

INDIAN INSTITUTE OF TECHNOLOGY ROORKEE**NAME OF DEPARTMENT/ CENTRE:** Department of Chemistry**Subject Code:** CYC-202**Course Title:** Coordination and Organometallic Chemistry**L-T-P:** 3-0-2**Credits:** 4**Subject Area:** PCC

Course Outlines: Theory: Introduction to Coordination chemistry with special emphasis on denticity of ligands and stability of coordination compounds, types of isomerism, nomenclature of coordination complexes; effect of crystal field theory for complexes of different geometries, application of this theory; organometallic chemistry, metal carbonyl and nitrosyl complexes, metal-alkyls, -aryls and -carbenes; important reaction mechanism of organometallic compounds in the catalytic applications such as hydrogenation, hydroformylation, Zeigler–Natta catalysis, olefin metathesis, carbonylation and decarbonylation; concept of hapticity, transition metal complexes of alkenes, Zeise's salt, allenes, alkynes, allyls, cyclic π - metal complexes, reaction and bonding in ferrocene.

INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

NAME OF DEPARTMENT/ CENTRE: Department of Chemistry

Subject Code: CYC-203

Course Title: Main Group and Cluster Chemistry

L-T-P: 3-0-0

Credits: 3

Subject Area: PCC

Course Outlines: *s* and *p* block elements; spectroscopic properties of alkali metals; chemical reactivities with water, air, acid and base; complexes such as oxides, hydroxides, peroxides, sulphates, sulfides, halides, hydrides and carbides containing *s* block elements, oxo salts, biological importance; complexes, clusters and their chemical properties containing *p* block elements within the same group; silicates and their applications, silicones, organosilicon compounds and polymers, structure and bonding of organosilicon compounds, silanes and polysilanes, low-oxidation state compounds of *p* block elements such as borylene, diborene, diboryne, nitrenes, phosphinidene, phosphazenes, cyclophosphazenes; nitrogen fixation, urea, phosphate fertilizers; properties of halides, halogen oxides, oxoacids of halogen, interhalogen compounds, polyhalides, pseudohalogens, pseudohalides; organometallics of *s* and *p* block elements.

INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

NAME OF DEPARTMENT/ CENTRE: Department of Chemistry

Subject Code: CYC-205

Course Title: Organic Chemistry-II

L-T-P: 3-0-2

Credits: 04

Subject Area: PCC

Course Outlines: Alkanes, Synthesis of alkanes, Wurtz reaction, Corey-House synthesis, Ring strain, Baeyer's strain theory, Banana bonds, Alkenes and Alkynes, Methods of synthesis, Reactivity, Electrophilic and nucleophilic addition, Oxidation (epoxidation, dihydroxylation, ozonolysis, hydroboration-oxidation, regioselectivity and stereoselectivity), Oxymercuration reduction, 1,2 *vs* 1,4-addition, Oligomerization, and polymerization reactions, Arenes and aromaticity, Birch reduction, Nucleophilic substitution reaction, Addition-elimination mechanism, S_N1 and benzyne mechanisms, S_N1 *vs* S_N2, Elimination reactions, E1 and E2 mechanisms, Stereoselectivity and regioselectivity in elimination, E1cB mechanism, Gilman reagents, S_N2' reactions and their stereochemistry.

INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

NAME OF DEPARTMENT/ CENTRE: Department of Chemistry

Subject Code: CYC-206

Course Title: Organic Chemistry-III

L-T-P: 3-0-0

Credits: 3

Subject Area: PCC

Course Outlines: Pericyclic Reactions, Diels-Alder reaction, Thermal cycloaddition reactions, 1,3-dipolar cycloadditions, Ene reaction, Sigmatropic rearrangement, [3,3]-sigmatropic rearrangement, [2,3]- and [1,5]-sigmatropic rearrangements, Electrocyclic reactions, Cope and aza-Cope rearrangements, Thermodynamic and kinetic requirements, Rate and equilibrium constants, Reaction coordinate diagram, Transition state (activated complex), Hammond postulate, Reactivity vs selectivity principle, Curtin-Hammett principle, Kinetic vs thermodynamic control, Isotope effects, Cannizzaro reaction, Ritter reaction and Beckmann fragmentation, Crossover experiments, Disconnection approach, Synthons and synthetic equivalents, functional group interconversions, Chemoselectivity, Reversal of polarity (umpolung), Cyclisation reactions, and Amine synthesis.

INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

NAME OF DEPARTMENT/ CENTRE: Department of Chemistry

Subject Code: CYC-301

Course Title: Advanced Coordination Chemistry

L-T-P: 3-0-0

Credits: 3

Subject Area: PCC

Course Outlines: Stereoisomerism chirality, nomenclature and measurement of chirality in inorganic complexes; application of group theory for construction of ligand group orbitals, molecular orbital energy diagrams of octahedral, tetrahedral, square planar complexes including both σ - and π -bonding; calculation of d orbital energies in the complexes; interpretation of electronic spectra of coordination complexes using the concepts of Orgel and Tanabe-Sugano diagrams of octahedral and tetrahedral d^n complexes, ligand field parameters; effect of triplet state stability in phosphorescent complexes; origin of magnetism other than unpaired electron spin, molecular magnetism - diamagnetic and paramagnetic behavior of transition metal complexes, spin-orbit coupling effects, orbital angular momentum, spin crossover phenomenon, spin admixed states, ferromagnetic, anti-ferromagnetic behavior of transition metal compounds, single molecular magnets; inorganic photochemistry, types of photochemical reactions of coordination compounds—substitution, decomposition, fragmentation, rearrangement and redox reactions; unimolecular charge-transfer Co(III) photochemistry, Cr(III) ligand-field photochemistry and few specific models of inorganic photochemistry.

INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

NAME OF DEPARTMENT/ CENTRE: Department of Chemistry

Subject Code: CYL-302

Course Title: Bioinorganic and Biomimetic Chemistry

L-T-P: 3-0-0

Credits: 3

Subject Area: PEC

Course Outlines: Origin of elements in biological systems, importance of essential and trace metal ions, classification of enzymes, contributing factors for the catalytic efficiency of enzymes, importance of alkali and alkaline earth metal ions in biological systems, importance of heme and non-heme proteins, synthetic models, beneficial and toxic effects of metal ions, examples for the biomimetic studies of the tetrapyrroles.

INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

NAME OF DEPARTMENT/ CENTRE: Department of Chemistry

Subject Code: CYL-520

Course Title: Inorganic Rings and Polymers

L-T-P: 3-0-0

Credits: 3

Subject Area: PEC

Course Outlines: Synthesis and applications of Inorganic heterocyclic rings based on P, N, Si, Sn, B, Al and S, e.g., cyclophosphazenes, carbophosphazenes, metallophosphazenes, cyclosiloxanes, stannoxanes, boranes, carboranes, metallacarboranes, borazines, alumoxanes, etc. Al-N rings and cages, Al-C rings and cages. Inorganic polymers based on homo and heterocatenated inorganic polymers. Anionic and cationic polymerization methods. Synthesis, structure, bonding, unique optical and electronic properties and applications of polyphosphazenes, polysilanes, polysiloxanes, polythiophenes, polythiazyls. Unique electronic and optical properties and its applications of polysilanes. Introduction to organometallic polymers: Ferrocenophanes, synthesis of poly(ferrocenylsilane) and their applications, synthesis, applications and electronic properties of polygermanes and polystannanes, polyynes Rigid-rod Organometallic Polymers.

INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

NAME OF DEPARTMENT/ CENTRE: Department of Chemistry

Subject Code: CYL-524

Course Title: Modern Organic Synthetic Methods

L-T-P: 3-0-0

Credits: 03

Subject Area: PEC

Course Outlines: Oxidation reactions, Oxidation of hydrocarbons (alkanes, alkenes and aromatic), Sharpless asymmetric epoxidation, Jacobsen epoxidation, Shi epoxidation, alkenes to diols (Manganese, Osmium based), Hydroboration-oxidation, Wacker oxidation, Baeyer-Villiger reactions, Baylis-Hillman reaction, Henry reaction, Nef reaction, Kulinkovich reaction, Ritter reaction, Sakurai reaction, Tishchenko reaction, Ugi reaction, Brook rearrangement and Tebbe olefination, Protection and deprotection of functional groups, and Retrosynthetic analysis.

INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

NAME OF DEPARTMENT/ CENTRE: Department of Chemistry

Subject Code: CYL-606

Course Title: Total Synthesis

L-T-P: 3-0-0

Credits:03

Subject Area: PEC

Course Outlines: Introduction to strategies for synthesis of complex molecular architectures, Synthesis of antibiotics penicillin V and tetracycline, Synthesis of alkaloids-reserpine and camptothecin. Synthesis of terpenoids- β -pinene, camphor, Abietic acid and β -amirine, Synthesis of steroids and hormones - cholesterol, progesterone and cortisone, Synthesis of prostaglandins PGFa and PGF2 α ; Glycosidic pigments anthocyanins and quercetin, Macrocyclic lactam fluvirucin-B1-aglycone, and Vitamin biotin.

INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

NAME OF DEPARTMENT/ CENTRE: Department of Chemistry

Subject Code: CYL-613

Course Title: Frontiers in Inorganic Biochemistry

L-T-P: 3-0-0

Credits: 3

Subject Area: PEC

Course Outlines: Homeostatic mechanism of metal ions in cells; prokaryotes to humans; metal transport and assembly of metalloproteins; role of metallochaperones, transcription factors, and heme synthesis in protein assembly; biocatalysis and electron transfer; molybdenum and tungsten in biology; iron in biosystems, non-heme iron proteins in cancer research, biocatalysis and industry applications; metal ions and diseases; protein aggregation and Alzheimer's disease; radiochemistry; manganese; inorganic NO-donors; bioinformatics and postgenomic era; metalloprotein and metal binding motif; , de novo protein design, and DNA intercalation and electron transfer; biomineralization in bone, teeth, and mollusk cells; NMR structural biology; metalloproteins; gene expression and protein purification; heme protein–cytochrome c vs cytochrome b; ^{15}N and ^{13}C protein labelling.

INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

NAME OF DEPARTMENT/ CENTRE: Department of Chemistry

Subject Code: CYL-615

Course Title: Crystal and Molecular Structure

L-T-P: 2-0-2

Credits: 3

Subject Area: PEC

Course Outlines: Theory: Crystal morphology and crystal symmetry, screw axis and glide plane, space groups, systematic absence; X-ray source, generation of monochromatic wavelength, Bragg equation, concept of reciprocal lattice, Bragg's law in reciprocal lattice, atomic scattering factor, structure factor equation and limiting conditions, intensity and intensity statistics, polarization and Lorentz correction, temperature factor and anisotropic effect, phase problem, small angle X-ray scattering/diffraction; Fourier techniques for electron density calculation in X-ray structure, electron density map, heavy atom method, Patterson function, direct method, normalized structure factor, Σ_2 relationship, least square refinement, anomalous dispersion, twinning in crystal, neutron diffraction, neutron sources and detection of neutrons, scattering cross sections.

INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

NAME OF DEPARTMENT/ CENTRE: Department of Chemistry

Subject Code: CYL-621

Course Title: Organic Structure Determination

L-T-P: 3-0-0

Credits:03

Subject Area: PEC

Course Outlines: Electronic spectroscopy, Electronic transitions in organic molecules, Woodward-Fieser rules, Infrared and Raman spectroscopy for simple organic molecules, Mass spectrometry, Basic principles, mass analyzer in ESI-MS and MALDI-MS, high-resolution MS, isotope abundance, molecular ion, fragmentation processes (McL) of organic molecules, and deduction of structure through mass spectral fragmentation, Nuclear magnetic resonance, chemical shift δ , spin-spin coupling, structural correlation to coupling constant J, first order and second order spectra, ^{13}C NMR, NOE effects, and Multinuclear NMR.

INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

NAME OF DEPARTMENT/ CENTRE: Department of Chemistry

Subject Code: CYL-625

Course Title: Proteins and Polypeptides

L-T-P: 3-0-0

Credits:03

Subject Area: PEC

Course Outlines: Proteins and peptides, Separation and purification methods, Electrophoresis, isoelectric focusing, gel filtration, affinity chromatography, Fragmentation of polypeptides, partial acid hydrolysis, Enzymic methods and protein modification reactions disulfide bond cleavage, modification of lysine and arginine residues, Specificity and conditions for trypsin, thrombin, chymotrypsin, thermolysin, pepsin papaine, Determination of peptide sequences, C-terminal sequence analysis, Applications of electron impact mass spectrometry, X-ray crystallography and electron microscopy.

INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

NAME OF DEPARTMENT/ CENTRE: Department of Chemistry

Subject Code: CYL-644

Course Title: High Energy Density Materials

L-T-P: 3-0-0

Credits: 3

Subject Area: PEC

Course Outlines: Historical overview, classification, properties, design and evaluation of high energy density materials. Military and civilian applications of high energy density materials; chemical safety of energetic materials. Classification, characterization and properties of explosives, synthetic routes to polynitro compounds. Chemistry of pentazole, energetic tetrazines and azoles based energetic compounds. Heat-resistant explosives, insensitive explosives, melt-cast explosives; energetic metal-organic frameworks (EMOFs) and energetic co-crystals; laser ignition of energetic transition metal complexes; nitrogen-rich energetic polymers and plasticizers. Classifications of propellants, liquid, solid, hybrid and thixotropic propellants. Ingredients of gun and solid rocket propellants: oxidizers, binders, metal fuels, plasticizers; hypergolic ionic liquids as green rocket propellants. General features of pyrotechnics; ingredients of pyrotechnic formulations and their important characteristics; types of pyrotechnic formulations; performance assessment of pyrotechnic formulations; recent trends in pyrotechnics.

INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

NAME OF DEPARTMENT/ CENTRE: Department of Chemistry

Subject Code: CYL-648

Course Title: Synthesis and Applications of Tetrapyrroles

L-T-P: 3-0-0

Credits: 3

Subject Area: PEC

Course Outlines: The pigments of life and their biological importance, IUPAC nomenclature, various synthetic routes to porphyrins and their analogues, synthesis of porphyrin dimers and oligomers, metal-organic and covalent-organic frameworks, spectral characterization, applications of porphyrinic materials in the diverse arena.

INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

NAME OF DEPARTMENT/ CENTRE: Department of Chemistry

Subject Code: CYL-608

Course Title: Chemical Biology

L-T-P: 3-0-0

Credits: 3

Subject Area: DHC

Course Outlines: Introduction to chemical biology, biological structures and its chemical constituents, spectroscopic tools to rationalize chemical reactions in biosystems, design of fluorescent and fluorogenic probes and optical biosensor molecules; solid phase peptide synthesis, bioorthogonal reactions, functional group specific ligation techniques, strategies for attachment of synthetic molecules to biomolecules, Staudinger ligation, native chemical ligation, click chemistry, site selective protein modification; Green fluorescence protein (GFP), fluorescein arsenical hairpin (FIAsH), SNAP tag, CLIP tag, mutant β -lactamase (BL) tag, halo tag, and their selective significant applications; synthetic membranes, vesicles – ion transport, unnatural amino acids and their incorporation, DNA chemistry and its uses, nucleic acid templated chemistry, chemistry of morpholino and locked nucleic acid (LNA), siRNA.

INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

NAME OF DEPARTMENT/ CENTRE: Department of Chemistry

Subject Code: CYL-902

Course Title: Advanced Inorganic Chemistry

L-T-P: 3-0-0

Credits: 3

Subject Area: DHC

Course Outlines: Symmetry and associated group theory, introduction to term symbols, spectroscopic term symbols for free ions and metal ions in complexes having different geometries, irreducible representations and their use in interpretation of IR and Raman transitions, advanced organometallic catalysis, water splitting reactions, mechanism, ammonia activation, oxygen atom transfer reactions, ligand design, catalyst design, multimetallic catalysis, latest trends in bioinorganic research, oxygen carrier, anticancer drugs based on platinum and their mode of activity, superoxide dismutases, active site structure, function and mechanism, dioxygen activation by iron and copper enzymes and biomimics.

INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

NAME OF DEPARTMENT/ CENTRE: Department of Chemistry

Subject Code: CYL-905 **Course Title:** Spectroscopic Methods of Structural Elucidation

L-T-P: 3-1-0

Credits: 4

Subject Area: DHC

Course Outlines: Instrumentation and principles of absorption and emission spectroscopy. Electronic transitions in inorganic complexes such as *d-d* transitions, charge transfer transitions. Fluorescence and phosphorescence emissions of metal complexes, delayed fluorescence, fluorescence quantum yield, lifetime, stokes shift, solvatochromism, photochromism, photocatalysis and photodynamic therapy. Instrumentation, principles, and interpretation of spectral data for various spectroscopic techniques such as IR, Raman, NMR including heteronuclei, solid state and paramagnetic NMR, GC, ESI-MS, HR-MS, MALDI-MS and EPR. Determination of isotopic abundance, isotopic distribution pattern, molecular ion, fragmentation processes of organic and inorganic molecules using mass spectrometry. Combinational spectral techniques for the structural elucidation of organic molecules and metal complexes.

INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

NAME OF DEPARTMENT/ CENTRE: Department of Chemistry

Subject Code: CYT-107

Course Title: Drug Design and Synthesis-I

L-T-P: 1-0-4

Credits:03

Subject Area: TEB

Course Outlines: Introduction to medicinal chemistry, classification of drugs, mode of action of drugs, concept of enzymes and receptors, Quantitative structure-activity relationships (QSAR) and computer-assisted drug design (CADD), Basics of spectroscopic elucidation of organic compounds, and application of IR and ^1H NMR spectroscopy in determining the structure of organic compounds.

INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

NAME OF DEPARTMENT/ CENTRE: Department of Chemistry

Subject Code: CYT-108

Course Title: Drug Design and Synthesis-II

L-T-P: 0-0-6

Credits:03

Subject Area: TEB

Course Outlines: Synthesis of paracetamol, Synthesis of diclofenac sodium salt (two-steps), Synthesis of metronidazole (two-step), Synthesis of phenytoin (two-step), Isolation of theobromine from cocoa powder, Synthesis of benzocaine (two-step), Synthesis of Lidocaine (two-step), Synthesis of flavone (three-step synthesis), Methylation of theobromine to caffeine, Isolation of piperine from black pepper, Estimation partition coefficient for iodine between CCl_4 and water

INDIAN INSTITUTE OF TECHNOLOGY ROORKEE**NAME OF DEPARTMENT/ CENTRE:** Department of Chemistry**Subject Code:** CYC-302**Course Title:** Organic Laboratory**L-T-P:** 0-0-8**Credits:** 4**Subject Area:** PCC

Course Outlines: Identification of organic mixtures by TLC, Preparation of p-nitroaniline from acetanilide, Diels-Alder reaction between anthracene and maleic anhydride, Preparation and uses of pyridinium dichromate, Conversion of benzil to quinoxaline, Cannizzaro reaction of p-nitrobenzaldehyde, Reduction of camphor, Synthesis of 2-iodobenzoic acid, Soxhlet extraction, Synthesis of ω -nitrostyrene, Aldol condensation, Preparation of cis- and trans-stilbenes, Synthesis of a chalcone, Bromination of acetanilide, Synthesis of phenyl acetylene, Preparation of meso-stilbene dibromide and diphenylacetylene, Fisher indole synthesis, Mechanochemical synthesis of 2,2'-dinitrobiphenyl via Ullman coupling, Preparation of 4-bromoacetanilide, Dieckmann condensation, Knoevenagel and Michael Reaction in PEG-400, Microwave synthesis of trans-cinnamic acid, Preparation of ionic liquid from N-methylimidazole.

INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

NAME OF DEPARTMENT/ CENTRE: Department of Chemistry

Subject Code: CYC-305

Course Title: Inorganic Laboratory

L-T-P: 0-0-8

Credits: 4

Subject Area: PCC

Course Outlines: Semi-micro qualitative analysis with interfering radicals; combination of volumetric and gravimetric analysis; syntheses and characterization such as electronic transition in metal complexes; estimation of metal content in the synthesized complexes to check the purity; comparison of the electronic spectra of metal complexes, verification of the spectrochemical series; use of Lambert-Beer's law, quantitative estimation of metal ion; estimation of stability constant from Job's plot and continuous ligand variation method; photochemical reaction of inorganic complexes; synthesis of chiral inorganic complexes and inorganic polymer; estimation of metal ion in ore; identification of linkage and geometrical isomerism; basic electrochemical studies.

INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

NAME OF DEPARTMENT/ CENTRE: Department of Chemistry

Subject Code: CYL-308

Course Title: Chemistry of Industrial Processes

L-T-P: 3-0-0

Credits: 3

Subject Area: PEC

Course Outlines: Industrial Processes in petroleum industries, shale gas, naphtha versus gaseous feed stocks, heavier oil fractions, steam cracking and petroleum refining reactions, oligomerization, alkylation, hydrotreating and coking, dehydrogenation, isomerization, metathesis, chemicals and polymers from ethylene, propylene, C4 and C5 stream, Homogeneous and heterogeneous catalysts, catalysis by acids, bases, metals and metal oxides, dual function catalysis, catalysis by semiconductors, and insulators, enzyme, shape-selective catalysts, phase-transfer and fluorobiphase catalysis, nanocatalysis, photocatalysts, green chemical methods, asymmetric hydrogenations, isomerization reactions, synthetic route to menthol, carbonylations, water-gas shift reaction, hydroformylation, Fischer-Tropsch reaction, carbon-carbon bond forming reactions, alkylations, activation of aryl and vinyl halides, metathesis of olefins, polymerization reactions, Phillips catalysts, Shell higher olefin process (SHOP), hydrocyanation, Ziegler-Natta, metallocene and Fenokishi-Imin catalysts.

INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

NAME OF DEPARTMENT/ CENTRE: Department of Chemistry

Subject Code: CYL-609

Course Title: Inorganic Biochemistry and Reaction Mechanism

L-T-P: 3-0-0

Credits: 3

Subject Area: PEC

Course Outlines: Substitution reactions in octahedral complexes, acid- and base-hydrolysis, annation, solvolytic and catalysed reactions. Substitution reactions in square-planar complexes, cis- and trans-effects, electron transfer reactions, solvated electron, inorganic photochemistry (Cr and Ru complexes), photochemical reactions in inorganic complexes, decomposition, fragmentation, rearrangement and redox reactions, charge transfer (CT) to mass (CTTM) photoreduction, applications of photochemical inorganic reactions, metalloproteins and enzymes, mechanistic studies of Mn-photosystem-II, catalase, pseudocatalase, oxygen carriers, haemoglobin, myoglobin, non-porphyrin oxygen carriers, hemerythrin, hemocyanin, Fe-ribonucleotide reductase, cytochrome c oxidases, cytochrome P-450s, Ni-urease, hydrogenase, nitrogen fixation, blue copper protein, tyrosinase, galactose oxidase, SOD, carbonic anhydrase, carboxypeptidase, alcohol dehydrogenase, Vitamin B₁₂ and coenzymes, Chemical toxicity and metallothrapy of arsenic, cadmium, lead, mercury, CO, cyanide, metal containing drugs in therapy, interaction of heavy metal ions with DNA, Organometallic drugs and enzyme inhibitors.

INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

NAME OF DEPARTMENT/ CENTRE: Department of Chemistry

Subject Code: CYL-612

Course Title: Carbon Nanomaterials and Their Applications

L-T-P: 3-0-0

Credits: 3

Subject Area: PEC

Course Outlines: Different synthetic approach such as arc discharge method, laser ablation method, chemical vapour deposition method, hydrothermal synthesis, high energy ball milling process etc of carbon anomaterials, nanodiamonds, fullerenes, single and multi-wall carbon nanotubes, carbon dots, carbon fibre and Peapods. Thermal, electrical and mechanical properties of carbon dots, Fullerene, Nanodiamond, Nanoonion, carbon fibre will be discussed. Carbon dots, nanotubes and graphene and fullerene for sensing applications in photodynamic therapy, environmental impact of carbon materials, toxicological effect on animals and living beings. Electronic and optoelectronic applications, photovoltaics application. Polymer and carbon nanotube composites for space applications like space elevator, solar sails.

INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

NAME OF DEPARTMENT/ CENTRE: Department of Chemistry

Subject Code: CYL-617

Course Title: Supramolecular Chemistry

L-T-P: 3-0-0

Credits: 3

Subject Area: PEC

Course Outlines: Types of non-covalent, concepts of host-guest complexation with examples from ionophore chemistry, complexation of ions, crown ethers, cryptands, calixarenes. Macrocyclic effect, complexation of neutral molecules, self-assembly. Synthesis of macrocycles, design and synthesis of receptors for cations, anions, and neutral molecules, supramolecular architecture—rotaxanes, catenanes. Spectroscopy in supramolecular chemistry, determination of stoichiometry, stability constants, and geometry of complexes, binding constant determination. Supramolecules in catalysis, as membrane transport, sensors, phase-transfer catalysts, supramolecular devices and switches, memories, logic gates and related systems, molecular machines (mechanical rotors, gears and brakes), conversion of light into fuels and light into electricity.

INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

NAME OF DEPARTMENT/CENTRE/SCHOOL: Department of Chemistry

Subject Code: CYC-201

Course Title: Thermodynamics and Electrochemistry

L-T-P: 3-0-0

Credits: 3

Subject Area: PCC

Course Outlines: Entropy and the Second Law of Thermodynamics, Carnot Engine and Efficiency, Gibbs-Helmholtz Equations, Thermodynamic Parameters from Free Energy Functions, Reversible and Irreversible Systems, Fugacity and Chemical Potential, Thermodynamic Treatment of Solutions, Phase Rule and Phase Diagrams, Statistical Thermodynamics, Surface and Interface Phenomena, Electrochemistry.

INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

NAME OF DEPARTMENT/CENTRE/SCHOOL: Department of Chemistry

Subject Code: CYC-207

Course Title: Quantum Chemistry and Chemical Bonding

L:T:P: 3-1-0

Credits: 4

Subject Area: PCC

Course Outlines: Wavefunctions and Operators, Particle in a box, Harmonic oscillator, Rigid rotor, Hydrogen like systems, Slater determinants, Many electron systems, Variation and perturbation methods, Hartree-Fock methods, Semi-empirical and *ab initio* methods, Bonding in H_2^+ and H_2 (Molecular and valence bond approach), Polyatomic molecules, Virial and Hellmann-Feynmann theorem, Hückel molecular orbital theory.