Course Details

General

All candidates in AcSIR Chemical Sciences Ph. D. programme should earn an aggregate of 20 credits (12 credits through course work, 4 credits for project proposal writing and 4 credits for activities related to CSIR 800). The different levels of courses offered are:

100 Level: Minimum 2 courses of total 4 credits

200 Level: Minimum 2 courses of total 4 credits

300 Level: Minimum 2 courses of total 4 credits

Part A – Compulsory Courses

Course description

100 Level Courses

A minimum of two courses of 4 credits in total. These courses will be on "Research Methodology and Communication" and "Analytical Methods and Instrumentation". These causes will be abbreviated as AcSIR-CS-501 and AcSIR- CS-502. These two courses are compulsory for all Chemical Science Ph. D. candidates.

AcSIR-NEIST-CS-101: Research Methodology and Communication (20-0-0-2)

Research Methodology

- Hypothesis: Literature survey, defining the question and formulating hypothesis/hypotheses.
- Methods: Generation of research data, tabulating and cataloging. sampling and methods of data analysis
- Record keeping and analysis: Interpreting results data and drawing conclusions
- Laboratory Safety Measures: Handling of radiation, bio-hazardous and other toxic experimental materials. Facilitation of scientific deliberations among students and faculty.

Communication

- Nature and importance of communication in Science. Preparation of manuscripts, review articles, research papers, books, monographs, research projects, review of manuscripts, Presentation of data, preparation of power point presentation, popularization of Science, Socio-Legal issues: Originality, Integrity, IPR, Patents, Plagiarism.

AcSIR-NEIST-CS-102: Analytical Methods and Instrumentation (15-5-0-2)

- Basic theory, instrumentation and analytical applications of the following physical methods: Spectroscopic techniques [NMR, ESR, MS (EI, FAB, MALDI-TOF), IR, UV-Vis, ICP, Fluorescence and Phosphorescence, Atomic Absorption, X-ray diffraction (single crystal, XRD)
- Chromatographic techniques**:** Introduction, classification of chromatographic methods, terms and relationships in chromatography, sample characterization.
- Hyphenated techniques: Principles and applications of: LC-MS, GC-MS, FTIR. Basic theory, instrumentation and analytical applications of the following physical methods: X-ray diffraction methods (powder method), Thermoanalytical methods (TGA, DSC, DTA), Microscopic methods (Polarized optical microscope, SEM, TEM, AFM), Surface Properties (XPS, BET), Mechanical Properties (DMA), rheological properties (viscometer, rheometer), electrical properties (conductivity, cyclic voltammetry).

PART B

200 LEVEL COURSES

A minimum of two courses of 4 credits in total. These courses may be on advanced topics in chemistry. For example: Advanced Organic Synthesis, Advanced Photochemistry, Advanced Polymer Synthesis, Advanced Quantum Mechanics, Advanced Coordination Chemistry etc. One course in this level should be compulsory to all and the other can be elective.

AcSIR-NEIST-CS-201: Frontiers in Chemical Sciences (20-0-0-2) (Compulsory)

- Introduction to the frontiers in chemical sciences, interface with chemistry, biology and medicine, materials and design, atmospheric and environmental chemistry, green chemistry, performance materials, nanomaterials, composite materials, ionic liquids, types of ionic liquids and their importance, electrochemical energy, energy storage.
- Emerging greener methodologies: Sonochemistry and green aspects; microwave in chemical synthesis: basic principles, advantages and examples; electrochemical synthesis: concepts and examples.
- Organic solvents: Environmentally benign solvents, solvent-free synthesis; water as a reaction solvent; ionic liquids.
- Phase transfer catalysis: Definition, mechanism, types of phase transfer catalysts, Synthesis and synthetic applications. Transition metal catalyzed organic reactions.
- Organocatalysis.

AcSIR-NEIST-CS-202: Stereochemistry (15-3-2-2) (Optional)

- Principles of stereochemistry: Configurational and conformational isomerism in acyclic and cyclic compounds, stereogenicity, stereoselectivity, enantioselectivity, diastereoselectivity and asymmetric induction, concept of absolute and relative configuration, EZ and RS system of nomenclature of stereoisomers, resolution of enatiomers, chirality in drugs.

AcSIR-NEIST-CS-203: Chemistry of Natural Products and Heterocyclic Compounds (14-2-4-2) (Optional)

- Extraction, isolation and characterization of natural products including different chromatographic methods. Chemistry of terpenes, steroids and alkaloids. Biogenesis of terpenoids, alkaloids and other type of secondary metabolites etc..
- Structure, reactivity and synthesis of common heterocyclic compounds containing one or more heteroatoms (O, N, S) starting from three to six membered heterocycles.

AcSIR-NEIST-CS-204: Reactive Intermediates, Reagents and Organic Transformations (17-3-0-2) (Optional)

- Generation, stability and reactivity of carbocations, carbanions, free radicals, carbenes, benzynes and nitrenes, ylides, enamines *etc*.
- Functional group interconversion including oxidations and reductions, common catalysts and reagents (organic, inorganic, organometallic and enzymatic). Chemo, and stereoselective transformations. Organotransition-metal reagents, General properties of lanthanides, use of lanthanide metal compounds at different oxidation states in synthesis, common oxidising agents such as PCC, PFC, swern oxidation, DCC, Desmartin-oxidation, Wacker oxidation *etc.* Hydride transfer reagents: Sodium borohydride, sodium cyanoborohydride, lithiumaluminium hydride, alkoxysubstituted LAH reducing agents, DIBAL, hydroboration (reduction, oxidation, carbonylation), Protection and deprotection of alcohol, carbonyl, carboxyl and amino groups.

AcSIR-NEIST-CS-205: Advance Coordination Chemistry (15-5-0-2) (Optional)

- The Valance Bond Theory(VBT), Crystal Field Theory(CFT), crystal field stabilization energy, Molecular Orbital Theory(MOT), sigma and pi bonding in tetrahedral and octahedral complexes.
- Bonding in Coordination Complexes: d-orbital splitting in octahedral, tetrahedral, square planar geometries; molecular orbital theory, Jahn-teller effect, spectrochemical series, nephelauxetic series, isomerism.

- Electronic Spectra: d-d transitions, Orgel and Tanabe-Sugano diagrams, charge-transfer spectra, Magnetism: Types, determination of magnetic susceptibility, Spin-only formula, Spin-orbit coupling, Spin-crossover, Russel-Saunders coupling, j-j coupling, selection rules for electronic spectra, electronic absorption spectra of spin paired complexes.

AcSIR-NEIST-CS-206: Structure and Bonding in solid (15-5-0-2) (Optional)

- Crystal structure of solids: Fundamental types of lattices, simple crystal structure, glasses, crystal diffraction by X-rays, neutrons and electrons, atomic form factor structure factor and integrated intensity, experimental diffraction methods, defects: band theory of solid, brilloin zones; metals: electrical, thermal and magnetic properties, semiconductors: intrinsic and extrinsic, junction properties, transistors, rectifiers, solar cells. Ferroelectric, piezoelectric and pyroelectric materials. Ferromagnetic and antiferromagnetic and ferrimagnetic materials and their properties. Crystal field effect and spinal structure of oxides
- Born-Oppenheimer approximation, MO and VB theories illustrated with H_2-molecule; Spectroscopic term symbols for diatomics, directed valence & hybridization in simple polyatomic molecules.

AcSIR-NEIST-CS-207: Petroleum Chemistry and Petrochemicals (15-5-0-2) (Optional)

- Petroleum Chemistry: Overview of oil and gas industry, introduction and origin of crude oil, crude oil and natural gas properties and evaluation ,composition and classification of crude oil, testing and evaluation of crude oil, pretreatment and distillation of crude oil, product from crude oil, chemical process in petroleum industry. rheological studies.
- Petrochemicals: Crude oil and natural gas as raw materials, petrochemical feed stocks from biomass resources, separation process for petrochemical feed stock, solvent extraction, catalysis in petroleum refining and their mechanisms.
- Chemical composition of crude oils and natural gas liquids, petroleum refining (cracking, hydrocracking, and catalytic reforming), catalysts for petrochemical processes (hydrogenation, isomerization, oxidation, hydroformylation, *etc.*), activation and catalytic transformation of hydrocarbons and other components of petroleum, natural gas, and other complex organic mixtures, new petrochemicals including lubricants and additives, environmental problems.

AcSIR-NEIST-CS-208: Oil Field Materials and Operations (18-2-0-2) (Optional)

- Oil well drilling, Clay based and oil based drilling fluids, clay structure and chemistry, Drilling Chemicals, Oil well cementing, formation of damage, Oil well simulation, Water injection, polymer flooding, Water shut off, EOR Chemicals, Fracturing Chemicals and Materials, Environmental aspects related to oil filed.

AcSIR-NEIST-CS-209: Transport Phenomena in Membrane Processes (15-5-0-2) (Optional)

- Different types of Membrane Processes: Principles and Application, Pervaporation, Dialysis, Electrodialysis, Reverse Osmosis, Ultrafiltration, Microfiltration, Nanofiltration and Emulsion Liquid Membrane: definition and Background, Theory and Design
- Navier Stokes Theory of Mass, Heat and Momentum Balances, Diffusion, Convection and Size Exclusion etc.
- Mathematical Modelling
- New Membrane Processes under Development: Membrane Based Solvent Extraction, Hollow Fibre, Membrane Reactors, Facilitated Transport
- Controlled release: Transport Principles, Diffusion in Polymers, Release Kinetics

AcSIR-NEIST-CS-210: Atomic Structure and Spectroscopy (15-5-0-2) (Optional)

- Approximate methods of quantum chemistry: Variational principle, LCAO approximation, Huckel theory, time-independent perturbation theory. Many electron atoms: Orbital approximation, Slater determinant; Hartree-Fock self-consistent field theory; Slater type orbitals. Angular momentum of many-particle systems. Spin orbital interaction, LS and JJ coupling. Spectroscopic term symbols for atoms. Molecules and chemical bonding: Born-Oppenheimer approximation, MO and VB theories illustrated with H_2-molecule; spectroscopic term symbols for diatomics, directed valence & hybridization in simple polyatomic molecules.
- Characterization of inorganic compounds : Electronic, IR and Raman spectroscopy, ^{1}H, ^{11}B, ^{19}F, ^{31}P NMR (including NMR of paramagnetic compounds), ESR (d^1 and d^9 only), Mossbauer and NQR spectral methods, photoelectron spectroscopy, fluoresence phenomenon.
- Spectroscopic techniques in organic chemistry: NMR- chemical shifts, factors influencing the chemical shift, spin-spin coupling, spin decoupling, shift reagent, NOE, ^{13}C, ^{15}N, ^{19}F and ^{31}P, COSY, NOESY, 2D NMR.

- General principles and utilization of mass spectrometry, fragmentation patterns of different organic compounds. Basic principles and utilization of GC, GC-MS, HPLC, LC-MS.

AcSIR-NEIST-CS-211: Frontier in Colloid and Interfacial Science (15-3-2-2) (Optional)

- Types of colloids: Lyophilic and lyophobic, different method of preparation: dialysis, electrophoresis etc., charge of colloid particles, electrokinetic properties of colloid particles, electrical double layer, Gouy Chapman model, DLVO (Derjaguin and Landau, Verwey and Overbeek) theory of colloid and interface, specific ion effect, Phase diagram,
- Surfactant system: micelles and vesicles, microemulsion: oil in water and water in oil, applications in drug delivery and cosmetics, microemulsion and vesicles: physicochemical properties and applications, microemulsion as a template for nanomaterials, concept of adsorption laboratory to practical day to day life, adsorption isotherm (solid/liquid and liquid/vapour): Langmuir, Freundlich, BET, Gibbs adsorption isotherm, adsorption kinetics: pseudo-first-order, pseudo-second-order (linear and non-linear method), intra-particle diffusion method, Surface tension, Surface free energy, Interfacial tension of solid-liquid, liquid-vapour, liquid-liquid, wettability of solid surfaces, So-gel chemistry, hydrogel formation, surface functionalization.

AcSIR-NEIST-CS-212: Advance Polymer Science (15-5-0-2) (Optional)

- Polymer reaction: Classification, addition polymerization, co-ordination polymerization, step polymerization, radical chain polymerization, chain polymerization kinetics, ionic polymerization, distinguishing between radical & ionic polymerization, group transfer polymerization, atom transfer radical polymerization, metathesis polymerization, ring opening polymerization, emulsion polymerization, chain copolymerization, green polymerization techniques.
- Copolymerization: Kinetics of co-polymerization equation-monomer reactivity ratios, types of behavior, random, alternating, and block co-polymers, integrated copolymerization equation, co-polymer microstructure, multi-component polymerisation, structural effects, Q-scheme.
- Molecular weight of polymers, molecular weight measurement end group analysis, viscometry, gel permeation chromatography, osmometry, light scattering, ultra centrifuge practical significance of molecular weight
- Classification of polymer – Mechanisms of polymerization - Some commercially important individual polymers – thermoplastics, elastomers, thermosets, engineering

plastics, liquid crystal polymers, conductive polymers, high performance fibers, miomedical applications, photonic polymers.

AcSIR-NEIST-CS-213: Clean Coal Chemistry (15-5-0-2) (Optional)

- Mining processes, mine safety, Sampling methods of coal and its importance, Coal classification systems and ASTM coal classification system, Physical characterization, proximate analysis, Ultimate analysis, Sulphur analysis, Ash fusion temperature, Low temperature Carbonization, Swell Index, Cacking Index, Thermo gravimetric analysis etc, Size Reduction and Size Classification of Coal, Structure of coal, Organic functionality of coal, aromatic Index, Mineral matter content, Mineralogy of coal. Geological origin of coal, petrographic analysis, geochemical processes during mining of coals, Coal Utilizationa (a) Coal Combustion Technology: Stoichiometry and Combustion Calculations, Properties of coal and combustion characteristics, Boiler designing (b) Coal Conversion processes: Introduction to coke making, coal to liquid conversion (c) Other useful product form coal, Environmental Issues: Acid Mine drainage, Emission Characterization, CO_2 Capturing, Management Plans

AcSIR-NEIST-CS-214 (3-2-15-2) (Compulsory)

- Project proposal Writing

PART C

300 LEVEL COURSES

A minimum of two courses of 4 credits in total. These courses may be in advanced topics in specified area of chemistry. For example, Reaction mechanism, Catalysis, Supramolecular chemistry, Drug design, Computational modeling etc. Candidates can choose courses of interests in consultation with the thesis supervisor and with the approval of the doctoral committee.

AcSIR-NEIST-CS-301: Drug Design and Discovery (16-4-0-2) (Optional)

- Definition of a drug molecule and factor affecting their biological activity, definition of chemotherapeutic index, therapeutic index, design of a drug molecule and relationship of functional groups, discovery of new drugs: drug discovery without a lead, lead discovery, random screen, non-random screen, concept of absorption, distribution, metabolism, and excretion (ADME), drug receptors, physicochemical properties, mechanism of a drug action, stereochemistry and drug action, synthetic and natural drugs and their mofications to increase oral bioavailability, chirality and drug action, bioisoterism, drug receptor-interactions, topographical and stereo-chemical considerations, concept of

drug resistance, drug synergism, enzyme inhibition and activation, molecular modeling and *insilico* drug design, concept of structure-activity relationship(SAR) and quantitative structure-activity relationship (QSAR), Lipinski rule of five, mechanism of action of some important drug molecules.

AcSIR-NEIST-CS-302: Green Chemistry (17-3-0-2) (Optional)

- Basic principles of green chemistry, designing green synthesis, green reagent, green catalysts, Phase transfer catalysis in green synthesis, microwave induced green synthesis, ultrasound assisted green synthesis, aqueous phase reactions, ionic liquid and water as green reaction media. Enzyme Mediated Reactions.

AcSIR-NEIST-CS-303: Medicinal Chemistry (16-4-0-2) (Optional)

- General Aspects of medicinal chemistry: Lead Compound discovery strategies, structure activity relationship, role of functional groups in drug-receptor interactions, receptor mapping and molecular modeling.
- Receptors: Drug receptor interactions, forces involved in the drug-receptor complexes, theories of drug-receptor interactions.
- Prodrugs and drug delivery systems: Types of prodrugs, mechanism of drug activation, carrier linked prodrugs.
- Drug metabolism: Pathway for drug deactivation and elimination, oxidative reactions, reductive reactions, carboxylation reactions, hydrolytic reactions.
- A brief idea of the common pharmaceuticals like chloramphenicol, artemisinine etc.

AcSIR-NEIST-CS-304: Frontiers in Catalysis (Homogeneous and Heterogeneous) (16-4-0-2) (Optional)

- General principles of catalysis, Types of catalysis, Significance, Promoters, Inhibitor, Poisons.
- Homogeneous catalysis: Organometallics directed towards organic transformations, Small molecules activations, Hemilability, Industrial application of homogeneous catalysis.
- Heterogeneous catalysis: Adsorption of molecules on solid surfaces, Adsorption isotherm, Surface Area, Porosity determination. Surface acidity and basicity of solid porous materials, Chemisorption on metals. Application of Zeolites, Mesoporous materials and Clays as heterogeneous catalysts and catalysts supports. Recycling of Catalysts.

AcSIR-NEIST-CS-305: Organic Synthesis (16-4-0-2) (Optional)

- Formation of carbon-carbon bond employing various kinds of organ metallic reagents, C-C double bonds through different reactions, oxidation, reduction through various kinds of reagents, functional group interconversion, by substitution including protection and deprotection, alkylation of enolates, and other carbon nucleophiles, reaction of carbon nucleophiles with carbonyl compounds, electrophilic addition to C-C multiple bonds, reactions of C-C multiple bonds. Concept of retrosynthetic analysis and its application to designing of organic molecules employing standard synthetic methods. Concepts in organic synthesis: Retrosynthesis, disconnection, synthons, linear and convergent synthesis, umpolung of reactivity and protecting groups.

AcSIR-NEIST-CS-306: Nutraceutical and Food Chemistry (15-5-0-2) (Optional)

- Raw material preparation, and characterization, extraction of valuable biomolecules, characterization of these molecules with stability study, preparation and formulations for functional foods. Characterization and stability study of neutraceuticals, properties and stability packaging of neutraceuticals.

AcSIR-NEIST-CS-307: Thermodynamics and Kinetic Stability (18-2-0-2) (Optional)

- First Law of Thermodynamics: heat, work, calculation of internal energy change, work in reversible and irreversible processes, heat capacity at constant pressure and constant volume, relation between heat capacities, enthalpy, measurement of enthalpy, Joule-Thompson expansion. 2nd law of Thermodynamics: Carnot cycle, efficiency of heat engine, entropy, change of entropy in reversible, and irreversible processes, entropy and spontaneous processes, probability and entropy, entropy change in chemical reactions, temperature and pressure effects, internal energy, Maxwells relations, Van't Hoff isotherm and isochore. 3rd Law of Thermodynamics: Nernst heat theorem, Gibbs free energy, and spontaneity, Helmholz free energy, variation of Gibbs free energy with temperature and pressure, Gibbs-Helmholz equation.

AcSIR-NEIST-CS-308: Macrocyclic Ligands and supramolecules (15-5-0-2) (Optional)

- Macrocyclic ligands: Nomenclature of macrocyclic ligands, chelate effect, macrocyclic effect, stability constant, Types: crown ether, cryptands, clathrates, ionophors, Applications of chelate compounds, biochemical and analytical application of macrocylic ligands. Role of weak interactions in supramolecules, supramolecular isomerism. Hydride sponge and related clathrates, co-ordination polymers, Liquid crystals. Host-

guest chemistry, Definition, classifications of host guest compounds, receptors, recognitions, nano-dimensional hosts.

AcSIR-NEIST-CS-309: Organometallic Compounds-16-4-0-2 (Optional)

- Organometallic compounds: Metal carbonyls, alkyls, carbenes, carbynes, and carbides; synthesis, bonding, structure and reactivity; electronic and magnetic properties, small molecule activation, organometallics in homogeneous catalysis. 18 electron rule, Bonding in ferrocene, aromaticity of cyclic C_nH_n ligands, nonaromatic alkene and alkyne complexes, metallocene, stereochemically nonrigid molecules, olefin metathesis, fluxional behaviour of organometallic compounds.

AcSIR-NEIST-CS-310: Nanoscience & Nanotechnology-14-4-2-2(Optional)

- Definition, historical development of nanoscience and nanotechnology, properties, synthetic approaches: top down and bottom up, importance of stabilizers / supports, sol-gel technique, surface plasmon resonance (SPR), quantum dots, metal nanoparticle, metal oxide nanoparticle, nanocomposites, nanohybrid, carbon nano-tube, graphene and their characterization tools: TEM, SEM-EDX, AFM, STM, AND XPS. etc. Application of nanoparticles and nanocomposites in different fields

AcSIR-NEIST-CS-311: Frontiers in Polymer Science-16-2-2-2 (Optional)

- Polymer Characterization: Molecular weight of polymers, molecular weight measurement, end-group analysis, viscometry, gel permeation chromatography, osmometry, light scattering, ultra centrifuge, practical significance of molecular weight, thermal analysis of polymers-thermal transition of polymers, X-ray diffraction study of polymers, instrumentation details of GPC, DSC, TGA, XRD on analysis of polymers, mechanical properties of polymers.
- Polymer processing: Polymer in special use, high temperature and fire resistance polymers, liquid crystalline polymers, poly electrolytes, biodegradable polymers, polymer composites, polyurethanes.
- Structure and prosperities of polymers: Mechanical, crystallization and microstructure, morphology, structure property correlation, viscoelasticity, dynamic mechanical properties
- Rheology: Phenomenon in polymeric flow systems, techniques of viscometric and viscoelastic measurements for polymeric fluids, rheological models, analytical solutions to flow problems, non-Newtonian viscosity, linear viscoelasticity.

- Operation in polymer industry: Film and molding technology, extrusion, blow molding, injection molding, mixing, fibre technology, laboratory equipments and demonstration

Project Proposal Writing

All candidates registering for Ph. D. programme in Chemical Sciences should write two research proposals of two credits each (total 4 credits).

AcSIR-NEIST-CS-312: 3-2-15-2 (Compulsory)

- Project Proposal Writing

CSIR-800 Programme

All candidates registering for Ph. D. programme in Chemical Sciences should participate in one of the appropriate CSIR-800 programme and write a report at the end of the programme. A successful completion of the programme will earn a total of 4 credits.

AcSIR-NEIST-CS-313: 6-4-30-4 (Compulsory)

- Project work (CSIR 800)