chemistry education, pollution control and pollution prevention-Principle of green chemistry.

Unit – II: Green Solvents:

Aqueous phase reactions: Mechanism and application of Baeyer-Villiger Oxidation, Claisen rearrangement, Claisen-Schmidt reaction, Diels-Alder reaction, Heck reaction, Knoevenagel condensation, Michael addition, Mukaiyama Reaction and Wurtz reaction. Ionic liquids: Properties of ionic liquids and applications in organic synthesis (illustrate with three examples such like Diels-Alder reaction, Heck reaction, Knoevenagel condensation, Michael addition, Witting reaction.

Unit – III: Non-conventional energy sources:

Microwave Solvent free reaction: Solid state reactions-Deacetylation, deprotection, Saponification of esters, alkylation of reactive methylene compounds, synthesis of nitriles from aldehydes, reductions. Microwave assisted reactions in water-Hoffmann elimination, hydrolysis, oxidation, saponification reactions. Microwave assisted reactions in organic solvents-Esterification reactions, Fries rearrangement, Orthoester rearrangement, Diels-Alder reaction, decarboxylation. Microwave assisted reactions under PTC conditions: Ultrasound assisted reaction: Introduction, substitution reactions, addition, oxidation and reduction reactions. Photochemical reactions using sunlight: Benzopionacol, conversion of trans azobenzene to cis azobenzene and conversion of trans stilbene to cis stilbene.

Unit – IV: Green catalysis:

Heterogeneous catalysis: use of zeolites, silica, alumina, clay, polymers, cyclodextrin and supported catalysts. Biocatalysis: enzymes, microbes etc Phase-transfer catalysis: micellar/surfactant etc.

Unit – V: Designing Green Synthesis:

Designing Green Synthesis- choice of starting materials, choice of reagents, choice of catalysts-biocatalysts, polymer supported catalysts, choice of solvents. Synthesis involving basic principles of green chemistry – Examples - Synthesis of ibuprofen, adipic acid, methyl methacrylate and paracetamol.

Reference Books:

1. Green Chemistry, Theory and Practical, Paul T.Anastas and John C.Warner, Oxford University Press.
2. New Trends in Green Chemistry by Ahluwalia and M. Kidwai.

3. Green Chemistry, Introductory Text, M.Lancaster, Royal Society of Chemistry, London.
4. Introduction to green chemistry, M.A. Ryan and M. Tinnesan, American Chemical Society, Washington.
5. Real World Cases in Green Chemistry, M.C. Cann and M.E. Connelly, American Chemical Society, Washington.
6. Alternative Solvents for Green Chemistry, F.M. Kerton, Royal Society of Chemistry, London.
7. Recoverable and Recyclable Catalysis, M. Benaglia, Wiley.
8. Handbook of Green Chemistry and Technology, J.Clark and D. Macquarrie, Black well Publication.
9. Solid-Phase Organic Synthesis, k. Burgess, Wiley-Interscience.
10. Eco-Friendly synthesis of Fine Chemicals, R. Ballini, Royal Society of Chemistry, London.

CHY5015	Environmental Chemistry	L	T	P	C
		5	1	0	4

Unit – I: Atmospheric Chemistry:

The structure of the earth's atmosphere- chemistry of the lower and upper atmosphere. The chemistry of air pollution- oxides of nitrogen- hydrogen sulphide and oxides of sulphur-Aerosols – ozone depletion and consequences- dioxins burning plastics- other atmospheric chemicals- smog- radio activity and fallout- air pollution abatement. Green house effect- Global warming, oxides of carbon.

Unit – II: The Earth:

The lithosphere- the chemical composition of earth- the structure and composition of inner earth- the mantle, and the crust. The exploitation of mineral resources and the abuse of earth – earth resources – changing the face of the land- the earth as a dump- recycl earth resource conservation steps. The hydrosphere : The fresh water chemistry – the structure and properties of liquid water –lakes, rivers, ponds and stream – river chemistry, pollution and aeration – water additives-isotopes- mercury pollution. The chemical constituents of sea water- organic matter and suspended material- ocean dumping- oil pollution. The role of water in our total environment-the hydrologic cycle- snow and ice – nucleation and precipitation – the chemical composition of rain water- phase changes and isotopic fractionation.

Unit – III: The Biosphere:

The structure of the biosphere, Man's perturbation of the biosphere – Man as a chemical factory – material use and waste – energy use and thermal pollution – ecological disruption –chemical sensation, hormonal imbalance and mutagens- internal pollution. Hydrosphere -lithosphere interaction: The structure of water at an interface – chemical composition of mineral water-weathering and the changing face of the land- the origin of the oceans-sedimentation and the deposition of materials from the hydrosphere – chemical exchange between sediments and the water column.

Unit – IV: Interactions:

Lithosphere- biosphere interaction: soil chemistry – the prospects of agriculture- agricultural pollution – pesticides and other persistent pollutants – the deposition of coal and petroleum – theories of origin of petroleum. Atmosphere – biosphere interaction and atmosphere –hydrosphere interaction: history of earth's atmosphere – the nitrogen cycle – the carbon cycle –air – sea interactions. Biosphere – hydrosphere interaction: The chemistry of water pollution – sewage treatment, primary, secondary- and tertiary – activated sledge – trickling filters- denitrification – biology and energy chain – reactor design theory – anaerobic digestion –eutrophication.

Unit – V: Pollution Control:

Pollution control in the following: Fertiliser, petroleum, pulp and paper, tanning, sugar, alcohol, electroplating and nuclear reactors. Analysis of pollutants: Sum, specific and group parameters BOD, COD, specific oxygen demand, DOC, DOCl, DOS, Fe, Cr, Cu, Pb, and Ni-SO_2, NO_x, H_2S, O_3 and CO.

Reference Books:

1. R. A. Horne.,The Chemistry of Our Environment. John Wiley & Sons Ltd., New York 1978.
2. A.K.De, Environmental chemistry, Fifth Edn., 2003, New age Intnateironal (P) limited, new Delhi,
3. S.P.Mahajan, Pollution control in process industries, TataMc Craw-Hill Enn.1985
4. Iain L, Marr and Malcom S. Cresser, Environmental chemical analysis, Intnational Text Book. Co., 1983 – science.

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