

M. Sc. in Industrial Chemistry  
Centre for Applied Chemistry  
Syllabus: 2016-2017

**Semester I**

**Total credits: 18 (A)**

<i>COURSE NO.</i>	<i>COURSE TITLE</i>	<i>COURSE CODE</i>	<i>CREDIT</i>
IC400	Organic Chemistry	1	3
IC401	Physical Chemistry	1	3
IC402	Inorganic Chemistry	1	3
IC403	Analytical Chemistry	1	3
IC404	Organic Chemistry Experiments-I	3	3
IC405	Physical Chemistry Experiments	3	3

**Semester II**

**Total credits: 18 (B)**

<i>COURSE NO.</i>	<i>COURSE TITLE</i>	<i>COURSE CODE</i>	<i>CREDIT</i>
IC425	Quality Control in Chemical Industry	1	3
IC426	Quantum Chemistry, Symmetry and Group Theory	1	3
IC427	Introduction to Materials Science	1	3
IC428	Reaction Mechanism and Stereochemistry	1	3
IC429	Analytical Chemistry Experiments	3	3
IC430	Organic Chemistry Experiments-II	3	3

**Semester III**

**Total credits: 18 (C)**

<i>COURSE NO.</i>	<i>COURSE TITLE</i>	<i>COURSE CODE</i>	<i>CREDIT</i>
IC450	Introduction to Polymer Materials	1	3
IC451	Energy and Environmental Chemistry	1	3
IC452	Molecular Spectroscopy	1	3
IC453-455	Elective*	2	3
IC456	Inorganic Chemistry Experiments	3	2
IC457	Instrumental Method of Chemical Analysis	3	2

IC458	Computational Chemistry Experiments	3	2
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**Semester IV**

**Total credits: 18 (D)**

<i>COURSE NO.</i>	<i>COURSE TITLE</i>	<i>COURSE CODE</i>	<i>CREDIT</i>
IC 475	High Energy Materials, Chemical Safety and Sensors	1	3
IC 476-478	Elective*	1	3
IC 479	Seminar	4	2
IC 480	Project work	3	10

\*Student can choose one elective in III<sup>rd</sup> and IV<sup>th</sup> Semester

<i>Grand Total Credit (A+B+C+D)</i>	72
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## Syllabus

**Semester I, 1<sup>st</sup> Year**

**Total credits: 18 (A)**

<i>COURSE NO.</i>	<i>COURSE TITLE</i>	<i>COURSE CODE</i>	<i>CREDIT</i>
<b>IC400</b>	<b>Organic Chemistry</b>	<b>1</b>	<b>3</b>
	<p>Nomenclature, General rules as applied to acyclic, mono and bicyclic compounds, Nature of reaction energy and kinetic considerations, types of organic reactions, reactive intermediates: formation and stabilization, electronic effects, Nucleophilic Substitutions, Linear free energy relationships, Neighboring group participation, Non- classic carbocations, Concept of resonance and aromaticity, Anti-aromaticity, Aromatic substitution reactions, Elimination reactions, Addition Reactions, Oxidation reactions, Reduction reactions</p> <p>Chemistry of heterocyclic compounds: Principle of heterocyclic synthesis including three, four, five, six and seven membered heterocycles; Natural products chemistry: Carbohydrates, terpenoids, flavonoids, steroids and alkaloids of recent pharmaceutical interest; Name reactions: Aldol condensation, Cannizzaro reaction and Grignard reaction; Comparison of the above with classical reactions; Green preparations, Applications: phase transfer catalysts; Introduction to Microwave organic synthesis, and Applications: environmental, solvents, time and energy benefits.</p>		
<b>IC401</b>	<b>Physical Chemistry</b>	<b>1</b>	<b>3</b>
	<p>Thermodynamics: Laws of thermodynamics. Entropy and its changes in various processes. Evaluation of absolute entropies. Free energy. thermodynamic relationships and applications: Partial molar quantities.</p> <p>Chemical kinetics: Reaction mechanism and kinetics for chemical reaction; Rate Equations; Kinetics of Complex Reactions; Chain Reactions; Explosive Reactions; Theories of Reaction Rates; Mechanisms from Rate Laws; Mechanisms of Photochemical and Oscillatory Reactions; Kinetics of Reactions in Solution: Catalysis: Acid-Base catalysis- Mechanisms. Enzyme catalysis. Electro Chemistry. Surface Chemistry. Study of Micelles &amp; Emulsions, Colloids and biocolloids: Definition, types, Tyndall effect, Brownian movement, electrophoresis, coagulation, and flocculation. Adsorption and surface Chemistry: Physisorption and chemisorption, Langmuir and B.E.T. equation and its significance of surface area determination, adsorption equation, and excess qualities</p>		

<b>IC402</b>	<b>Inorganic Chemistry</b>	<b>1</b>	<b>3</b>
	<p>Shapes of molecules: VSEPR theory and hybridization; Coordination Chemistry: Crystal field theory, Jahn-Teller theorem, Spectrochemical series, Molecular orbital theory, Nephelauxetic series, L-S &amp; j-j coupling scheme, Terms and Microstates, Orgel and TS diagrams, Electronic spectra of metal complexes, Stability constants of metal complexes, Carbonyls and Metallocenes. Inorganic Reaction Mechanisms, Hydrolysis Reactions, Trans Effect, Electron Transfer Reactions, Bioinorganic Chemistry: Iron Sulfur Clusters, Porphyrins and Corrins, Metal-Nucleotide Complexes, Dioxygen Binding, Photosynthesis; Metallo-Enzymes: Model Compounds; Magnetic Properties:</p> <p><i>Organometallic chemistry and catalysis in industry:</i> Industrial applications of organotransition metal compounds; <i>Important catalytic reactions:</i> Hydrogenation, Wacker process, Ziegler-Natta catalysis; Metal carbonyls compounds; <i>Organometallic reagents in organic synthesis:</i> Principle, preparation and applications of Li, Mg, Hg, Zn, Ni, Pd, Fe, Co and boron compounds in organic synthesis; Medicinal application of organometallic chemistry</p>		
<b>IC403</b>	<b>Analytical Chemistry</b>	<b>1</b>	<b>3</b>
	<p>Role of statistical methods in data analysis; Errors and Statistical Treatment of Data: Accuracy, precision and errors, error distributions, finite data analysis, standard deviation, Correlation vs. regression, Hypothesis testing and criteria for rejection of data, method of least squares. Protocol and procedures.</p> <p>Thermoanalytical Methods: Types, Thermogravimetry, Differential Thermal Analysis (DTA), and Differential Scanning Calorimetry: DSC. Separation Techniques: Heterogeneous Equilibria; solvent extraction, solid phase extraction Ion exchange. Chromatography (planar and Column.), Electroanalytical Methods: Electro-gravimetry - Coulometry - Voltammetry - polarography, Amperometry</p>		
<b>IC404</b>	<b>Organic Chemistry Experiments-I</b>	<b>3</b>	<b>3</b>
	(a) <i>Qualitative analysis:</i> (i) Separation and identification of components of binary organic mixture (ii) Thin layer chromatography (TLC) (iii) Column chromatography (iv) simple, fractional and vacuum distillation techniques (v) Recrystallization Techniques.		
<b>IC405</b>	<b>Physical Chemistry Experiments</b>	<b>3</b>	<b>3</b>
	Experiments to understand the principles of Phase equilibria, thermodynamics, conductance, electrochemistry, kinetics, pH metry.		

**Semester II, 1<sup>st</sup> Year****Total credits: 18 (B)**

<b>COURSE NO.</b>	<b>COURSE TITLE</b>	<b>COURSE CODE</b>	<b>CREDIT</b>
<b>IC425</b>	<b>Quality Control in Chemical Industry</b>		<b>3</b>
	Statistical Quality Control Techniques: Statistical treatment of data. Control charts, Performance Evaluation uncertainties in measurement. Validation of analytical methods. Quality Assurance: Elements of quality Assurance, Quality Management System Quality management concepts and principles: ISO 9001:2000 QMS Case studies on ISO 9001: 2000 in chemical industries. ISO 14000 Series of Standards. TQM in Chemical Industry. Six Sigma Approach to Quality: Applying Six Sigma to chemical Industries. Good Laboratory Practices: Principles of GLP, GMP in Drugs and Pharmaceutical Industries Accreditation of QC laboratories: Tools and Mechanisms ICH Guidelines on Drug substances and Products.		
<b>IC426</b>	<b>Quantum Chemistry, Symmetry and Group Theory</b>	<b>1</b>	<b>3</b>
	Basic principles of quantum mechanics: postulates, operators algebra, exactly solvable system, particle in a box, harmonic oscillator and hydrogen atom, shapes of the atomic orbitals, orbital angular momenta, tunnelling. Approximate methods of quantum mechanics, vibrational principle, perturbation theory up to second order in energy, applications, Born interpretation, Time dependent and time independent Schrödinger equations. Elementary concept of MO and VB theory, Huckel theory for conjugated $\pi$ electron system, Molecular spectroscopy: Rotational and vibrational spectra of diatomic molecules; electronic spectra; IR and Raman activities – selection rules; basic principles of magnetic resonance. Molecular Symmetry and Group theory: Symmetry Operations Symmetry and Stereoisomerism, Symmetry Criteria for Optical Activity and Dipole Moment, Group Theory and Properties, Point Groups, Matrix Representations of Symmetry Operations, Character Tables, Symmetry of Normal Modes of Vibrations of Molecules. Application of group theory in quantum mechanical calculations.		
<b>IC427</b>	<b>Introduction to Materials Science</b>	<b>1</b>	<b>3</b>
	Introduction, Atomic structure, Chemical bonding, Crystal structure, Polycrystalline, Lattice defects, Diffusion, Solid State, Solid Solutions, Phase diagrams, Phase Transformation, Properties; Mechanical, Thermal, Electrical, Magnetic. Applications of Materials.		
<b>IC 428</b>	<b>Reaction Mechanism and Stereochemistry</b>	<b>1</b>	<b>3</b>
	Stereochemistry: Stereoselectivity, stereospecificity, conformational and optical isomerism, optical activity, molecular symmetry and asymmetry, and geometrical isomerism; classification of chiral molecules based on symmetry. Asymmetric synthesis. Retrosynthetic analysis. Application of symmetry in photochemistry and photochemical and pericyclic reactions. Atom economical reactions.		

<b>IC429</b>	<b>Analytical Chemistry Experiments</b>		<b>3</b>
	Inorganic quantitative Analysis: Experiments based on redox, iodometric and complexometric titrations and Gravimetric analysis.		
<b>IC430</b>	<b>Organic Chemistry Experiment-II</b>		<b>3</b>
	(a) Synthesis and resolution of BINOL (b) Hydrolytic Kinetic Resolution of epoxides (c) Synthesis of following drugs: aspirin, and paracetamol (d) Synthesis of heterocyclic compounds (two) (e) Synthesis of dyes (one) (f) Benzyl chloride to Benzoic acid, (g) Nitro benzene to aniline, 7-hydroxy-4-methyl-cumarine.		

**Semester III, 2<sup>nd</sup> Year****Total credits: 18 (C)**

<b>IC450</b>	<b>Introduction to Polymer Materials</b>		<b>3</b>
	Basic concepts, nomenclature, degree of polymerization, classification of polymerization reactions, thermodynamic and transit properties of polymer. Types of polymerization: dendrimer, copolymerization, block copolymerization, graft copolymerization, stereo isomers, isotactic and syndiotactic polymers. Mechanism of polymerization: Free radical and ionic; characterization and rheology of polymers, heterogeneous polymerization, Zeigler-Natta catalysis, polymer degradation. Processing techniques: Calendaring, die casting, rotational casting, film casting, injection molding, blow molding, extrusion molding, thermoforming, foaming, reinforcing and fiber spinning, film and laminates. <i>Commercial polymers and their importance:</i> Nylon, polyesters (terylene and dacron), rubber, vulcanization of rubber, synthetic rubber, Bun 2N rubber, copolymers of butadiene, PVC, acrylic, teflon, polyethylene and acrylonitrile; Silicone polymers: silicone oils, rubber, grease and resin; Resins: Phenol-formaldehyde resins, urea-formaldehyde resins, epoxy resins, melamine-formaldehyde resins; Biomedical polymers: implants, contact lens and dental polymers.		
<b>IC451</b>	<b>Energy and Environmental Chemistry</b>		<b>3</b>
	Chemistry of Atmosphere: Composition and structure of atmosphere, Greenhouse effect, Ozone depletion, Photochemical smog, Air sampling techniques, Sources, effects and monitoring of air pollutants by Instrumental methods, Control of air pollution, Water Pollution, Different types of water pollutants, Sources, characteristics and effects of water pollutants, Monitoring of Water Pollutants, Treatment of Municipal Waste Water, Treatment of Industrial Waste Water, Environmental Impact Assessment process in India, Basic principles of Green Chemistry. Energy harvesting and source of energy Renewable Energy, Sustainability and the Environment		
<b>IC452</b>	<b>Molecular Spectroscopy</b>		<b>3</b>
	Interaction of Radiation with Matter: Molecular Quantum Properties, Transition Moment Integrals; Schematic of a Spectrometer; Microwave Spectroscopy: Molecular Rotational Energy; Applications of Microwave Spectroscopy. Infrared Spectroscopy: Molecular Symmetry; Instrumentation; Applications of Infrared Spectroscopy; Raman Spectroscopy: Electronic Spectroscopy, Nuclear Magnetic Resonance (NMR) Spectroscopy: <sup>1</sup> H-NMR Spectroscopy: Instrumentation of NMR Spectroscopy; <sup>13</sup> C NMR Spectroscopy: Electron Spin Resonance (ESR) Spectroscopy: Mossbauer Spectroscopy: Mass Spectrometry.		
<b>IC453</b>	<b>Elective-I: Drug Design and Synthesis-I</b>		<b>3</b>
<b>IC454</b>	<b>Elective-II: Dye Sensitised Solar Cells-I</b>		<b>3</b>
<b>IC455</b>	<b>Elective-III: Molecular Modelling-I</b>		<b>3</b>
<b>IC456</b>	<b>Inorganic Chemistry Experiments</b>		<b>2</b>
	Preparation and characterization of metal complexes by various physico chemical methods. Determination of metal ion by spectrophotometric and potentiometric methods.		

<b>IC457</b>	<b>Instrumental Method of Chemical Analysis</b>		<b>2</b>
	Demonstration of UV, IR, NMR, LCMS, SEM, HPLC		
<b>IC458</b>	<b>Computational Chemistry Experiments</b>		<b>2</b>
	Introduction to programming language, Numerical methods in chemistry, use of computer for predicting IR, Raman, NMR, bonding and structure of simple chemical compounds.		

<b>IC475</b>	<b>High Energy Materials, Chemical Safety and Sensors</b>		<b>3</b>
	<i>Explosives:</i> Definition, classification, synthesis and uses: nitrobenzene, TNT, PETN, picric acid, mono and ethylene glycol, glycol dinitrate, nitroglycerine, nitrocellulose, manitol, RDX, guanidine nitrate. <i>Fire retardants:</i> Definition, classification, synthesis and uses. <i>Industrial hygiene:</i> Concept, air and biological monitoring, occupational disease, operational control measures, personal protective equipments; <i>Industrial hazards and Safety:</i> Process hazards checklists, hazard surveys, safety program, Hazop safety reviews. <i>Industrial pollution:</i> Classification of hazards chemicals, storage, transportation, handling, risk assessments, challenges/solutions. <i>Eco-friendly effluents disposal:</i> Water pollutants, health hazards, sampling and analysis of water, water treatment, different industrial and domestic effluents and their treatment and disposal, advanced waste water treatment, effluent quality standards and laws, chemical industries, tannery, dairy, textile effluents, common treatment. <i>Sensors:</i> Concept of molecular sensors its properties and applications		
<b>IC476</b>	<b>Elective-I: Drug Design and Synthesis-II</b>		<b>3</b>
<b>IC477</b>	<b>Elective-II: Dye Sensitised Solar Cells-II</b>		<b>3</b>
<b>IC478</b>	<b>Elective-III: Molecular Modelling-II</b>		<b>3</b>
<b>IC481</b>	<b>Seminar</b>		<b>2</b>
<b>IC482</b>	<b>Project work</b>		<b>10</b>

**References**

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