REVISED COURSE STRUCTURE

Sem.	Course No.	Courses	L T P	Credit Hr.
I	**Theory**			
	ACC 31131	Group Theory	3 – 0 – 0	6
	ACC 31132	Organic Reaction, Mechanism and Stereochemistry	3 – 0 – 0	6
	ACC 31133	Coordination Chemistry	3 – 0 – 0	6
	ACC 31134	Kinetics & Thermodynamics	3 – 0 – 0	6
	ACC 31135	Molecular Spectroscopy	3 – 0 – 0	6
	Sessional			
	HSC 21103	Scientific Writing	2 – 1 – 0	5
	Practical			
	ACC 31231	Inorganic Chemistry Lab – I	0 – 0 – 6	6
	ACC 31232	Organic Chemistry Lab – I	0 – 0 – 6	6
	Total		17– 1 – 12	47

Sem.	Course No.	Courses	L T P	Credit Hr.
II	**Theory**			
	ACC 33141	Applications of Spectroscopic Methods	3 – 0 – 0	6
	ACC 32137	Synthetic Organic Chemistry	3 – 0 – 0	6
	ACC 32138	Main Group Chemistry	3 – 0 – 0	6
	ACC 32139	Instrumental Methods of Analysis	3 – 0 – 0	6
	ACC 32140	Organometallic Chemistry	3 – 0 – 0	6
	Practical			
	ACC 32233	Physical Chemistry Lab – I	0 – 0 – 6	6
	ACC 32234	Organic Chemistry Lab – II	0 – 0 – 6	6
	Total		15 – 0 – 12	42

Sem.	Course No.	Courses	L T P	Credit Hr.
III	**Theory**			
	ACC 32136	Quantum Chemistry	3 – 0 – 0	6
	ACC 33142	Photochemistry & Pericyclic Reactions	3 – 0 – 0	6
	ACC 33143	Bio-inorganic Chemistry	3 – 0 – 0	6
	ACC 33144	Modern Methods in Organic Synthesis	3 – 0 – 0	6
	ACC 33145	Solid State Chemistry	3 – 0 – 0	6
	Practical			
	ACC 33235	Inorganic Chemistry Lab – II	0 – 0 – 6	6
	ACC 33236	Physical Chemistry Lab-II	0 – 0 – 6	6
	Seminar			
	ACC 33401	Seminar	0 – 0 – 0	2
	ACC 33501	Project Work	0 – 0 – 0	0
	Total		15 – 0 – 12	44

Sem.	Course No.	Courses	L T P	Credit Hr.
IV	**Elective Courses (Any three)**			
	ACE 34146	Advanced Electrochemistry	3 – 0 – 0	6
	ACE 34147	Computational Chemistry	3 – 0 – 0	6
	ACE 34148	Biophysical Chemistry	3 – 0 – 0	6
	ACE 34149	Science of Corrosion and Corrosion Control	3 – 0 – 0	6
	ACE 34150	Surface Science & Catalysis	3 – 0 – 0	6
	ACE 34151	Electro & Photo-chemical Energy Systems	3 – 0 – 0	6
	ACE 34152	Advanced Characterization Techniques	3 – 0 – 0	6
	ACE 34153	X-Ray Crystallographic Techniques	3 – 0 – 0	6
	ACE 34154	Nuclear & Radiation Chemistry	3 – 0 – 0	6
	ACE 34155	Chemistry of Lanthanides and Actinides	3 – 0 – 0	6
	ACE 34156	Heterocyclic Chemistry	3 – 0 – 0	6
	ACE 34157	Polymer Chemistry	3 – 0 – 0	6
	ACE 34158	Chemistry of Natural Products	3 – 0 – 0	6
	ACE 34159	Medicinal Chemistry	3 – 0 – 0	6
	ACE 34160	Carbohydrate Chemistry	3 – 0 – 0	6
	ACE 34161	Asymmetric Synthesis	3 – 0 – 0	6
	ACE 34162	Supramolecular Chemistry	3 – 0 – 0	6
	ACE 34163	Green Chemistry	3 – 0 – 0	6
	Project/(Seminar & Dissertation)/Viva-voce			
	ACC 34502	Project Work	0 – 0 – 15	15
	ACC 34503	Seminar and Dissertation	0 – 0 – 0	6
	ACC 34504	Grand Viva-voce	0 – 0 – 0	2
	Total		9 – 0 – 15	41

SEMESTER-I

ACC 31131 Group Theory (3-0-0)

Group Theory: Symmetry elements and symmetry operations, Algebraic Operators, Point groups and it's determination in various molecules. Matrix mathematics & Matrix representation symmetry operation. Definition of a Group, Subgroup, Abelian group, Cyclic group. Rearrangement Theorem, Group multiplication Tables, Lagrange's Theorem. Classes, Similarity transforms, Reducible & Irreducible representations. The Great Orthogonality Theorem and its importance. Character table& its construction. Standard reduction formula. Translational, rotational symmetry elements & operators, Mulliken symbols.
Applications: Classification & Determination of normal vibrational modes, Transition moment integral and selection rules. Projection operator, Application to atomic orbitals, molecular orbitals, hybridization, LCAO Approximation, π-electron approximation, Hückel π-orbital method and applications. Construction of SALCs for different geometry of molecules. SALCs for σ and π bonding. Molecular orbitals of sandwich compounds.

References:

1. Chemical Applications of Group Theory, F. Albert Cotton, 3rd Edition, John Wiley & Sons, 2008.
2. Group Theory and Chemistry, David M. Bishop, 1st edition, Dover Publications; Una Rev Edition, 1993.
3. Introduction to Symmetry and Group Theory for Chemists, Arthur M. Lesk, Kluwer Academic Publishers, 2004.
4. Symmetry and Structure, Readable Group Theory for Chemists, Sidney F. A. Kettle, 3rd Edition, John Wiley & Sons, 2008.
5. Molecular Symmetry, David J. Willock, 1st Edition, John Wiley & Sons, 2009.
6. Symmetry through the Eyes of a Chemist, Magdolna Hargittai and István Hargittai, 3rd Edition, Springer, 2009.
7. Symmetry and spectroscopy of molecules, K. V. Reddy, 2nd Edition, New Age International Publishers, 2009.
8. Molecular Symmetry & Group Theory, R. L. Carter, 1st Edition, John Wiley & Sons, 1997.

ACC 31132 Organic Reaction, Mechanism & Stereochemistry (3-0-0)

Conformation analysis of cycloalkanes, decalines and hydrindanes, effect of conformation on reactivity, threo and erythro isomers, methods of resolution, optical purity, enatiotopic and diastereotopic atoms, groups & faces.
Stereoselectivity and stereospecificity – 1,2-induction and 1,3-induction – Cram's rule and beyond – chelation-control and non-chelation-control – directed functionalization – directed biomimetic polyene cyclization (Johnson). Sterospecific and stereoselective synthesis
Baldwin's Rule and Dunitz's angle of attack, Cram's Model, Felkin-Ahn Model, Cieplak Model. Optical activity in absence of chiral carbon (biphenyls, allenes and spirans), chirality due to helical shape. Stereochemistry of organo nitrogen-, sulfur- and phosphorus- compounds.
Optical rotatory dispersion, circular dichroism, Cotton effect, axial haloketone rule, octant rule. Aromaticity in benzenoid and non-benzenoid compounds.
Reaction Mechanism: Structure and Reactivity. Types of mechanism, types, of reaction, thermodynamic and kinetic requirements, kinetic and thermodynamic control, Hammond's

postulate, Curtin-Hammett principle, potential energy diagrams, transition states and intermediates, methods of determining mechanisms, isotope effects.

Reference:

1. Advanced Organic Chemistry, J. March, 4th Edition, John Wiley and Sons, 1992.
2. Stereochemistry of Organic Compounds, D. Nasipuri, 2nd Edition, New Age International, 1994.
3. Stereochemistry of Organic Compounds, P. S. Kalsi, 6th Edition, New Age International, 2004.
4. Organic Chemistry, J. Clayden, N. Greeves, S. Warren and P. Wothers, 1st Edition, Oxford University Press, 2001.
5. Stereochemistry of Organic Compounds, E. Eliel and S. H. Wilen, Wiley India Edition, John Wiley & Sons, 1994.

ACC 31133 Coordination Chemistry (3-0-0)

CFT and its limitations, LFT, MOT. Classification of ligands by donor atoms, stability, reactivity, bond types, geometry and coordination compounds. Kinetics and mechanism of reactions of transition metal complexes: substitution reactions, electron transfer redox processes, acid base and related processes.

Electronic Spectra of transition metal complexes: Spectroscopic ground states, Orgel, Tanabe-Sugano, Correlation diagram, Charge transfer spectra. Spectroscopic method of assignment of absolute configuration of metal chelates and their stereochemical information.

Definition of magnetic properties, Curie and Curie-Weiss Law, Orbital and spin contribution to magnetic susceptibility, Introduction to magnetic properties of lanthanides, Magnetic exchange coupling, Spin cross over phenomena.

Inorganic photochemistry of coordination compounds.

References:

1. Shriver & Atkins: Inorganic Chemistry, P.W. Atkins, T. Overton, J. Rourke, M. Weller and F. Armstrong; 5th Edition, Oxford University Press, 2013.
2. Advanced Inorganic Chemistry,F. A. Cotton, G. Wilkinson, C. A. Murillo and M. Bochmann; 6th Edition, Wiley, 1999.
3. Inorganic chemistry, K. F. Purcell and J.C. Kotz, Holt Saunders international, 1980.
4. Reaction Mechanism of Inorganic and Organometallic Systems, R. B. Jordan, 2nd Edition, Oxford University Press, 1998.
5. Photochemistry of coordination compounds, V. Balzaniand, V. Carassiti. Academic Press, 1970.
6. Inorganic Chemistry Principles of structure and reactivity, J. E. Huheey, E. A. Keiter, R. L. Keiter and O. K. Medhi, 4th Edition, Pearson, 2013.
7. Inorganic Chemistry, C. E. Housecroft and A. G. Sharpe, 4th edition, Prentice-Hall, 2012.
8. Elements of Magnetochemistry, R. L. Dutta and Arun Syamal, 2nd edition, East-West Press, 2010.

ACC 31134 Kinetics & Thermodynamics (3-0-0)

Review of classical thermodynamics; Third law of thermodynamics and residual entropy; Non equilibrium thermodynamics: Thermodynamic criteria for non-equilibrium states, entropy

production, flow, irreversible processes, Electrokinetic phenomena, Diffusion, Electric conduction, Coupled reactions. Theory of electrolytes, Ionic strength, Derivation of Debye Hückel limiting law. Introduction to Statistical thermodynamics, various ensembles, Fluctuations, Partition functions, Applications to gases. Chemical equilibrium; Chemical kinetics and applications. Theories of chemical reaction rates. Elementary reactions in solutions and surface. Fundamentals of Homogeneous and heterogeneous catalysis.

References:

1. Physical Chemistry: Thermodynamics, Structure, and Change, P.W. Atkins, Julio de Paula, 10th Edition, W. H. Freeman, 2014.
2. Physical Chemistry: Statistical mechanics, H. Metiu, Taylor & Francis; Pap/Cdr edition, 2006.
3. Chemical Kinetics, K. J. Laidler, 3rd Edition, Pearson Education India, 1987.
4. Statistical Mechanics, D. A. McQuarrie, 1st Edition, University Science Books, 2000.
5. Thermodynamics for chemists, Samuel Glasstone, Narahari Press, 2007.

ACC 31135 Molecular Spectroscopy (3-0-0)

Introduction to spectral energy domains and measurement of spectra, Implications of discrete energy levels, Population of States – Boltzman Distribution, Interaction of radiation with matter, origin of linewidths in molecular spectra, Transition dipole moment, Molecular electronic spectra, Electronic transitions, Franck-Condon principle. Polarization of transitions, Molecular vibrations - Infrared spectroscopy, harmonic and anharmonic oscillators, Morse potential, IR selection rules, Raman spectroscopy, polarizability and Raman selection rules, Lasers and Masers; Rotational (Microwave) spectroscopy: The rigid diatomic rotor, intensity of rotational transitions, degeneracy, allowed rotational energy levels. Classification of polyatomic rotors and the non-rigid rotor, symmetric and asymmetric tops. Photophysical processes, Non-Linear Spectroscopy, Nuclear Magnetic Resonance, Relaxation times, FT-NMR, spin-spin coupling, Nuclear Quadrupolar Resonance, Overhauser effect. ESR Spectroscopy: line shapes, isotropic and anisotropic interactions, theory of *g*-factors & hyperfine interactions.

References:

1. Fundamentals of Molecular Spectroscopy, C. N. Banwell and E. M. McCash, 4th Edition, Tata McGraw-Hill Education, 1994.
2. Molecular Quantum Mechanics, P. W. Atkins and Ronald S. Friedman, 4th Edition, Oxford University Press, 2010.
3. Spectra of Atoms and Molecules, P. F. Bernath, 2nd Edition, Oxford University Press, 2005.
4. Molecular Vibrations: The Theory of Infrared and Raman Spectra, E. B. Wilson, Jr., J. C. Decius and P. C. Cross, Dover Publications, 1980.
5. Electron Paramagnetic Resonance: Elementary Theory and Practical Applications, J. A. Weil and J. R. Bolton, (Eds), 2nd Edition, John Wiley & Sons, Inc., 2007.
6. Modern NMR Techniques for Chemistry Research, A. E. Derome, Pregamon, 1987.
7. Principles of Magnetic Resonance, C. P. Slichter, 3rd Edition, Springer-Verlag, 1990.
8. Introduction to Molecular Spectroscopy, Gordon M. Barrow, McGraw-Hill, 1962

SESSIONAL

HSC 21103 Scientific Writing (2-1-0)

To receive and interpret written information: academic texts; journals and reference materials; manuals and laboratory instruction sheets; graphical information, viz. maps, tables, charts, graphs, diagrams, flow-charts, sketches, plans and statistical data.
Understanding interactive writing process and scientific writing with word, sentence and paragraph sense.
Writing physical descriptions, writing instructions and report; defining, describing processes; writing narratives, classifications, explanations; hypothesis, prediction and conclusion; generalizing and exemplifying; using graphical information and using thought connectors.
Note taking; outlining, paraphrasing, summarizing and writing abstracts; organizing references and writing assignments and revision of grammar.

PRACTICAL

ACC 31231 Inorganic Chemistry Lab-I (0-0-6)

1. Detection of common and less common cations. Mo, W, Ti, Zr, Th, V, U, Li.
2. Hydrothermal synthesis of MOFs.
3. Volumetric Experiments
   a) Estimation of alkali present in Antacid Tablet.
   b) Estimation of calcium in milk powder by complexometry.
4. Inorganic Preparations:
   a) Hexamminecobalt(III) Chloride
   b) Potassium tris(oxalato)ferrate(III)

References:

1. Vogels Textbook Of Quantitative Chemical Analysis, J. Mendham, R. C. Denney, J. D. Barnes, M. J. K. Thomas, 6th edition, Pearson, 2006..
2. Advanced Practical Inorganic Chemistry, Gurdeep Raj, 22nd Edition, Krishna Prakasan M. (Pvt.) Ltd., 2010.
3. Integrated Approach to Coordination Chemistry: An Inorganic Laboratory Guide, R. A. Marusak, Kate Doan, S. D. Cummins, 2007, Wiley, NY.

ACC 31232 Organic Chemistry Lab-I (0-0-6)

Separation of organic compounds from a binary mixture and identification of the functional groups present. Identification of the individual organic compounds by physical, chemical and spectroscopic means.
Organic quantitative analysis. Estimation of phenol, acetone, ethyl alcohol, aniline, etc.

References:

1. Systematic Identification of Organic Compounds, a lab. Manual, R. L. Shriner, R. C. Fuson and D.Y. Curtin, 6th edition Wiley, New York.
2. Vogel's Textbook of Practical Organic Chemistry revised- B. S. Furniss, A. J. Hannaford, P. W. G. Smith, A. R. Tatchell, 5th Edition, Addision Wesley Longman Limited, UK, 1997.
3. Experimental Organic Chemistry- L. M. Harwood and C.J.Moody, Blackwell Scientific, London, 1989. 5. Practical Organic Chemistry – W. Kemp, McGraw Hill, London, 1962.

SEMESTER-II

ACC 33141 Applications of Spectroscopic Methods (3-0-0)

Unit I

Electronic spectroscopy: Types of electronic transitions in organic compounds, solvent effects, effect of extended conjugation, Woodward-Fieser rules, stereochemistry and electronic absorption.

Infrared spectroscopy: Group frequencies of organic functionality, factors affecting the group frequencies.

Nuclear Magnetic Resonance Spectroscopy: Karplus relationship of J on dihedral angle. First order splitting patterns and structure correlation. Off-resonance decoupling, chemical shift reagents, restricted rotation (DMF, biphenyls, annulenes), long range coupling, NOE effects. ^{13}C-NMR: Natural abundance and sensitivity, 2D NMR.

Mass spectrometry: Base peak, metastable peak, fragmentation processes of organic molecules and deduction of structural information.

Structure elucidation by spectroscopic techniques.

Unit II

Infrared and Raman spectroscopy: Vibrational spectra of ionic, coordination and metal carbonyl compounds.

Mass spectrometry: Applications of CSI, EI, FAB and MALDI in organometallic and supramolecular chemistry.

EPR spectroscopy: EPR spectra of transition metal complexes.

Special Techniques:

CD and ORD, Faraday Effect, Cotton Effect and Magnetic Circular Dichorism (MCD). Basic principles and applications of Mossbauer spectroscopy.

References:

1. Organic spectroscopy, William Kemp, 3rd edition, Macmillan, 2011.
2. Introduction to Spectroscopy – D. L. Pavia, G.M. Lampman, G. S. Kriz, 4th Edition, Cengage Learning, 2008.
3. Spectrometric identification of organic compounds, Robert M. Silverstein, Francis X. Webster, David Kiemle, 7th Edition. Wiley, 2005.
4. Spectroscopic methods in organic chemistry - D. H. Williams and I. Flemming, 6th Edition, Mc Graw Hill, 2011.
5. Organic structure Analysis- Phillip Crews, Rodriguez, Jaspars, Oxford University Press, 1998
6. Physical Methods for Chemists, R. S. Drago, 2nd Edition, Saunders (W.B.) Co Ltd, 1992.
7. Electron Paramagnetic Resonance: Elementary Theory and Practical Applications, John A. Weil, James R. Bolton, 2nd Edition, Wiley, 2007.

ACC 32137 Synthetic Organic Chemistry (3-0-0)

Oxidation: Different oxidative processes, Oxidation of hydrocarbons, alcohols, carbonyl compounds and amines. (Sharpless Asymmetric epoxidation, Corey's reagent, Hypervalent iodine reagents, Wacker oxidation)

Reduction: Different reductive processes, Reduction of hydrocarbons, carbonyl compounds, nitro compounds (Reduction with hydride and modified hydride reagents, Birch reductions, Shapiro reaction)

Common named reactions and reagents – C-C bond formations for alkanes, alkenes, Csp^2-Csp^2 couplings.

Organic main group chemistry:

Organoboron chemistry: carboranes, hydroboration, reaction of organoboranes, unsaturated hydrocarbon synthesis, allyl boranes, allyl enolates.
Organosilicon chemistry: α-and β- effects, hydrosilylation, synthesis and reactivity of vinylsilanes, allylsilanes.
Organophosphorous chemistry: phosphorus ylides- Wittig reaction and its modifications; phosphine oxides and its applications.
Organosulfur chemistry: sulfur-stabilization of anions and cations, sulfur ylides, sulfoxides and sulfones. Organotin chemistry.

References:

1. Strategic Applications of Named Reactions in Organic Synthesis, L. Kürti and B. Czakó Elsevier Academic Press, 2005.
2. Favaloro -Name Reactions and Reagents in Organic Synthesis, B. P. Mundy, M. G. Ellerd and Jr. F. G, Wiley-Interscience, 2nd Edition, 2005.
3. Advanced Organic Chemistry Part B, F.A. Carey and R.J. Sundberg, 5th Edition, Springer, 2008.
4. Organic chemistry J. Clayden, N. Greeves, S. Warren and P. Wothers 2nd Edition Oxford Press, 2012.
5. Modern methods of organic synthesis, W. Carruthers & I. Coldham, 4th edition, Cambridge, 2004

ACC 32138 Main Group Chemistry (3-0-0)

Synthesis, Properties, Structure and Bonding of: Nitrogen, Phosphorous, Sulfur, Pseudohalogen, Interhalogen and Xenon Compounds, Borazines, Phosphazenes, Sulfur-Nitrogen compounds, Silicones, bonding and reactions in higher boranes, Wades rules and styx numbers, Carboranes, Metallocarboranes. Isolobal analogy, metal carbonyl and halide clusters, compounds with metal-metal multiple bonds. Preparation, structure, PSEPT theory, Capping principle, Electron precise molecules. Cluster assigned ligand transformation, Polyhedral rearrangements, Fragmentation reactions, Isopoly & heteropoly acids & salts.
Introduction, properties, structure, bonding, organometallic chemistry, synthesis and reactivity of organo lithium, beryllium, and magnesium compounds. Boron, aluminum, gallium, indium organyls, germanium, tin and lead organyls, multiple bonded compounds, cages, clusters, applications in organic synthesis.

References:

1. Concepts and Models of Inorganic Chemistry, Bodie E. Douglas, Darl H. McDaniel and John J. Alexander, 3rd Edition, John Wiley and Sons, 1994.
2. Inorganic Chemistry Principles of structure and reactivity, J. E. Huheey, E. A. Keiter, R. L. Keiter and O. K. Medhi, 4th Edition, Pearson, 2013.
3. Inorganic Chemistry, Gary L. Miessler, Donald A. Tarr, 3rd Edition, Pearson, 2004.
4. Organometallic Chemistry, C. Elschenbroich, 3rd Edition, Wiley VCH, 2006.
5. Cluster Chemistry, D. M. P. Mingos, David J. Wales, Prentice Hall, 1990.
6. Inorganic and Organometallic Polymers, V. Chandrasekhar, Springer India, 2005.
7. Basic Organometallic Chemistry: Concepts, Syntheses and Applications, Dr. B.D. Gupta, Dr. Anil J. Elias, 2nd Edition, University Press, 2013.

ACC 32139 Instrumental Methods of Analysis (3-0-0)

Basic principles and instrumentation of: Chromatographic methods of separation, Mass spectroscopy: FAB, ESI, CSI, MALDI. Atomic Spectroscopy; X-ray methods of analysis: XRD, XRF, Thermal Analysis: DTA, DSC, TG, DMA.
Potentiometric techniques, Voltammetry: Polarographic methods, Dropping Mercury Electrode, Current-voltage relationship, Cyclic voltammetry, Theory of electro-gravimetric analysis, electrode reactions, overpotential, completeness of deposition, electrolytic separation of metals by controlled potential electrolysis/electrodeposition.
Introduction to Microscopic Techniques: SEM, TEM, STM, AFM, EPMA.

References:

1. Scanning Probe Microscopy and Spectroscopy, R. Wiesendanger, 1st Edition, Cambridge University Press, 1994.
2. Handbook of instrumental techniques for analytical chemistry, Frank A. Settle, 1st Edition, Prentice Hall, 1997.
3. Surface science: Foundations of catalysis and nanoscience, K. W. Kolasinski, 3rd Edition, Wiley, 2012.
4. Fundamentals of analytical chemistry, Douglas Skoog, Donald West, F. Holler, Stanley Crouch, 9th Edition, Cengage Learning, 2013.
5. Atkins' physical chemistry, P. Atkins and J. de Paula, 8th Edition, Oxford University Press, New Delhi, 2008.
6. Nano: The essentials, T. Pradeep, McGraw-Hill Education, New Delhi, 2010.
7. Electroanalytical Methods, F. Scholz, Springer, 2nd Edition. 2010.

ACC 32140 Organometallic Chemistry (3-0-0)

Basic Concept of organometallic chemistry, Metal carbonyl, phosphine, alkenes, alkynes, and allyl complexes. Hydrides, carbenes, carbynes Metallocenes, metal arene complexes.
Fluxionality in organometallic compounds.
Homogeneous & Heterogeneous Catalysis: Oxidative addition and reductive elimination, insertion reactions. Agostic interaction, Hydroformylation, Ziegler-Natta catalyst, Wilkinson's catalyst, Synthesis gas, Monsanto process, and Wacker process. Catalytic asymmetric synthesis and introduction to heterogeneous catalysis.
Organometallic polymers & Bio-organometallic chemistry.

References:

1. Basic Organometallic Chemistry: Concepts, Syntheses and Applications, Dr. B.D. Gupta, Dr. Anil J. Elias, 2nd Edition, University Press, 2013.
2. Inorganic Chemistry Principles of structure and reactivity, J. E. Huheey, E. A. Keiter, R. L. Keiter and O. K. Medhi, 4th Edition, Pearson, 2013.
3. The Organometallic Chemistry of the Transition Metals, Robert H. Crabtree, John Wiley & Sons: New York, 2nd Edition, 1994.
4. Organometallics by Ch. Elschenbroich, A. Salzer, 2nd Edition, VCH, 1995.
5. Organotransition Metal Chemistry: Fundamental Concepts and Applications by A. Yamamoto, John Wiley 1986.
6. Organometallic Chemistry, A Unified Approach, R. C. Mehrotra and A. Singh, New Age International, 2009.

PRACTICAL

ACC 32233 Physical Chemistry Lab-I (0-0-6)

Adsorption: To study surface tension – concentration – relationship for solutions (Gibbs equation)
Chemical Kinetics: Determination of the velocity constant of hydrolysis of an ester/ ionic reaction in micellar media.
Chemical Kinetics: Determination of the effect of (a) change of temperature (b) change of concentration of reactants and catalyst and (c) ionic strength of the media on the velocity constant of hydrolysis ester/ ionic reaction. Determination of the velocity constant of hydrolysis of an ester/ ionic reaction in micellar media.
Determination of the rate constant for the oxidation of iodide ions by hygrogen peroxide studying the kinetics as an iodine clock reaction.
Determination of the primary salt effect on the kinetics of ionic reaction and testing of the Bronsted relationship (iodide ion is oxidized by persulphate ion)
Solutions: Determination of the degree of dissociation of weak electrolyte and to study the deviation from ideal behaviour that occurs with a strong electrolyte.
Electrochemistry: Conductometry: Determination of solubility and solubility product of sparingly soluble salts (e.g. $PbSO_4$, $BaSO_4$) conductometrically. *Potentiometry / pH metry:* Determination of the strength of strong and weak acid in a given mixture.
Determination of the velocity constant, order of the reaction and energy of activation for saponification of ethyl acetate by sodium hydroxide conductometrically.
Electrochemistry: Determination of the activity coefficient of zinc ions in the solution of 0.002 M Zinc sulphate using Debye Huckel's limiting law.
To study the effect of solvent on the conductance of $AgNO_3$/Acetic acid and to determine the degree of dissociation and equilibrium constant in different solvents and in their mixtures (DMSO, DMF, dioxane, acetone, water) and to test the validity of Debye-Huckel-Onsager theory.
Determination of temperature dependence of EMF of a cell.

References:

1. A Handbook of Instrumental techniques for analytical chemistry, F. A Settle, Prentice Hall, 1997.
2. Introduction to Instrumental Analysis by R. D. Braun, McGraw-Hill Int. Ed, 1987.

ACC 32234 Organic Chemistry Lab-II (0-0-6)

Multistep organic synthesis. Characterization and identification of the products of the individual steps by physical and spectroscopic means.

References:

1. Practical Organic Chemistry, 4 th ed, Mann & Saunders, Longmans, (1960).
2. A Handbook of Quantitative & Qualitative Analysis- Arnold Heinemann, Clarke, H. T (1975):
3. Advanced Organic Chemistry: Reactions, Mechanisms and Structure, 5th edition, March, J., Wiley, (2000).
4. A Textbook of Practical Organic Chemistry, 5th ed., Vogel, A. I, Prentice Hall, (1996).
5. Reagents in Organic Synthesis, Fieser and Fieser, Wiley, 2006.

SEMESTER-III

ACC 32136 Quantum Chemistry (3-0-0)

Review of essential mathematical concepts. Origin of the quantum theory. Blackbody radiation and Heisenberg uncertainty principle, Postulates of quantum mechanics and Schrödinger equation; Operator algebra. its application on some model systems viz., free-particle and particle in a box, three dimensional system, tunneling, Hermitian operator, Laplacian operator, the harmonic oscillator, power series and Ladder operator method, hermite polynominals; the rigid rotator, and the hydrogen atom, hydrogen like atom, Zeemann effect. The variation theorem; linear variation principle; perturbation theory; applications of variational methods and perturbation theory to the helium atom. Ordinary angular momentum, generalized angular momentum, basis functions and representation of angular momentum operators, Electron Spin, Hartee-Fock SCF method, Born-Oppenheimer approximation; Valence-bond (VB) and Molecular orbital (MO) treatment for homonuclear and heteronuclear diatomic molecules. Hückel molecular orbital theory; application of quantum mechanics to molecular spectroscopy, introduction to density functional theory.

References:

1. Advanced Engineering Mathematics, E. Kreyszig, 5th Edition, Wiley Eastern, 1989.
2. Mathematical methods for physicists, G. Arfken and Hans J. Weber, Prism Indian Edition, 1995.
3. Quantum Chemistry, D. A. McQuarrie, 2nd Edition, University Science Books, 2007.
4. Molecular Quantum Mechanics, P. W. Atkins, 5th Edition, Oxford University Press, 2010.
5. Quantum Chemistry, I. N. Levine, 7th Edition, Prentice Hall, 2013.
6. Introduction to Quantum Mechanics, D. J. Griffiths, 2nd Edition, Pearson Prentice Hall, 2004.
7. Principles of Physical Chemistry, H. Kuhn, H.-D. Försterling, and D.H. Waldeck, 2nd Edition. Wiley, 2009.
8. Quantum Chemistry, J. P. Lowe, K. A. Peterson, 3rd Edition, Academic Press, 2006.
9. Modern Quantum Chemistry, A. Szabo and N. Ostlund, 1st Edition, Dover Publication, 1996.
10. Elementary Quantum Chemistry, Frank L. Pillar, 2nd Edition, Dover Publication, 2001.

ACC 33142 Photochemistry and Pericyclic Reactions (3-0-0)

Pericyclic Reaction: 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 reactions- conrotatory and disrotatory motion, 4n, 4n+2 and allyl systems. Cycloadditions – antarafacial and suprafacial addition ,4n and 4n+2 systems, Diels-Alder reactions, 2+2 addition of ketenes, 1,3, dipolar cycloadditions. Sigmatropic rearrangements- suprafacial and antarafacial shifts of H, sigmatropic shifts involving carbon moieties, 3,3, and 5,5 sigmatropic rearrangements. Ene reaction.
Photochemistry: Photochemical reactions; determination of reaction mechanism; photochemistry of alkenes, carbonyl compounds, enones and aromatic compounds. Reactions of anilides. Photochemical Rearrangements, Lumiketone rearrangement, Type A and Type B rearrangement, Di-pi-methane rearrangement, Oxa-di-pi-methane rearrangement, Barton reaction, reaction of hypohalites, Photo-Fries rearrangement. Photoinduced electron transfer (PET) reactions. Photoredox catalysis. Photochemistry of vision. Photosynthesis.

References:

1. Organic chemistry – J. Clayden, N. Greeves, S. Warren and P. Wothers 2nd Edition Oxford Press, 2012.
2. Frontier Orbitals and Organic Chemical Reactions, I. Flemming, Wiley, London, 1976.
3. Photochemistry of organic compounds, Petr Klan, Jakob Wirz, 1st Edition, Wiley, 2009,
4. Organic photochemistry, O.L. Chapman, Vol. I & II, Marcel Decker, 1969.
5. Orbital Symmetry: A problem solving approach, R. E. Lehr and A. P. Marchand; Academic press, 1972.
6. Organic reactions and orbital symmetry, T. L. Gilchrist and R. C. Storr; 2nd Edition, Cambridge University Press, 1979.
7. Conservation of orbital symmetry, R. B. Woodward and R. Hoffmann; Verlag Chemie, Weinheim, 3rd printing 1971.

ACC 33143 Bio-inorganic Chemistry (3-0-0)

Essential and trace elements in biological processes, Metal Storage Transport and Biomineralization: Ferritin, transferrin, and siderophores, ionophores. Biological role of alkali and alkaline earth metal ions, transport and regulation, molecular aspects of intramolecular processes, extracellular binding proteins. Metalloenzymes, Iron enzymes, SODs, Molybdenum containing enzymes, Coenzyme vitamin B_{12}, Zinc in transcription and regulation.

Photosynthesis, Oxygen Evolution Complex (OEC), Oxygen Binding and transport: metalloporphyrins, artificial dioxygen carriers, Electron-transfer proteins, long distance electron transfer.

Metal-Nucleic Acid Interactions: Metals in Medicine, Metal deficiency and disease, toxic effects of metals, metals used for diagnosis and chemotherapy with particular reference to anticancer drugs

References:

1. Bioinorganic Chemistry, Ivano Bertini, Harry B. Gray, Stephen J. Lippard, Joan Selverstone Valentine, University Science Books, 1994.
2. Principles of Bioinorganic Chemistry, Stephen J. Lippard, Jeremy M. Berg, University Science Books, 1994.
3. Bioinorganic Chemistry – An Introduction. E.-I. Ochiai, Allyn and Bacon Inc. 1977.
4. Bioinorganic Chemistry: A Survey, Ei-Ichiro Ochiai, academic press, 2008.
5. Bioinorganic Chemistry: Inorganic Elements in the Chemistry of Life, W. Kaim & B. Schwederski, John Wiley, 1994.
6. Bio-inorganic Chemistry: A short course, Rossette M. Roat –Malone, 2nd edition, Wiley, NY, 2007.

ACC 33144 Modern Methods in Organic Synthesis (3-0-0)

Disconnection approach: basic principles, one-group, two-group disconnections, selectivity aspects: Chemoselectivity, regioselectivity, stereoselectivity, Retron, Umpolung concepts; uses of aliphatic nitro, amines; radical reactions in synthesis- FGA and its reverse, Protection and deprotection of common functional groups (hydroxy, carbonyl, carboxylic and amino groups). Synthetic strategies – linear and convergent synthesis, Multicomponent reactions, One-pot reactions, Domino, Cascade and tandem reactions.

Directed ortho-metallation, Metathesis reactions, C-H activation and functionalization, organometallic reagents, formation of C-X bond. Common catalysts and reagents (organic, inorganic and enzymatic)
Protecting groups: Protection of alcohol, carbonyl and carboxyl groups, amine and amino acids. Phase transfer catalysis.

References:

1. Organic Synthesis: The Disconnection Approach, S. Warren,2nd Edition, Wiley, 2008.
2. Reactions, Rearrangements and Reagents, S. N. Sanyal, bharati bhawan pub.& dis-new delhi, 2014.
3. Advanced Organic Chemistry Part B, F.A. Carey and R.J. Sundberg, 5th Edition, Springer, 2008.
4. Designing Organic Syntheses – A programmed Introduction to the synthon approach, Stuart Warren, Wiley India Pvt. Ltd.
5. The Logic of Chemical Synthesis, E. J. Corey and X-M. Cheng, Wiley, 1995.
6. Classics in Total Synthesis. Targets, Strategies, Methods. Nicolaou, K. C.; Sorensen, E. J. VCH. Weinheim, 1996.
7. Organic Synthesis, M. Smith, Mc Graw Hill, 2nd Edition, 2004.

ACC 33145 Solid State Chemistry (3-0-0)

Crystal structure of solids: Fundamental of lattices, unit cell, atomic coordinates, Bravais lattices, symmetry elements in crystals, crystal direction and planes, reciprocal lattices, packing efficiency, radius ratios; structure and types of solid. Crystal diffraction by X-rays, Structure factor, Neutrons and Electrons; Structure determination by X-ray diffraction, Semiconductors (intrinsic & extrinsic), and Devices, Electronic properties and Band theory of solids. Fermi level; Imperfections in Solids: Point, Line, Surface; Thermodynamics of the Defects; Ionic Conductivity & Photoconductivity; Colour Centers, Traps, Phosphors; Electrical and Magnetic Properties (Hall Effect); BCS-type superconductivity. Preparative techniques of solids.

References:

1. Solid State Chemistry and its applications, A. R. West, Wiley, 1st Edition, 2001.
2. Solid State Chemistry – An Introduction, L. Smart and E. Moore, Taylor & Francis Group, 4th Edition, 2012.
3. Solid State Chemistry, D. K. Chakrabarty, New Age Science, 2nd Edition, 2010.
4. Principles of the Solid State, H. V. Keer, 1st Edition, New Age International Publishers, 2005.

PRACTICAL

ACC 33235 Inorganic Chemistry Lab-II (0-0-6)

1. Determination of ligand field strength of series of transition metal complexes.
2. Synthesis and magnetic moment determination of series of transition metal complexes.
3. Preparation and catalytic study of transition metal complexes.
4. Preparation and spectroscopic characterization of different isomers of copper (II) glycinato complex.
5. Determination of Composition and stability constant by Job's Method.
6. Synthesis of $[Co(NH_3)_5Cl]Cl_2$ and its reducing properties.
7. Estimation of phosphoric acid in cold drinks by molybdenum blue method.

8. Thermal analysis: Thermal decomposition of calcium oxalate, copper sulphate, calcium sulphate hydrate in cement.
9. Applications of UV-Vis spectrophotometry in simultaneous analysis of two component systems.
10. IR spectrophotometry: Sample preparation, identification of functional groups.

References:

1. Vogels Textbook Of Quantitative Chemical Analysis, J. Mendham, R. C. Denney, J. D. Barnes, M. J. K. Thomas, 6th edition, Pearson, 2006.
2. Integrated Approach to Coordination Chemistry: An Inorganic Laboratory Guide, R. A. Marusak, Kate Doan, S. D. Cummins, 2007, Wiley, NY.
3. Collection of Interesting General Chemistry Experiments, Anil J Elias, Universities Press, 2008.
4. Handbook of instrumental techniques for analytical chemistry, Frank A. Settle, 1st Edition, Prentice Hall, 1997.
5. Fundamentals of analytical chemistry, Douglas Skoog, Donald West, F. Holler, Stanley Crouch, 9th Edition, Cengage Learning, 2013.
6. Atkins' physical chemistry, P. Atkins and J. de Paula, 8th Ed., Oxford University Press, New Delhi, 2008.

ACC 33236 Physical Chemistry Lab-II (0-0-6)

Determination of thermodynamic constants ΔG, ΔS and ΔH for the reaction by EMF method.
Determination of activity and activity coefficients of electrolytes.
Viscosity: Determination of molecular weight of a polymer
Adsorption: Acetic acid on charcoal.
Determination of the temperature dependence of the solubility of a compound in two solvents having similar intermolecular interactions (benzoic acid in water and in DMSO water mixture) and calculate the partial molar heat of solution. Determinations of CMC by Conductometry and Fluorimetry.
UV-Vis spectrophotometry: Applications.
The students will learn to how to operate a PC and how to run standard programmer and packages – for chemistry applications.
Role of computer in research, data organization, software selection and its applications, solving problems by using scientific software & tools, sample programmes for analysis of data.
Execution of linear regression such as X-Y plot, numerical integration and differentiation as well as differential equation solution programmer (EXCEL/origin, Chemdraw).

References:

1. A Handbook of Instrumental techniques for analytical chemistry, F. A Settle, Prentice Hall, 1997.
2. Introduction to Instrumental Analysis by R. D. Braun, McGraw-Hill Int. Ed, 1987.

SEMESTER-IV

Electives

ACE 34146 Advanced Electrochemistry (3-0-0)

Electrodics: Electrified interface, Electrical double layer and its determination, current-voltage curves - reversible and irreversible electrode processes - factors contributing to the decomposition voltage - different kinds of overvoltage -hydrogen and oxygen overvoltage. Cottrell equation, Cyclic voltammetry, Butler-Volmer equation for simple electron transfer reactions, transfer coefficient, exchange current density, rate constants - Tafel equation, electrocapillarity, potential of zero charge, pzc of solid electrodes, polarization: types of polarization, the charge transfer resistance, kinetics of hydrogen evolution reaction. Mechanism of electrode processes: Multielectron processes, chemical reactions initiated by electron transfer, standard mechanistic schemes. Quantum aspects of charge transfer at electrodes – solution interfaces, quantization of charge transfer, tunnelling. Semiconductor interfaces, Electro-catalysis, Bio-electrochemistry, Electron transfer in homogeneous system and in heterogeneous system. Electrosynthesis: Reductive elimination reactions, Kolbe's Hydrocarbon synthesis. Industrial processes: electroplating, anodization, Al production, electroorganic and electroinorganic syntheses, electrosynthesis of some industrial chemicals.

References:

1. Handbook of instrumental techniques for analytical chemistry, Frank A. Settle, Prince Hall, New Jersey, 1997.
2. Surface science: Foundations of catalysis and nanoscience, K. W. Kolasinski, John Wiley and Sons, West Susses, 2002.
3. Fundamentals of analytical chemistry, Douglas Skoog, Donald West, F. Holler, Stanley Crouch, 9th Edition, Cengage Learning, 2013.
4. Atkins' physical chemistry, P. Atkins and J. de Paula, 8th Edition, Oxford University Press, New Delhi, 2008.
5. Nano: The essentials, T. Pradeep, 1st Edition, McGraw-Hill Professional, 2008.
6. Electroanalytical Methods, F. Scholz, 2nd Edition, Springer, 2010.

ACE 34147 Computational Chemistry (3-0-0)

A brief outline of molecular mechanics, semi-empirical approximations, ab initio methods, basis sets and Z-matrix; Application of these computational methods for prediction of structural and electronic properties of molecules by using standard programs; FMOs in organic chemistry, crystal and ligand field calculations, computation of potential energy surfaces. Conformational analysis by molecular mechanics; Dynamical and structural studies of molecules using molecular dynamics simulations; Monte Carlo simulations of molecules.

References:

1. Computational Chemistry and Molecular Modeling: Principles and Applications, K. I. Ramachandran, G. Deepa, K. Namboori,Springer, 2008.
2. Introduction to Computational Chemistry, Frank Jensen, 2nd Edition, Wiley, 2007.
3. Computational Chemistry, Introduction to Theory and Application of Molecular and Quantum Mechanics, Errol Lewars, Springer, 2004.
4. Molecular Modelling: Principle and Application, 2nd Edition. Andrew R. Leach, Addison-Wesley Longman Ltd, 2001.

ACE 34148 Biophysical Chemistry (3-0-0)

Biological relevance of chemical potential. Hydrophobic and hydrophilic interactions in biological systems. Protein-Solvent Interactions - preferential binding, hydration and exclusion. Protein-Ligand Binding. Structure-Function relationships.
Concept of drug delivery. Traditional and controlled drug delivery system. Carrier based drug delivery pathways. Common modes of drug delivery. Targeted drug delivery. Responsive polymers for drug delivery. Application of nanotechnology in drug delivery.

References:

1. Protein-Solvent Interactions, R. B. Gregory, Marcel Dekker, Inc., 1995.
2. Conformations and Forces in Protein Folding, American Association for the Advancement of Science, B. T. Nall and K. A. Dill, ed., 1991.
3. Introduction to Protein Structure, C. Branden and J. Tooze, 2nd Edition, Garland Science, 1995.
4. Binding and Linkage: Functional Chemistry of Biological Macromolecules, J. Wyman and S. J. Gill, University Sciences Books, 1990.

ACE 34149 Science of Corrosion & Corrosion Control (3-0-0)

Definition of corrosion, economic aspects of corrosion, theories of corrosion. Factors affecting corrosion. Kinetics of corrosion. Evan's diagram. Thermodynamics of corrosion-Pourbaix diagram. Forms of corrosion. Corrosion testing techniques. Evaluation of corrosion effect: XRD, ESCA, FTIR and surface techniques. Corrosion prevention: modification of materials, corrosion inhibitors, protective coatings, Cathodic and anodic protection. Corrosion problems in industries.

References:

1. An Introduction to Science of Corrosion and Its Inhibition, S. N. Banerjee, Oxonian Press, 1985.
2. Principles and prevention of corrosion, Denny A. Jones, 2nd Edition, Prentice Hall, 1995.
3. Corrosion and Corrosion Control, R. Winston Revie, 4th Edition, John Wiley & Sons, 2007.
4. Corrosion Engineering, Mars. G. Fontana, 3rd Edition, McGraw-Hill, Inc. 1987.

ACE 34150 Surface Science and Catalysis (3-0-0)

Kinetics of Gas-solid reaction; LH and LR Mechanism, Adsorption and adsorption isotherm; Physisorption and Chemisorption of gas molecules to the solid surface; determination of particle size from chemisorptions measurement, TPR/TPD/TPO techniques; elementary gas phase reaction, spillover effect, multiplet theory brief overview of catalytic reactor, fixed bed and batch reactor, mass transfer and heat transfer on the catalyst surface; promotional and poisoning effect on catalyst surface; selected organic reaction e,g selective oxidation, hydrogenation, dehydrogenation, dehydration, alkylation, aromatization etc. and their mechanism in gas phase, energy related catalysis, petroleum refining, hydrotreating, methane decomposition, steam reforming, cracking and isomerization reaction; Fischer-Troph synthesis; bio-fuel.
Nanomaterials, surface energy, nucleation and growth mechanism, sol-gel synthesis, mesoporous material, Organic-inorganic hybrid material, thin film, PVD, CVD, Molecular beam epitaxy techniques, Langmuir-blodget thin film, self-assembled monolayer.

References:

1. The Surface Science of Metal Oxides, Victor E. Henrich, P. A. Cox, Cambridge University Press; New Ed edition, 1996.
2. Current Trends of Surface Science and Catalysis, Jeong Young (Ed.) Park (Author), Jeong Young Park(editor), 1st Edition, Springer, 2013.
3. Handbook of Heterogenous Catalysis, G. Ertl, H. Knozinger, F. Schuth, J. Weitkamp, WILEY-VCH Verlag GmbH & Co. KGaA, ISBN 978-3-527-31241-2
4. Nanotechnology in Catalysis, Spinger,; ISBN-0387-34687-2; Edited by G A Somorjai Vol-1-3
5. Nanostructures and Nanomaterials, Cao and Wang, 2nd Edition, World Scientific Publishing Company, 2011.

ACE 34151 Electro & Photo-Chemical Energy Systems (3-0-0)

Basic Principles of Electrochemical Engineering: Thermodynamics and kinetics of electrochemical systems, electrochemical analytical methods, fundamentals of typical electrochemical energy systems: batteries, fuel cells, solar system. Fuel Cells Technology and applications. Pourbaix diagram & its features. Mimic of NAD^+/NADH function through electrochemical method, electrochemical analogues of Water-gas shift reaction; Electrochemical, photochemical and chemical methods for: CO_2 Reduction, Proton Reduction and Water Splitting.

References:

1. Energy Production and Storage: Inorganic Chemical Strategies for a Warming World (Inorganic Chemical Strategies for a Warming World), edited by Robert H. Crabtree ISBN: 978-0-470-74986-9, Wiley Publications.
2. Molecular Water Oxidation Catalysis, edited by Antoni Llobet ISBN: 978-1-118-41337-1, Wiley Publications.
3. Electrochemical and Electrocatalytic Reactions of Carbon Dioxide; Edited by: B.P. Sullivan, K. Krist and H.E. Guard; ISBN: 978-0-444-88316-2.
4. Non-Conventional Energy Resources, B. H. Khan 2nd Edition, Tata McGraw Hill Education Private Limited, 2010.
5. Fuel Cell Technology, Nigel Sammes, Springer, 2006.

ACE 34152 Advanced Characterization Techniques (3-0-0)

Microscopic Techniques: SEM and TEM: Principle, Instrumentation, Specimen Preparation and Applications. Elemental Analysis with SEM and TEM.
STM, AFM, EPMA: principle, Instrumentation and applications.
Electron Energy Loss Spectroscopy (EELS), Auger Electron Spectroscopy (AES): Principle, Instrumentation and applications.

References:

1. Electron Energy-Loss Spectroscopy in the Electron Microscope, R. F. Egerton, 3rd Edition, Springer, 2011.
2. Scanning Probe Microscopy and Spectroscopy, R. Wiesendanger, Cambridge University Press, 1994.
3. Materials Characterization, Introduction to Microscopic and Spectroscopic Methods, Y Leng, 2nd Edition, Wiley, 2008.
4. Advanced Scanning Electron Microscopy and X-Ray Microanalysis, D. E. Newbury, D. C. Joy, P, Echlin, C. E. Fiori, J.I. Goldstein, Springer, 1986.
5. Atomic Force Microscopy, P. Eaton, P. West, Oxford University Press, 2013.

ACE 34153 X-Ray Crystallographic Techniques (3-0-0)

Reciprocal lattice concept, determination of space groups, Hermann-Mauguin Symbolism. X-ray diffraction Techniques: SCXRD: Ehwald's sphere, the phase problem, Structure factor, Patterson Fourier synthesis, Direct methods, Isomorphous replacement, Harkar-Kasper inequalities, refinement of crystal structures. R factor, Difference fourier maps. PXRD: Application of Powder XRD in identification of phase, phase analysis, determination of cell parameters, particle size, Reitveld refinement. Other X-ray based techniques.

References:

1. X-Ray Structure Determination: A Practical Guide, George H. Stout, Lyle H. Jensen, 2nd Edition, Wiley-Blackwell, 1989.
2. Crystal Structure Determination, Werner Massa, Robert O. Gould, 2nd Edition, Springer; 2004. Corr. 5th printing 2010 edition, 2010.
3. Introduction to macromolecular crystallography, Alexander McPhearson, Wiley-Liss, 2003.
4. Crystals and crystal structures, Richard Tilley, John Wiley & Sons, 2006.

ACE 34154 Nuclear & Radiation Chemistry (3-0-0)

Structure of Nucleus, Shell Model, liquid drop model, Collective model, optical model, merits and demerits. Radioactivity: Decay kinetics, α, β decay, γ emission, Parent –daughter decay – growth relationship, secular and transient equilibrium, Theory of α, β and γ decay, selection rules. Artificial radioactivity. Nuclear Reactions: Elastic, inelastic, Photonuclear, radiative capture, evaporation, spallation, Fragmentation, and Transfer reactions. Nuclear fission and fusion; Theory of Nuclear fission, fission energy and fission cross-section, Nuclear Reactors: Classification of reactors, reactor power, critical size, Breeder reactor. Application of radioactivity: Tracers in medicine, agriculture, chemical investigations; Analytical applications, Industry and in age determinations. Neutron Activation Analysis, advantages and applications. Radiation detectors: Wilson cloud chamber, Geiger-Muller counter, scintillation detectors, semiconductor detectors, thermionic detectors. Radiolysis of water, Dosimeters

References:

1. Essentials of Nuclear Chemistry H. J. Arnikar, 4th edition, New Age Publishers, 1995
2. Nuclear and Radiochemistry, G. Friedlander, J. W. Kennedy, E. S. Macias and J. M. Miller, John Wiley & Sons, 1985
3. Nuclear and Radiochemistry: Fundamentals and Applications, Karl H. Lieser, 2nd edition, 2001, Wiley, NY
4. Nuclear Physics, I. Kaplan, 2nd edition, Narosa Book Distributors Pvt. Ltd.

ACE 34155 Chemistry of Lanthanides and Actinides (3-0-0)

Introduction, Characteristics, Extraction, Lanthanide Contraction, energetics, binary compounds, coordination chemistry, General Principles, Coordination numbers in lanthanide and actinide complexes, electronic and magnetic properties, Electronic Spectra, Luminescence Spectra, organometallic chemistry, applications in organic synthesis. Transactinides.

References:

1. Lanthanide and Actinide Chemistry, Simon Cotton, Wiley & Sons Ltd, 2006.

2. Shriver & Atkins: Inorganic Chemistry, P.W. Atkins, T. Overton, J. Rourke, M. Weller and F. Armstrong; 5th Edition Oxford University Press, 2013.

ACE 34156 Heterocyclic Chemistry (3-0-0)

Synthesis and reactions of heteroaromatics containing one hetero atom. General approaches to heterocycle synthesis – cyclisation and cycloaddition routes. Synthesis, reactions and their mechanisms of aziridine, azetidine; pyrazines and their analogues; oxazole, thiazole, imidazole, iso-oxazole, isothiazole and corresponding fused systems; pteridines, folic acid. Nomenclature of bicyclic and tricyclic fused system. Synthesis of uracol, thymine and cytosine. Synthesis of adenine and guanine. Synthesis of uric acid, caffeine, pyrazine, synthesis of furanones, tetrazole.

References:

1. I .L. Finar, Organic Chemistry, Vol.II, 5th Edition, ELBS, 1975.
2. Heterocyclic Chemistry J. A. Joule and K. Mills, 5th Edition, Wiley-Blackwell publishing, 2010.
3. Heterocyclic Chemistry T. Gilchrist 3rd edition, Prentice Hall, 1997.
4. Modern Heterocyclic Chemistry, Julio Alvarez-Builla, Juan Jose Vaquero, José Barluenga, Wiley-VCH, 2011.

ACE 34157 Polymer Chemistry ` (3-0-0)

Introduction and common applications of polymers. Classification of polymers. Kinetics and mechanism of chain growth and step growth polymerisation. Polymerisation processes (Bulk, Solution, Emulsion and Suspension). Molecular weight, molecular weight distribution and degree of polymerization. Experimental methods for determination of molecular weight. Glass transition temperature: significance and determination. Copolymers: Classification, synthesis and application. Synthesis and applications of biodegradable, biomedical polymers. Conducting Polymers. Inorganic Polymers. Polymer synthesis procedures – ATRP, ROMP, MP, ROP. Commercial thermoplastic and thermosetting polymers- Synthesis, properties and applications. Spectral and Instrumental analysis of Polymers (IR, UV, NMR, XRD, DSC, TGA, POM). Advanced Polymers: Shape Memory Polymers, Self-Healing Polymers, LCP. Branched polymers (star, dendritic and hyper branched polymers).

References:

1. Principles of polymerization, George G. Odian, 4th Edition, A John Wiley & Sons, Inc., Publication, 2004.
2. Textbook of Polymer Science, W. F. Billmeyer, 3rd Edition, A John Wiley & Sons, Inc., Publication, 2007.
3. The Chemistry of Polymers, John W. Nicholson, 3rd Edition, RSC Publishing, 2006.
4. Polymer Chemistry: Properties and Application. A.J Peacock, A. Calhoun. Hanser Gardner Publications, 2006.
5. Polymer Science & Technology – Plastics, Rubbers, Blends and Composites. Premamoy Ghosh. 3rd Edition, McGraw Hill Education (India) Private Limited, 2010.

ACE 34158 Chemistry of Natural Products (3-0-0)

Structural types; Biogenesis; Structure Elucidation and chemistry of representative examples of the following classes of natural products.
Alkaloids, Terpenoids, Steroids, Prostaglandins and Marine natural products

References:

1. Organic Chemistry: Stereochemistry and the chemistry of Natural Products, I.L. Finar, 5th Edition, Vol.II, ELBS, 1975.
2. The Chemistry of Terpenes, A.R. Pinder, 1st Edition, Chapman and Hall, 1960.
3. Organic Chemistry, S. H. Pine, J.B. Hendrickson, D. J. Cram and G. S. Hammond, 4th Edition. McGraw-Hill Company, 1980.
4. The Alkaloids-chemistry and Physiology, R.H.F. Maniske and H.L. Holmass, 1st Edition, Academic Press Inc., 1950.
5. An Introduction to the Chemistry of the Terpenoids and Steroids, W.Templeton, Butterworth, Butterworth & Co Publishers Ltd 1970.

ACE 34159 Medicinal Chemistry (3-0-0)

Drugs and drug targets – introduction. Proteins, Enzymes, receptors and nucleic acids as drug targets.

Pharmacodynamics and pharmacokinetics

Drugs: Classification of drugs, Drugs based on enzyme inhibition: Sulfa drugs, penicillin antibiotics and fluorouracil (Mechanism of drug action). Drug targets on nucleic acids (Alkylating agents and intercalating agents). Drugs based on receptors, Definition of antagonist, agonist, prodrugs, pharmacokinetics and pharmacodynamics, concept of structure-activity relationship (SAR) and quantitative structure and relationship (QSAR).

Drug discovery- target selection, finding leads, identification of pharmacophore, structure optimization, optimizing target access. Preclinical and clinical trials, patenting and regulatory affairs.

Classification of drugs: Based on structure or pharmacological basis with examples. Mode of action and synthesis of Antibacterials, Antivirals, Anticancer agents, cholinergics, anticholinergics and anticholineserases, adrenergic drugs, opioid drugs and antiulcer agents. Synthesis of a few drugs.

References:

1. Medicinal Chemistry-An Introduction, Gareth Thomas, 2nd edition, 2007, Wiley, NY.
2. An introduction to medicinal Chemistry, Graham L. Patrick, 4th Edition, Oxford, 2009
3. Strategies for Organic Drug Synthesis and Design, Daniel Lednicer, 2 Edition, Wiley, 2008.
4. Medicinal Chemistry, Ashutosh Kar, 1st edition, New Age International, 2007.
5. Medicinal Chemistry, Sriram and Yogeeswari, 2nd edition, Pearson education, 2007.

ACE 34160 Carbohydrate Chemistry (3-0-0)

Monosaccharides, synthetic aspects of rare sugars and Deoxysugars, aminosugars, glycalsugars protecting group strategies, glycosylation, glycosyl donors and acceptors, stereoselective glycosylation, glycosylation strategies – one pot glycosylation, iterative glycosylation. Structure, relevance and synthesis of some important carbohydrates such as GAGs.

References:

1. Carbohydrates- the sweet molecules of life R. V Stick, Academic press, 2001.
2. Essentials of Carbohydrate Chemistry and Biochemistry, T. K. Lindhorst, Wiley VCH, 2000.

ACE 34161 Asymmetric Synthesis (3-0-0)

Introduction – Scope of the study
Chiral induction – Diastereoselective synthesis:
Chiral Pool approach – Diastereoselective Synthesis:
"Chirons"– terpenes and carbohydrates as chiral source material – Steven‟s steroid intermediate synthesis – alkaloid synthesis – limitations
Chiral auxiliary – Diastereoselective synthesis:
Basic requirements of a chiral auxiliary – "chiral pool" sources – popular and generally adaptable chiral auxiliaries (Oppolzer, Evans, Enders, Davies, 8-phenyl-menthol, BINOL, etc.) – kinetic resolution by chiral auxiliary – boronic ester mediated homologation – disadvantages of "auxiliary" approach:
Asymmetric hydroboration; Asymmetric aldol condensation and Alkylations reducing agents like boron/aluminium hydrides – allylation and crotylation – oxazaborilidines – TADDOL – chiral lithium amides – chiral Lewis acids in enolate reactions, cycloadditions and sigmatropic rearrangements – enantioselective deprotonation and protonation – "chiral cavity" for enentioselection
Asymmetric catalysis; Asymmetric organocatalysis; enzymatic catalysis

References:

1. Principles of Asymmetric Synthesis – R. E. Gawley and J. Aub, Pergamon, 1996.
2. Catalytic Asymmetric Synthesis, I. Ojima(ed.), 3rd Edition, Wiley, 2010.
3. Asymmetric Catalysis in Organic Synthesis, R. Noyori, Wiley, 1994.
4. Asymmetric Synthesis, vol 1-5, H. S. Mosher and J. D. Morrison (ed.), Academic Press.
5. Asymmetric Synthesis: The Essentials -, M. Christmann and S. Bräse (ed.), Wiley-VCH, 2007.
6. Asymmetric Synthesis with Chemical and Biological Methods, D. Enders and K. E. Jaeger, Wiley-VCH, 2007.
7. Comprehensive Asymmetric Catalysis, I-III, E. N. Jacobsen, A. Pfaltz and H. Yamamoto, Springer, 1999.

ACE 34162 Supramolecular Chemistry (3-0-0)

Introduction to supramolecular chemistry (concepts and definitions), non-covalent forces and interactions in supramolecules, macrocycles and supramolecules (crown ethers, cryptates, cryptands, carcerands, calixarenes, cyclodextrins, fullerenes, dendrimers, rotaxanes, cucurbiturils, porphyrins), self-assembly and preorganization, coordination driven self-assembly of supramolecular two and three dimensional architectures, host-guest chemistry, molecular devices and functional supramolecular structures – molecular wires, sensors, switches and logic gate devices, metal-organic frameworks and their applications, nucleobases as supramolecular motifs.

References:

1. Core Concepts in Supramolecular Chemistry and Nanochemistry, J. W. Steed, D. R. Turner, K. Wallace, 1st Edition, Wiley, 2007.
2. Supramolecular Chemistry: Concepts and Perspectives, J. M. Lehn, 1st Edition, VCH, 1995.
3. H. Dodziuk, Introduction to Supramolecular Chemistry, 1st Edition, Springer, 2001.
4. Supramolecular Chemistry: Fundamentals and Applications, Katsuhiko, 1st Edition Springer, 2006.

ACE 34163 Green Chemistry (3-0-0)

Introduction, Principles & Concepts of Green Chemistry. Waste: Production, Problems, Prevention. Catalysis and Green Chemistry: Oxidations and Reductions, C-C Bond Formation, Organometallic Chemistry & Catalysis Organic Solvents: Environmentally Benign Solutions (Focus on water, ionic liquid, fluorous solvents and super critical CO_2).
Design for energy efficiency Renewable Resources: Chemicals from Biomass, Utilization of CO_2 and other feed stocks. Focus on the application of innovative technology the development of greener" routes to improve industrial processes and to produce important products.

References:

1. Green Chemistry: Theory and Practice, Anastas, P. T.; Warner, J. C. Oxford University Press: New York, 1998.
2. Renewables-Based Technology: Sustainability Assessment; Dewulf, J.; Langenhove, H. V., Eds.; John Wiley & Sons, Ltd, 2006.
3. Green Chemistry and Engineering, Doble, M.; Kruthiventi, A. K.; Elsevier, 2007.
4. Handbook of Green Chemistry and Technology, James Clark and Duncan Macquarrie, Blackwell Science, 2002.
5. The Chemistry of Waste Minimization, J.H. Clark, Blackie Academic, 1995.
6. Multi Component Reactions Jeiping Zhu and Hugues Bienayme (Ed.), Wiley VCH Velag GmbH & Co., 2005.
7. Green Chemistry: Environmentally Benign Reactions; Ahluwalia, V. K., CRC Press: Boca Raton, FL, 2008.