

**Sardar Vallabhbhai National Institute of Technology (SVNIT) Surat**  
**Department of Chemistry**  
**Five Years Integrated M.Sc. Chemistry**

**(M. Sc. III) (Sem. – V)**

Sr. No.	Subject	Code	Scheme L-T-P	Credits (Min.)	Notional hours of Learning (Approx.)
<b>Fifth Semester (3<sup>rd</sup> year of MSc)</b>					
1	Organometallic Chemistry	CY301	3-0-2	4	85
2	Pericyclic Reactions and Photochemistry	CY303	3-0-4	5	115
3	Analytical Chemistry	CY305	3-0-4	5	115
4	Physical Methods of Structure Determination	CY307	3-0-0	3	55
5	Open Elective	CY3AA	3-0-0	3	55
			<b>Total</b>	<b>20</b>	<b>425</b>
6	Purification of Liquids and Solids Vocational Training / Professional Experience (Optional) (mandatory for exit)	CYV05 / CYP05	0-0-10	5	200 (20 x 10)

Sr. No.	Open Elective	Code	Scheme L-T-P
1	Unit Process in Chemical Industries	CY309	3-0-0

Subject Code: ##nXX; ##: Department Identity, n: Year, XX: Subject Sequence number XX: last digit 0 (subject offered in both ODD and EVEN semesters, XX: 01 to 30 – last digit ODD and EVEN for ODD and EVEN semesters (Mandatory Core), XX: 31 to 50 (Optional Core), XX: 51 to 99 (Elective), Subjects list for Minor and Honor (M/H#1-4), Subjects list for Specialization track (#1-4) EG: Engineering Subject, SC: Science Subject (offered combinedly by departments) (SVNIT Surat)

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**Five Years Integrated M.Sc. Chemistry**

M.Sc.– III (Chem), Semester – V <b>ORGANOMETALLIC CHEMISTRY</b> CY301	Scheme	L	T	P	Credit
		3	0	2	04

<b>1.</b>	<b>Course Outcomes (COs):</b> <b>At the end of the course, the students will be able to</b>
CO1	Interpret the structure and bonding aspects of organometallic compounds.
CO2	Discuss the stability and reactivity of organometallic complexes.
CO3	Predict the chemical behavior and reactivity of transition metal organometallic compounds.
CO4	Apply different electron counting rules to predict the shape/geometry of metal carbonyl clusters.
CO5	Explore the applications of organometallics in catalysis.

<b>2.</b>	<b>Syllabus</b>
	<b>METALLOORGANIC CHEMISTRY-I (12 Hours)</b>
	Introduction, Classification based on the nature of metal-carbon bond including $\eta$ -metal complexes, Hapticity ( $\eta$ ), General methods of preparations and properties, Organometallic compounds of alkali metals, Be, Mg, Al, Metal olefin complexes; Metal-alkynyl complexes, Cyclopentadienyl complexes: Metallocenes, Synthesis and properties of ferrocene, Reactions of ferrocene, Synthesis, structure and properties of metal-sandwich compounds, Synthesis and reactions of metal-hydrides.
	<b>METALLOORGANIC CHEMISTRY-II (12 Hours)</b>
	Organometallic compounds: Metal alkyls, Metal aryls, Electron-deficient Organometallic compounds, Electron-rich organometallics, Agostic interaction, Transition metal $\pi$ complexes with unsaturated organic ligands, Fluxionality in organometallic complexes, 18-electron rule and stability of organotransition metal compounds. Important reactions of Grignard reagent and Organo copper reagent, Synthesis and reactions of metal-carbenes and carbynes.
	<b>METAL CARBONYLS AND CLUSTERS (12 Hours)</b>
	Metal carbonyls, Structure and bonding in mononuclear metal carbonyls, Metal clusters, Carbonyl clusters, Low nuclearity carbonyl clusters, High nuclearity carbonyl clusters, Electron counting scheme, Wade's rules, Halide type clusters, Boranes and metalloboranes, Carboranes, Metal-metal single and multiple bond clusters, Isolobal analogy.
	<b>ORGANOMETALLIC COMPOUNDS IN HOMOGENEOUS CATALYSIS (9 Hours)</b>
	Homogeneous catalysis: Hydrogenation, Hydroformylation, and Polymerization of olefins (Ziegler-Natta catalysis), Mechanism of homogeneous catalysis reactions – Oxidative-addition, Reductive-elimination, $\beta$ -migratory insertion, Sigma bond metathesis, Transmetallation, Ligand substitution reactions, Wacker's oxidation, Water gas shift reactions and Fischer-Tropsch process, Monsanto acetic acid process, Olefin metathesis.
	<b>Practical will be based on the coverage of the above topics separately (30 Hours)</b>
	<b>(Total Contact Time: 45 Hours + 30 Hours = 75 Hours)</b>

<b>3.</b>	<b>Practical will be based on</b>
1	Analysis of Ternary mixtures: $\text{Ag}^+$ , $\text{Cu}^{2+}$ , and $\text{Ni}^{2+}$
2	Analysis of Ternary mixtures: $\text{Cu}^{2+}$ , $\text{Ni}^{2+}$ and $\text{Zn}^{2+}$

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3	Analysis of Ternary mixtures: Fe <sup>3+</sup> , Mg <sup>2+</sup> , and Ca <sup>2+</sup>
4	Given a solution of BaCl <sub>2</sub> and CaCl <sub>2</sub> determine the amount of Ba gravimetrically and Ca volumetrically by oxalate method.
5	To prepare the tetra amine copper (II) sulfate monohydrate complex [Cu(NH <sub>3</sub> ) <sub>4</sub> (H <sub>2</sub> O)]SO <sub>4</sub> from copper sulfate (CuSO <sub>4</sub> .5H <sub>2</sub> O). To estimate the amount of Cu in the prepared sample volumetrically.
6	To estimate gravimetrically, the amount of lead present in the whole of the given solution of lead acetate (or lead nitrate) by precipitating it as lead chromate.
7	Preparation and characterization of metal complex K <sub>3</sub> [Cr(C <sub>2</sub> O <sub>4</sub> ) <sub>3</sub> ]
8	Preparation and characterization of metal complex Mn(acac) <sub>2</sub>
9	Preparation and characterization of metal complex Prussian blue
10	Preparation and characterization of metal complex Turnbull blue

<b>4.</b>	<b>Books Recommended</b>
1	B. D. Gupta and A. J. Elias, Basic Organometallic Chemistry- Concepts, Synthesis, and Applications, Universities Press Private Limited, India, 2011.
2	J. Hartwig, Organotransition Metal Chemistry: From Bonding to Catalysis, 1 <sup>st</sup> Edition, University Science Books, USA, 2009.
3	R. H. Crabtree, The Organometallic Chemistry of the Transition Metals, 6 <sup>th</sup> Edition, John Wiley & Sons, New York, 2014.
4	D. F. Shriver and P. W. Atkins, Inorganic Chemistry, Oxford University Press, 4 <sup>th</sup> Edition, London, 2006.
5	J. E. Huheey, E. A. Keiter, R. L. Keiter and O. K. Medhi, Inorganic Chemistry-Principles of Structure and Reactivity, 4 <sup>th</sup> Edition, Pearson Education, London, 2006.

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<b>M.Sc.– III (Chem), Semester – V</b> <b>PERICYCLIC REACTIONS AND PHOTOCHEMISTRY</b> <b>CY303</b>	<b>Scheme</b>	<b>L</b>	<b>T</b>	<b>P</b>	<b>Credit</b>
		<b>3</b>	<b>0</b>	<b>4</b>	<b>05</b>

<b>1.</b>	<b>Course Outcomes (COs):</b> <b>At the end of the course, the students will be able to</b>
CO1	Demonstrate the knowledge of the basic concept of various Photochemical reactions
CO2	Learn the concept of pericyclic reactions.
CO3	Predict the stereochemical outcome of pericyclic reactions.
CO4	Utilize the knowledge of free radical reactions.
CO5	Apply the use of synthetic reagents in various organic reactions.

<b>2.</b>	<b>Syllabus</b>	
	<b>PERICYCLIC REACTIONS</b>	<b>(10 Hours)</b>
	Molecular orbital symmetry, Frontier molecular orbitals approach, 1,3-butadiene, 1,3,5-hexatriene. Classification of pericyclic reactions, FMO and PMO approach, correlation diagrams, Woodward-Hoffman rules, Electrocyclic reactions-conrotatory and disrotatory motions, 4n and 4n+2 systems, Cycloadditions-antrafacial and suprafacial additions in 4n and 4n+2 systems. Sigmatropic rearrangements-suprafacial and antrafacial shifts of H	
	<b>PHOTOCHEMISTRY</b>	<b>(15 Hours)</b>
	Quantum yields, techniques in photochemistry, photosensitization, and quenching mechanism. Laws of photochemistry, thermal and photochemical reactions. Photochemistry of olefins: cis-trans isomerization, dimerization reactions, Di- $\pi$ methane rearrangement, Photochemistry of aromatic compounds and its isomerization. Photochemistry of carbonyl compounds: Representation of excited states of ketones, Reactivity of electrically excited ketones, Photo reduction, Norrish type I & II reactions, Reactions of cyclic ketones, oxetane formation (Paterno-Buchi reaction). Photochemistry of aromatic compounds and nitrogen-containing organic compounds. Reaction of singlet-oxygen and photocatalytic oxygenation reactions.	
	<b>FREE RADICAL REACTIONS</b>	<b>(10 Hours)</b>
	Generation of free radicals - thermolysis, photolysis, redox methods, abstraction, addition and fragmentation; Generation of radical intermediates and its (a) addition to alkenes, alkynes (inter- and intra- molecular) for C-C bond formation and Baldwin's rules (b) fragmentation and rearrangements. Barton deoxygenation and decarboxylation, McMurry coupling. Electron transfer catalysis; Factors influencing radical reactivities- radical stability, polar influences, solvent and steric effects on radical reactions.	
	<b>REAGENTS</b>	<b>(10 Hours)</b>
	Mechanism of action, selectivity and utility of following reagents: Selenium dioxide, Aluminium isopropoxide, Diazomethane, Lead tetra acetate, Sodamide, N-Bromosuccinimide, Lithium aluminium hydride, Osmium tetroxide, Raney nickel, Sodium borohydride, Manganese dioxide, Lithium diisopropylamide (LDA), DCC, DDQ, HIO <sub>4</sub> .	
	<b>Practical will be based on the coverage of the below topics separately</b>	<b>(60 Hours)</b>
	<b>(Total Contact Time: 45 Hours + 60 Hours = 105 Hours)</b>	

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<b>3.</b>	<b>Practical will be based on</b>
1	Systematic qualitative analysis of binary organic mixture: water-insoluble phenol + water-insoluble acid
2	Systematic qualitative analysis of binary organic mixture: water-soluble phenol + water-insoluble acid
3	Systematic qualitative analysis of binary organic mixture: water-insoluble neutral + water-insoluble base
4	Systematic qualitative analysis of binary organic mixture: water-insoluble acid + water-insoluble neutral
5	Systematic qualitative analysis of binary organic mixture: water-soluble neutral + water-insoluble neutral
6	Systematic qualitative analysis of binary organic mixture: water-soluble neutral + water-insoluble acid
7	Systematic qualitative analysis of binary organic mixture: water-insoluble phenol + water-insoluble base
8	Systematic qualitative analysis of ternary organic mixture: water-soluble neutral + water-insoluble base
9	Systematic qualitative analysis of ternary organic mixture: water-insoluble acid + water-insoluble base + water-insoluble neutral
10	Systematic qualitative analysis of ternary organic mixture: water-soluble neutral + water-insoluble phenol + water-insoluble neutral

<b>4.</b>	<b>Books Recommended</b>
1	N. J. Turro, V.Ramamurthy, J.C.Scaiano, Modern Molecular Photochemistry of Organic molecules, University Science Books, Sausalito, California, 2010.
2	R.K. Parashar, V. K. Ahluwalia, Organic Reaction Mechanism, 4 <sup>th</sup> Edition, Narosa Publishing House, India, 2018.
3	I. Fleming, Pericyclic Reactions, 2 <sup>nd</sup> Edition, Oxford University Press, Oxford, 2015.
4	J. Singh, J.A. Singh Photochemistry and Pericyclic Reaction, 4 <sup>th</sup> Edition, New Age International Publishers, India, 2019.
5	R.T. Morrison, R. N. Boyd, S. Bhattacharjee, Organic Chemistry, 7 <sup>th</sup> Edition, Pearson Education, India, 2010.

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<b>M.Sc.– III (Chem), Semester – V</b> <b>ANALYTICAL CHEMISTRY</b> <b>CY305</b>	<b>Scheme</b>	<b>L</b>	<b>T</b>	<b>P</b>	<b>Credit</b>
		<b>3</b>	<b>0</b>	<b>4</b>	<b>05</b>

<b>1.</b>	<b>Course Outcomes (COs):</b> <b>At the end of the course, the students will be able to</b>
CO1	Demonstrate the basics of Thermal Methods of Analysis in analytical chemistry.
CO2	Learn the quantitative approaches through conventional methods of analysis.
CO3	Utilize the knowledge on electrophoresis and its applications in multidisciplinary areas.
CO4	Develop the basic concepts and applications of atomic spectrometry.
CO5	Establish the correlation between conventional and modern approach for quantitative analysis.

<b>2.</b>	<b>Syllabus</b>
	<b>THERMAL METHODS</b> <span style="float: right;"><b>(10 Hours)</b></span>
	Theory, methodology and applications of thermogravimetric analysis (TGA), Differential Thermal Analysis (DTA), and Differential scanning calorimetry (DSC). Principles, techniques and applications of thermometric titration methods. Derivative thermal gravimetry – introduction and instrumentation – thermometric titration – titration of mixture of Ca <sup>2+</sup> and Mg <sup>2+</sup> with EDTA – titration of sodium melanate with HClO <sub>4</sub> – direct injection enthalpy.
	<b>POLAROGRAPHY</b> <span style="float: right;"><b>(08 Hours)</b></span>
	Origin of polarography, Current-voltage relationship, Theory of polarographic waves (DC and sampled DC polarograms), Instrumentation, Ilkovič equation, Qualitative and quantitative applications
	<b>CYCLIC VOLTAMMETRY AND AMPEROMETRY</b> <span style="float: right;"><b>(07 Hours)</b></span>
	Principle, instrumentation, Randles Sevcik equation, Applications (cyclic voltamogram of K <sub>3</sub> [Fe(CN) <sub>6</sub> ]), amperometric titrations
	<b>ELECTROPHORESIS</b> <span style="float: right;"><b>(08 Hours)</b></span>
	Introduction – migration rates and plate heights in CE – electroosmotic flow - various types of electrophoresis -instrumentation – detectors – microchip electrophoresis – CE-MS - applications.
	<b>ATOMIC SPECTROMETRY</b> <span style="float: right;"><b>(12 Hours)</b></span>
	Flame spectrometry: introduction, elementary theory, instrumentation, type of burners, interferences, type of interferences, background correction method and applications. Atomic Absorption Spectrometry (AAS): Principle, instrumentation, production of atoms and ions, burners, detectors, advantage and disadvantage of AAS, standard addition method, internal standard method. Atomic Emission Spectrometry (AES): Principle, instrumentation, qualitative and quantitative analysis with AES, plasma emission spectrometry, direct current plasma, inductively coupled plasma, ICP-AES, high energy sources (plasma, arc, and spark), sample introduction and measurements.
	<b>Practical will be based on the coverage of the below topics separately</b>
	<b>(Total Contact Time: 45 Hours + 60 Hours = 105 Hours)</b>

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<b>3.</b>	<b>Practical will be based on</b>
1	TG and DTA Techniques to Study of Reaction Mechanism of Potassium Tetraoxalate at Elevated Temperatures
2	Thermo-gravimetric Determination of Calcium as $\text{CaC}_2\text{O}_4 \cdot \text{H}_2\text{O}$
3	Thermo-gravimetric Determination of Iron as $\text{Fe}_2\text{O}_3$
4	Measuring Vitamin C in Fruit Juice by Voltammetry with Standard Addition
5	Use of coated graphite electrodes for the potentiometric monitoring of precipitation reaction
6	Use of coated graphite electrodes for the potentiometric monitoring of acid-base reaction
7	Use of coated graphite electrodes for the potentiometric monitoring of complexation reaction
8	Measuring Manganese in Steel by Atomic Absorption Using a Calibration Curve
9	Spectrophotometric Analysis of a Mixture: Caffeine and Benzoic Acid in Soft Drink
10	Spectrophotometric Determination of Iron in Vitamin Tablets

<b>4.</b>	<b>Books Recommended</b>
1	S. M. Khopkar, Basic Concepts of Analytical Chemistry, 4 <sup>th</sup> Edition, New Age International, New Delhi, 2020.
2	D. A. Skoog, D. M. West, Holler, Crouch, Fundamentals of Analytical Chemistry, 8 <sup>th</sup> Edition, Cengage Learning, USA, 2013
3	J. H. Kennedy, Analytical Chemistry: Principles, 2 <sup>nd</sup> Edition (India Edition), Cengage Learning India Pvt Ltd., New Delhi, 2011.
4	G. D. Christian, P. K. Dasgupta, K. A. Schug, Analytical Chemistry, 7 <sup>th</sup> Edition, Wiley-Interscience, New Jersey, 2013.
5	D. C. Harris, Quantitative Chemical Analysis, 9 <sup>th</sup> Edition, W.H. Freeman and Company, New York, 2015.

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M.Sc. - III (Chem) Semester – V PHYSICAL METHODS OF STRUCTURE DETERMINATION CY307	Scheme	L	T	P	Credit
		3	0	0	03

<b>1.</b>	<b>Course Outcomes (COs):</b> <b>At the end of the course, the students will be able to</b>
CO1	Learn fundamentals of crystal growth and crystal habits.
CO2	Articulate profound knowledge in crystal systems.
CO3	Execute X-ray crystallographic knowledge for solving structures.
CO4	Discuss spectral behaviour of a molecule with unpaired electrons.
CO5	Interpret magnet properties of a molecule.

<b>2.</b>	<b>Syllabus</b>	
	<b>CRYSTAL GROWTH</b>	<b>(09 Hours)</b>
	Nucleation phenomenon – Homogenous and Heterogeneous nucleation, Theories of crystal growth. Defects, Classification of crystal growth methods: Melt, solution and Vapour Growth Techniques. Crystal habits and aggregates.	
	<b>CRYSTAL STRUCTURE</b>	<b>(20 Hours)</b>
	Crystal symmetry, Cell parameters and Crystal systems, Cubic crystal system & lattices; Density & Packing Fraction; Miller indices of crystallographic planes & directions; interplanar distance, Determination of crystal structure using X-ray diffraction techniques viz. Laue method, rotating crystal method (Bragg method) & powder method. X-ray Diffraction pattern of a cubic system: Indexing of powder diffraction patterns. Coordinates of Points, Structure factor calculation, Diffraction Intensity, preparation of structure plots including ORTEP and lattice structures including packing diagrams. Crystal packing and <b>Visualisation through MERCURY and DIAMOND software</b> , diffractometer instrumentation, Practical exercise of structure determination using standard packages. Basic Refinement exercise.	
	<b>EPR SPECTROSCOPY AND MAGNETIC PROPERTIES</b>	<b>(16 Hours)</b>
	Basic principles, zero field splitting and Kramer's degeneracy, factors affecting the 'g' value. Isotropic and anisotropic hyperfine coupling constants spin Hamiltonian, spin densities and Mc Connell relationship, applications. Structure characterization of Cu(II) complexes using EPR spectroscopy, Isotropic, axial and rhombic EPR spectra and interpretation. Magnetic properties -Determination of Magnetic moments and their applications to the elucidation of structures of inorganic compounds – temperature independent paramagnetism, Field-dependent magnetization, Magnetic properties of transition metals. Spin crossover in coordination compounds – Single molecule magnets, Plotting MPMS Data.	
	<b>(Total Contact Time: 45 Hours)</b>	

<b>3.</b>	<b>Books Recommended</b>
1	G. S. Girolami, X-ray Crystallography, 1 <sup>st</sup> Edition, Univ. Science Books, New York, United States, 2015.
2	J. M. D. Coey, Magnetism and Magnetic Materials, Illustrated edition, Cambridge University Press, Cambridge, United Kingdom, 2010.
3	J. W. Mullin, Crystallization, 5th Edition, Elsevier Butterworth-Heinemann, London, 2019.

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4	W. Carter, Crystals & Crystal Growth, UK edition, Nova Science Publishers Inc, New York, United States, 2015.
5	R. S. Drago, Physical Methods in Inorganic Chemistry, 2 <sup>nd</sup> Edition, International Edition East-West Press Pvt. Ltd. New Delhi, 2016.

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<b>M.Sc.– III (Chem), Semester – V</b> <b>UNIT PROCESS IN CHEMICAL INDUSTRIES</b> <b>CY309</b>	<b>Scheme</b>	<b>L</b>	<b>T</b>	<b>P</b>	<b>Credit</b>
		<b>3</b>	<b>0</b>	<b>0</b>	<b>03</b>

<b>1.</b>	<b>Course Outcomes (COs):</b> <b>At the end of the course, the students will be able to</b>
CO1	Develop an introductory knowledge of chemical industry and unit processes.
CO2	Build a bridge between theoretical and practical concept used in industry.
CO3	Explore the various synthetic methods of producing industrial chemicals and their applications.
CO4	Appraise knowledge about the basic chemistry of production.
CO5	State the industrial chemical process of transforming raw materials to desired products.

<b>2.</b>	<b>Syllabus</b>
	<b>NITRATION</b> <span style="float: right;"><b>(06 Hours)</b></span>
	Introduction, Nitrating Agents, Aromatic Nitration, Process Equipment for Technical Nitration, Batch Nitration, Continuous Nitration, manufacturing of nitrobenzene by batch and continuous process using fortified spent acid, m-dinitrobenzene and p-nitro acetanilide.
	<b>AMINATION BY REDUCTION &amp; AMMONOLYSIS AND HALOGENATION</b> <span style="float: right;"><b>(08 Hours)</b></span>
	Amination: Introduction, Different types of reduction reactions, Schimdt and Biazzi nitrators, different reduced products of nitrobenzene, manufacturing of aniline by Bechamp reduction, m-nitro aniline and aniline by ammonolysis. Halogenation: Introduction, different halogenating agents and halogenation reactions, mechanism and manufacturing of BHC and chlorobenzene.
	<b>SULFONATION &amp; SULFATION</b> <span style="float: right;"><b>(05 Hours)</b></span>
	Introduction, Sulfonating & Sulfating agents, Sulfonation of Aromatic Compounds. Chemical and physical factors in sulfonation and sulfation, Commercial manufacturing of benzene sulfonic acid (Barbet process) and naphthalene sulfonic acid
	<b>OXIDATION</b> <span style="float: right;"><b>(06 Hours)</b></span>
	Introduction, Types of oxidizing agents and reactions, Oxidation of toluene with MnO <sub>2</sub> . Manufacture of acetaldehyde from acetic acid and acetic acid from ethanol. Commercial manufacturing of benzoic acid and phthalic anhydride
	<b>HYDROGENATION AND ALKYLATION</b> <span style="float: right;"><b>(10 Hours)</b></span>
	Hydrogenation: Introduction and scope, properties and sources of hydrogen, gas catalytic hydrogenation and hydrogenolysis, factors affecting hydrogenation, industrial hydrogenation of fat and oil, manufacture methanol from CO <sub>2</sub> and H <sub>2</sub> . Alkylation: Introduction, Types of alkylation, alkylating agents, factors controlling alkylation, equipment for alkylation, manufacture of alkyl aryl sulphonates and ethylbenzene by continuous process.
	<b>ESTERIFICATION AND HYDROLYSIS</b> <span style="float: right;"><b>(10 Hours)</b></span>
	Esterification: Introduction, Esterification of organic acids. Commercial manufacture of some important compounds.

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	Hydrolysis: Introduction, Hydrolysing agents, Equipment for hydrolysis, industrial hydrolysis of fat, manufacture of ethanol from ethylene (Shell process) and phenol from benzene sulfonic acid.
	<b>(Total Contact Time: 45 Hours)</b>

<b>3.</b>	<b>Books Recommended</b>
1	M. Gopala Rao, M. Sittig, Dryden's Outlines of Chemical Technology, 3 <sup>rd</sup> Edition, East-West Press, 2010.
2	G. T. Austin, Shreve's Chemical Process Industries, 5 <sup>th</sup> Edition, McGraw-Hill Pub., New York, 2017.
3	R. M. Felder, R. W. Rousseau, L. G. Bullard Elementary Principles of Chemical Processes, 4 <sup>th</sup> Edition, John Wiley, New York, 2016.
4	J. A. Kent (Ed.) Riegel's Handbook of Industrial Chemistry, 10 <sup>th</sup> Edition, Kluwer Academic Publishers, New York, 2003.
5	P. H. Groggins, Unit Processing of Organic Synthesis, 5 <sup>th</sup> Edition, Tata-McGraw Hill, New Delhi, 2001.

Subject Code: ##nXX; ##: Department Identity, n: Year, XX: Subject Sequence number XX: last digit 0 (subject offered in both ODD and EVEN semesters, XX: 01 to 30 – last digit ODD and EVEN for ODD and EVEN semesters (Mandatory Core), XX: 31 to 50 (Optional Core), XX: 51 to 99 (Elective), Subjects list for Minor and Honor (M/H#1-4), Subjects list for Specialization track (#1-4) EG: Engineering Subject, SC: Science Subject (offered combinedly by departments) (SVNIT Surat)

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**(M. Sc. III) (Sem. – VI)**

Sr. No.	Subject	Code	Scheme L-T-P	Credits (Min.)	Notional hours of Learning (Approx.)
<b>Sixth Semester (3<sup>rd</sup> year of MSc)</b>					
1	Interpretative Molecular Spectroscopy	CY302	3-1-0	4	70
2	Molecules in Motion and Reaction Dynamics	CY304	3-1-2	5	100
3	Polymer Chemistry	CY306	3-0-4	5	115
4	Chemistry in Industries	CY308	3-0-0	3	55
5	Open Elective	CY3BB	3-0-0	3	55
			<b>Total</b>	<b>20</b>	<b>395</b>
6	Vocational Training / Professional Experience (Optional) (mandatory for exit)	CYV06 / CYP06	0-0-10	5	200 (20 x 10)

Sr. No.	Open Elective	Code	Scheme L-T-P
1	Materials Chemistry	CY312	3-0-0

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<b>M.Sc.– III (Chem), Semester – VI</b> <b>INTERPRETATIVE MOLECULAR SPECTROSCOPY</b> <b>CY 302</b>	<b>Scheme</b>	<b>L</b>	<b>T</b>	<b>P</b>	<b>Credit</b>
		<b>3</b>	<b>1</b>	<b>0</b>	<b>04</b>

<b>1.</b>	<b>Course Outcomes (COs):</b> <b>At the end of the course, the students will be able to</b>
CO1	Define the theories and basic principles of spectroscopic techniques.
CO2	Distinguish the effect of solvent and hydrogen bonding on vibrational frequencies.
CO3	Identify the organic functional groups by spectroscopic techniques.
CO4	Learn gas-phase reactions and to predict the fragmentation of organic molecules by mass spectrometry.
CO5	Evaluate unknown structure, or solve a structure-related problem by utilizing spectroscopic data.

<b>2.</b>	<b>Syllabus</b>
	<b>UV-VISIBLE ABSORPTION AND EMISSION SPECTROSCOPY</b> (10 Hours)
	Mechanism of absorption and emission of radiation by organic compounds, shape of absorption and emission bands and Franck-Condon principle. Various electronic transitions, Lambert-Beer law, effect of solvent on electronic transition, Ultraviolet bands for carbonyl compound, unsaturated carbonyl compounds, conjugated unsaturated compounds, Woodward-Fieser's rules for conjugated dienes and unsaturated carbonyl compounds, UV spectra of aromatic and heterocyclic compounds steric effect in biphenyls. Principles, origin of fluorescence and phosphorescence spectra, instrumentation and applications.
	<b>INFRARED SPECTROSCOPY</b> (08 Hours)
	Principle, Instrumentation and sample handling, modes of vibrations, force constant and bond strengths, characteristic vibrational frequencies of alkanes, alkenes, alkynes, aromatic compounds, alcohols, ethers, phenols, amines, carbonyl compounds, esters, amides, anhydrides, lactones and lactams. Effect of solvent and hydrogen bonding on vibrational frequencies, overtones, IR of gaseous, solids and polymeric materials.
	<b>NUCLEAR MAGNETIC RESONANCE SPECTROSCOPY</b> (16 Hours)
	NMR phenomenon, spin $\frac{1}{2}$ nuclei, ( $^1\text{H}$ , $^{13}\text{C}$ , $^{31}\text{P}$ and $^{19}\text{F}$ ), Zeeman splitting, effect of magnetic field strength on sensitivity and resolution, chemical shift $\delta$ , inductive and anisotropic effects on $\delta$ , chemical structure correlations of $\delta$ , chemical and magnetic equivalence of spins, spin-spin coupling, structural correlation to coupling constant J, selective decoupling, use of chemical shift reagents for stereochemical assignments. $^{13}\text{C}$ NMR, introduction to FT technique, relaxation phenomena.
	<b>MASS SPECTROMETRY</b> (11 Hours)
	Basic principles, ionization techniques, isotope abundance, molecular ion, fragmentation processes of organic molecules, deduction of structure through mass spectral fragmentation, high resolution MS, soft ionization methods, ESI-MS and MALDI-MS, illustrative examples from macromolecules and supramolecules, Fragment ions of odd and even electron types – rearrangement ions – factors affecting cleavage patterns – simple and multicentre fragmentation – McLafferty rearrangement – Retro Diels-Alder fragmentation.

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	Mass spectra of hydrocarbons, alcohols, phenols, aldehydes, ketones, carboxylic acids, amines and their derivatives.	
	<b>Tutorials will be based on the coverage of the above topics separately</b>	<b>(15 Hours)</b>
	<b>(Total Contact Time: 45 Hours + 15 Hours = 60 Hours)</b>	

<b>3.</b>	<b>Tutorials will be based on</b>
1	Calculations based on Woodward-Fieser rules for Absorption maxima of various organic compounds
2	Spectral problems for identification of organic compound 1
3	Spectral problems for identification of organic compound 2
4	Spectral problems for identification of organic compound 3
5	Spectral problems for identification of organic compound 4
6	Spectral problems for identification of organic compound 5
7	Spectral problems for identification of organic compound 6
8	Spectral problems for identification of organic compound 7
9	Spectral problems for identification of organic compound 8
10	Identification of organic functional groups based on IR and UV spectral data
11	Identification of isomers by $^1\text{H}$ and $^{13}\text{C}$ NMR spectral data
12	Identification of aromatic compounds by $^1\text{H}$ and $^{13}\text{C}$ NMR spectral data
13	Structure determination by NMR and mass spectral data
14	Identification of metal complex structures by mass spectra
15	Structure determination by mass spectrometry

<b>4.</b>	<b>Books Recommended</b>
1	K. W. Silverstein, F. X. Webster, D. J. Kiemle, D. L. Bryce, Spectrometric Identification of Organic Compounds, 8 <sup>th</sup> Edition, John Wiley & Sons, New York, 2014.
2	J. R. Lakowicz, Principles of Fluorescence Spectroscopy, 3 <sup>rd</sup> Edition, Springer, USA, 2006.
3	M. Sauer, J. Hofkens, J. Enderlein, Basic Principles of Fluorescence Spectroscopy, Wiley-VCH, New York, 2011.
4	J. H. Gross, Mass Spectrometry, 2 <sup>nd</sup> Edition, Springer Berlin Heidelberg, Germany, 2011.
5	G. M. Lampman, D. L. Pavia, G. S. Kria, J. R. Vyvyan, Spectroscopy International Edition, 4 <sup>th</sup> Edition, Cengage Learning India Pvt. Ltd., New Delhi, 2012.

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<b>M.Sc. -III (Chem) Semester – VI</b> <b>MOLECULES IN MOTION AND REACTION DYNAMICS</b> <b>CY304</b>	<b>Scheme</b>	<b>L</b>	<b>T</b>	<b>P</b>	<b>Credit</b>
		<b>3</b>	<b>1</b>	<b>2</b>	<b>05</b>

<b>1.</b>	<b>Course Outcomes (COs):</b> <b>At the end of the course, the students will be able to</b>
CO1	Interpret rate of reactions through various kinetic theories and understand mechanism of enzyme catalysis.
CO2	Learn the advances in electrodes and electrolytic reactions.
CO3	Demonstrate the deep theoretical knowledge of colligative properties.
CO4	Develop the theoretical basics of statistical thermodynamics
CO5	Execute the experiments related to physical chemistry approach which includes Kinetics, Conductometry, Colorimetry, pH-metry, Potentiometry and Titration.

<b>2.</b>	<b>Syllabus</b>
	<b>CHEMICAL KINETICS</b> <span style="float: right;"><b>(12 Hours)</b></span>
	Collision theory, Arrhenius equation, rate determining step (RDS), activation energy concept, transition state theory, steady state and equilibrium approximation, parallel and consecutive reactions, reversible reactions. Temperature dependence and the Arrhenius theory of reaction rates, Collision theory of bi-molecular gaseous reaction, collision and the steric effects, limitations, The transition-state theory, derivation of rate equation, Thermodynamic formulation of transition state theory, Unimolecular gas reactions: Lindeman theory, the Hinshelwood's theory, Rice-Ramsperger-Kassel theory. Mechanism and Kinetics of Enzyme catalysis. Numericals.
	<b>ELECTROCHEMISTRY</b> <span style="float: right;"><b>(13 Hours)</b></span>
	Different types of electrodes and electrolyte concentration cell, liquid junction potential (LJP), methods for elimination of LJP, salt bridge, concentration cell with and without transference (with derivation of equation for EMF of cell and LJP). Debye-Huckel theory, activity coefficients, Ionic strength, Transport number, Applications of EMF in the determination of: solubility product and solubility of sparingly soluble salts, ionic product of water by galvanic cell, transport number of ions, equilibrium constant, pH by hydrogen, glass and quinhydrone electrodes. Numericals.
	<b>COLLIGATIVE PROPERTIES</b> <span style="float: right;"><b>(10 Hours)</b></span>
	Vapour pressure lowering, Osmosis and osmotic pressure, Determination of Molar mass from osmotic pressure measurements, Relation between osmotic pressure and vapour pressure lowering of an ideal solution, Theories of semi-permeability, Reverse osmosis, Boiling point elevation, Boiling point elevation, Freezing point elevation, Freezing point elevation depression, Abnormal Results and the van't Hoff factor.
	<b>STATISTICAL THERMODYNAMICS</b> <span style="float: right;"><b>(10 Hours)</b></span>
	Distribution laws: Boltzmann, Bose-Einstein, and Fermi-Dirac, limitations of applicability of various distribution laws. Partition function and its significance. Translational, rotational, vibrational, and electronic partition functions of diatomic molecules and their evaluation. Relation between partition and their thermodynamic function, average internal energy, heat

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	capacity, Helmholtz free energy and entropy of mono- and di-atomic molecules, Sackur-Tetrode equation.	
	<b>Tutorials will be based on the coverage of the above topics separately</b>	<b>(15 Hours)</b>
	<b>Practical will be based on the coverage of the above topics separately</b>	<b>(30 Hours)</b>
	<b>(Total Contact Time: 45 Hours + 15 Hours + 30 Hours = 90 Hours)</b>	

<b>3.</b>	<b>Tutorials will be based on</b>
1	Problem based on Arrhenius equation, rate determining step (RDS) and activation energy.
2	Problems based on Collision theory.
3	Problem based on transition-state theory, Lindeman theory, the Hinshelwood's theory and Rice-Ramsperger-Kassel theory.
4	Problems based steady state and equilibrium approximation.
5	Problems on electrodes and electrolyte concentration cell.
6	Problems on Debye-Huckel theory, activity coefficients, Ionic strength, Transport number.
7	Problem based on solubility product and solubility of sparingly soluble salts, ionic product of water by galvanic cell, transport number of ions, equilibrium constant and pH.
8	Problems based on Vapour pressure lowering, Osmosis and osmotic pressure.
9	Determination of Molar mass from osmotic pressure measurements.
10	Problems based on theories of semi-permeability, Reverse osmosis, Boiling point elevation, Boiling point elevation, Freezing point elevation, Freezing point elevation depression.
11	Problems based on the van't Hoff factor.
12	Derivation of distribution laws: Boltzmann, Bose-Einstein, and Fermi-Dirac.
13	Problems based on Partition function.
14	Problems based on Sackur-Tetrode equation.

<b>4.</b>	<b>Practical will be based on</b>
1	Determine the order and rate constant of the reaction between $K_2S_2O_8$ and KI. Also study the influence of ionic strength on the rate constant.
2	Study of the effect of substituent on the dissociation constant of weak acid by conductance (Acetic acid, mono-, di-, and tri-chloro acetic acid).
3	Determine the dissociation constants ( $pK_a$ values) of tribasic acid by pH-metry (e.g. ortho Phosphoric acid).
4	Determination of the freezing point depression and boiling point elevation of water by addition of sodium chloride.
5	To determine normality and neutralization point of HCl in the given solution by conductometric titration against $NH_4OH$ Solution.
6	To determine the solubility product of $BaSO_4$ conductometrically.
7	Verify the Onsager equation using KCl, $K_2SO_4$ and $BaCl_2$ as electrolytes and determine their equivalent conductivity at different dilutions and from them find out the equivalent conductivity of a weak electrolyte at infinite dilution.
8	To determine the CMC of any surfactant at room temperature in aqueous solution by conductance method.
9	To find out amount of ferrous ammonium sulphate in given flask potentiometrically using ceric salt.
10	Determination of adsorption isotherm of oxalic acid on activated charcoal.

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<b>5.</b>	<b>Books Recommended</b>
1	S. Glasstone, Thermodynamics for Chemists, 1 <sup>st</sup> Edition, Affiliated East-West Press Pvt. Ltd., New Delhi, 2009.
2	R. P. Rastogi, R. R. Misra, An Introduction to Chemical Thermodynamics, 6 <sup>th</sup> Edition, Vikas Publishing House Pvt. Ltd., New Delhi, 2009.
3	B. R. Puri, L. R. Sharma, Principles of Physical Chemistry, 49 <sup>th</sup> Edition, Vishal Publications, New Delhi, India, 2020.
4	S. Maity, N. Ghosh, Physical Chemistry Practical, 1 <sup>st</sup> Edition, New Central Book Agency (P) Ltd., India, 2012.
5	M. C. Gupta, Statistical Thermodynamics, 3 <sup>rd</sup> Edition, New Age International Pvt. Ltd., Daryaganj, New Delhi, 2021.

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<b>M.Sc. - III (Chem) Semester - VI</b> <b>POLYMER CHEMISTRY</b> <b>CY306</b>	<b>Scheme</b>	<b>L</b>	<b>T</b>	<b>P</b>	<b>Credit</b>
		<b>3</b>	<b>0</b>	<b>4</b>	<b>05</b>

<b>1.</b>	<b>Course Outcomes (COs):</b> <b>At the end of the course, the students will be able to</b>
CO1	Explain the general reaction course and reaction mechanism for common polymerizations.
CO2	Describe and compare the polymerization principles.
CO3	Calculate parameters and outcomes of polymerizations.
CO4	Evaluate polymerizations from a green chemistry perspective.
CO5	Demonstrate different types of polymerizations.

<b>2.</b>	<b>Syllabus</b>
	<b>INTRODUCTION</b> <span style="float: right;"><b>(05 Hours)</b></span>
	Introduction, classification of polymers, general characteristics of polymers in comparison with organic compound, distinction between plastics, elastomers, fibres and liquid resins, properties of polymers.
	<b>CHAIN POLYMERIZATION</b> <span style="float: right;"><b>(10 Hours)</b></span>
	Preparative methods, properties and application: Low density (branched) polyethylene, polypropylene, high density (linear), polyethylene, polypropylene, natural rubber, rubbers derived from butadiene–acrylic acid copolymers, stereo-regular polybutadienes, polychloroprene (neoprene), styrene- butadiene –acrylonitrile copolymers. Carbon–carbon polymers- polystyrene, copolymers of polystyrene, acrylic polymers–acrylic fibers, acrylic adhesives, poly acrylates, polymethyl methacrylate (PMMA), polyvinyl acetate (PVA), polyvinyl alcohol, poly vinyl chloride, fluorocarbon polymers.
	<b>CONDENSATION POLYMERIZATION</b> <span style="float: right;"><b>(10 Hours)</b></span>
	Preparative methods, properties and application: Polyamides, Nylon 6, Nylon 66, Nylon 610, polyesters, polyether and related polymers – poly ethylene terephthalate (PET), polybutylene terephthalate (PBT), aromatic polyesters, polycarbonate, polyurethanes – Flexible and rigid polyurethane, polyurethane elastomers, coatings, adhesives, Sulphur containing polymers. Thermosetting resins – phenolic resins, amino resins epoxy resins.
	<b>POLYMER PROCESSING</b> <span style="float: right;"><b>(08 Hours)</b></span>
	Basic processing operations, extrusion, calendaring, sheet forming, stamping, casting, fibre spinning, injection moulding, thermoforming, vulcanisation of elastomers.
	<b>POLYMER CHARACTERIZATION</b> <span style="float: right;"><b>(12 Hours)</b></span>
	Identification and characterization of polymers: tensile strength, impact strength, elongation at break, water resistance, hardness, heat distortion temperature, brittleness, flexural strength, molecular weight and molecular weight distribution-number, weight and viscosity average molecular weights of polymers, methods of determining, molecular weight, Rheology of polymer, Fractionation of polymers, chemical analysis of polymers, mechanical properties of polymers glassy state, glass transition temperature, factor's affecting glass transition temperature, degradation of polymers by thermal, oxidative, mechanical and chemical methods.

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	Practical will be based on the coverage of the above topics separately	(60 Hours)
(Total Contact Time: 45 Hours + 60 Hours = 105 Hours)		

<b>3.</b>	<b>Practical will be based on</b>
1	To study synthesis of Polyester resin.
2	To study synthesis of Acrylic polymer.
3	To study synthesis of Polyurethane resin.
4	To study synthesis of Polystyrene by emulsion polymerization.
5	To study synthesis of Polystyrene by suspension polymerization.
6	To perform FT-IR analysis of synthesized polymers.
7	Demonstration: To perform TGA of synthesized polymers.
8	To study synthesis of phenol-formaldehyde resin.
9	To prepare composite from unsaturated Polyester resin using Jute / Glass fiber as reinforcing material.
10	To study synthesis of urea-formaldehyde resin.

<b>4.</b>	<b>Books Recommended</b>
1	F. W. Billmeyer, Textbook of Polymer Science, 3 <sup>rd</sup> Edition, Wiley-Interscience, 2017.
2	J. S. Walker, Physical Chemistry of Macromolecules - Basic Principles and Issues, 2 <sup>nd</sup> Edition, Pearson, 2004.
3	V. R. Gowariker, N. V. Viswanathan, J. Sreedhar, Polymer Science, 4 <sup>th</sup> Edition, New Age International Pvt Ltd., 2021.
4	V. K. Ahluwalia, Anuradha Mishra, Polymer Science: A Textbook, 1 <sup>st</sup> Edition, CRC Press, 2008.
5	Charles E. Carraher, R. Seymour, Introduction to polymer chemistry, 4 <sup>th</sup> Edition, CRC Press, 2017.

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<b>M.Sc.– III (Chem), Semester – VI</b> <b>CHEMISTRY IN INDUSTRIES</b> <b>CY308</b>	<b>Scheme</b>	<b>L</b>	<b>T</b>	<b>P</b>	<b>Credit</b>
		<b>3</b>	<b>0</b>	<b>0</b>	<b>03</b>

<b>1.</b>	<b>Course Outcomes (COs):</b> <b>At the end of the course, the students will be able to</b>
CO1	Explain process technologies of various organic and inorganic process industries.
CO2	Discuss the process flow diagram and various process parameters.
CO3	Explore various synthetic methods of producing industrial chemicals, their applications.
CO4	State the basic chemistry of production.
CO5	Appraise knowledge about laboratory and plant safety and management.

<b>2.</b>	<b>Syllabus</b>
	<b>NITROGEN INDUSTRY</b> <span style="float: right;"><b>(06 Hours)</b></span>
	Introduction, manufacture of synthetic nitrogen products and miscellaneous chemicals such as ammonia, hydro amine, fluorocarbon and various types of nitrogenous fertilizers such as urea, ammonium sulphate, ammonium nitrate, calcium ammonium nitrate.
	<b>FERMENTATION INDUSTRY</b> <span style="float: right;"><b>(05 Hours)</b></span>
	Introduction, culture development, inoculum preparation, nutrients for microorganisms, toxic effects on culture, manufacture of industrial alcohol, absolute alcohol, vinegar, downstream processing.
	<b>PERFUMERY INDUSTRY</b> <span style="float: right;"><b>(06 Hours)</b></span>
	Compounds used for different perfumes, vehicles, fixatives, odorous substances, preparation of phenyl ethanol, synthesis of musk ketone, musk xylene, vanillin, perfume formulation.
	<b>AGROCHEMICAL AND PESTICIDE INDUSTRY</b> <span style="float: right;"><b>(06 Hours)</b></span>
	Classification of agrochemicals, classification of insecticide, ammonium phosphate, super phosphate, BHC, Uses of agrochemicals and environments.
	<b>INDUSTRIAL GASES</b> <span style="float: right;"><b>(06 Hours)</b></span>
	Industrial Gases – Manufacture of hydrogen, oxygen, nitrogen, carbon dioxide, chlorine and sulphur dioxide.
	<b>LABORATORY SAFETY AND PROCESS SAFETY</b> <span style="float: right;"><b>(08 Hours)</b></span>
	Personal protective equipment, nature of the hazard and the task, compatibility with other PPE, chemicals being used, including concentration and quantity, hazards posed by the chemicals, routes of exposure for the chemicals, material the PPE is constructed of, safety signs, hazard assessment.
	<b>INDUSTRIAL SAFETY AND HAZARDS</b> <span style="float: right;"><b>(08 Hours)</b></span>
	Industrial hazards and safety considerations in chemical industries, mechanical, electrical and chemical hazards, fire and explosion hazards, health hazards, laboratory safety, control of plant hazards, safety practice.
	<b>(Total Contact Time: 45 Hours)</b>

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<b>3.</b>	<b>Books Recommended</b>
1	G. T. Austin, Shreve's Chemical Process Industries, 5 <sup>th</sup> Edition, McGraw Hill Education (India) Private Limited, 2017.
2	Jain and Jain, Engineering Chemistry, 17 <sup>th</sup> Edition, Dhanpat Rai publishing company, 2015.
3	B. K. Sharma, Industrial Chemistry, 3 <sup>rd</sup> Edition, Krishna Prakashan Media (P) Ltd., Meerut, 2016.
4	Ash, Michael and Irene, Formulary of Cosmetic Preparations, 1 <sup>st</sup> Edition, Chemical Publishing Co, 1977.
5	F. V. Wells, M. Billot, Perfumery Technology, 2 <sup>nd</sup> Edition, Longman Higher Education, 1981

<b>4.</b>	<b>Additional Reading Materials</b>
1	J. A. Kent (Ed.) Riegel's Handbook of Industrial Chemistry, 10 <sup>th</sup> Edition, Kluwer Academic Publishers, New York, 2003.
2	M. L. Srivastava, Fermentation Technology, Narosa Publisher, 2008.

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M.Sc. -III (Chem) Semester – VI MATERIALS CHEMISTRY CY312	Scheme	L	T	P	Credit
		3	0	0	03

**1. Course Outcomes (COs):**

At the end of the course the students will be able to:

CO1	Discuss basic concepts of chemical processing and synthesis routes of various materials.
CO2	Distinguish and compare variety of materials based on their structures and functions
CO3	Memorize the fundamentals of the materials properties
CO4	Develop skills for material processes for device integration
CO5	Learn the different classes of materials used in engineering applications

<b>2.</b>	<b>Syllabus</b>	
	<b>HYBRID MATERIALS</b>	<b>(12 Hours)</b>
	Introduction to materials chemistry, compounds vs materials, nanoscale porosity in organic and inorganic materials, Synthesis, structural features and potential applications of metal organic frameworks, covalent organic frameworks and porous organic frameworks in adsorption, sensing and storage applications.	
	<b>INORGANIC FIBRES</b>	<b>(07 Hours)</b>
	Structure, properties and applications of boron fibres, carbon fibres, silicon carbide fibres, alumina fibres. Inorganic polymers.	
	<b>ELECTRONIC MATERIALS</b>	<b>(08 Hours)</b>
	Semiconductors, Superconductors and High temperature superconductors, topological insulators, conducting oxides materials and their applications in devices.	
	<b>PHOTONIC MATERIALS</b>	<b>(10 Hours)</b>
	Basic design and applications of photo-luminescent materials, dye-sensitized solar cells (DSCs), light-emitting diodes (LED), organic light-emitting diodes (OLED), photovoltaics, and chiroptical materials and photorefractive materials.	
	<b>ENERGY MATERIALS</b>	<b>(08 Hours)</b>
	Basic concepts of batteries and Super capacitors, fuel cells, hydrogen generation, hydrogen and methane storage materials, carbon capture and sequestration materials.	
	<b>(Total Lecture Hours: 45)</b>	

<b>3</b>	<b>Books Recommended</b>
1	Lalena, J.N.; Cleary, D.A. Principles of Inorganic Materials Design; Wiley: New York, 2010
2	Sam-Shajing Sun, Larry R. Dalton, Introduction to Organic Electronic and Optoelectronic Materials and Devices, CRC Press, London, 2017.
3	Organic Electronics Materials and Devices by S. Ogawa, Springer, Tokyo, 2015.
4	B. D. Fahlman, Ed, Materials Chemistry, Elsevier, Switzerland, 2018
5	B. K. Sharma, Industrial Chemistry, Goel Publishing House, India, 2014.

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**(M. Sc. IV) (Sem. – VII)**

Sr. No.	Subject	Code	Scheme L-T-P	Credits (Min.)	Notional hours of Learning (Approx.)
<b>Seventh Semester (4<sup>th</sup> Year of M. Sc.)</b>					
1	Reaction Mechanism in Coordination Chemistry	CY401	3-0-4	5	115
2	Synthetic Approaches in Organic Chemistry	CY403	3-0-4	5	115
3	Atomic Spectroscopy and Electron Microscopic Techniques	CY405	3-1-0	4	70
4	Computational Chemistry	CY407	3-0-4	5	115
5	Core Elective-1	CY4AA	3-0-0	3	55
6	MOOC Course*	CY453	3-0-0/ 3-1-0	3/4	
			<b>Total</b>	<b>25-26</b>	<b>470</b>
7	Skill Development on Computational Tools Vocational Training/ Professional Experience (Optional) (Mandatory for exit)	CYV07/CYP07	0-0-10	5	200 (20x10)

Sr. No.	Core Elective	Code	Scheme L-T-P
1	Surfactant Chemistry	CY451	3-0-0
2	Chemistry of Nanomaterials	CY452	3-0-0

\*Students will be required to opt any one Massive Open Online Courses (MOOC) course through NPTEL / SWAYAM platform in Semester- VII or Semester VIII excluding the courses of the existing curriculum of five years integrated programme in chemistry. Necessary approval from the department is required before the registration of the courses on above platform. The credit of the courses through above platform will be considered as per the norms of the institute.

Subject Code: ##nXX; ##: Department Identity, n: Year, XX: Subject Sequence number XX: last digit 0 (subject offered in both ODD and EVEN semesters, XX: 01 to 30 – last digit ODD and EVEN for ODD and EVEN semesters (Mandatory Core), XX: 31 to 50 (Optional Core), XX: 51 to 99 (Elective), Subjects list for Minor and Honor (M/H#1-4), Subjects list for Specialization track (#1-4) EG: Engineering Subject, SC: Science Subject (offered combinedly by departments) (SVNIT Surat)

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M.Sc. - IV (Chem), Semester – VII REACTION MECHANISM IN COORDINATION CHEMISTRY CY401	Scheme	L	T	P	Credit
		3	0	4	05

<b>1.</b>	<b>Course Outcomes (COs):</b> <b>At the end of the course, the students will be able to</b>
CO1	Explore thermodynamic and kinetic of complex formation in solution.
CO2	Study on reaction mechanisms of complexation in solution.
CO3	Explore redox processes in metal complexes.
CO4	Discuss on possible electronic transitions in metal complexes.
CO5	Write photochemical reaction of metal complexes.

<b>2.</b>	<b>Syllabus</b>	
	<b>THERMODYNAMIC AND KINETIC BEHAVIOR OF METAL COMPLEXES</b>	<b>(15 Hours)</b>
	Stability, step wise formation constants and overall formation constants. Kinetic versus Thermodynamic stability, labile and inert octahedral complexes according to valence bond and crystal field theory. factors affecting stability constants, Chelates and macrocyclic effects, Irving Williams order, determination of stability constant by various methods (spectrophotometric and pH-metric), conditional stability constants and their importance in complexometric EDTA titration of metal ions, statistical and non-statistical factors affecting stability of complexes in solution.	
	<b>REACTION MECHANISMS IN TRANSITION METAL COMPLEXES</b>	<b>(15 Hours)</b>
	Substitution reactions in octahedral and square planar complexes, Reaction mechanism of ligand substitution reactions in octahedral complexes: $SN_1$ (D-process), $SN_2$ (A-process), solvent intervention, ion pair formation, conjugate base formation $SN_1CB$ . Solvolysis reactions: acid and base hydrolysis, Trans effect, theories of Trans effect, Redox (one and two-electron transfer) reactions, inner sphere and outer sphere processes, Creutz-Traube complexes.	
	<b>INORGANIC PHOTOCHEMISTRY</b>	<b>(15 Hours)</b>
	Introduction of inorganic photochemistry, Photochemically excited states and excited state processes for transition metal complexes, Types of photochemical reactions in transition metal complexes, Ligand-field photochemistry of chromium(III) complexes, Photo substitution reactions, Adamson's rules, photochemistry of Cobalt(III) complexes, Mechanism of photoreduction: photophysics and photochemistry of Ruthenium-polypyridine complexes, Applications of photochemical inorganic reactions in synthesis, Catalysis, Biological processes, chemical actinometer and in laser.	
	<b>Practical will be based on the coverage of the above topics separately</b>	<b>(60 Hours)</b>
	<b>(Total Contact Time: 45 Hours + 60 Hours = 105 Hours)</b>	

<b>3.</b>	<b>Practical will be based on</b>
1	Preparation and characterization (UV-Vis, FT-IR, etc.) of potassium tris(oxalato) aluminate (III)
2	Preparation and characterization (UV-Vis, FT-IR, etc.) of potassium tris(oxalato) chromate (III)
3	Preparation and characterization (UV-Vis, FT-IR, etc.) of sodium hexa(nitro) cobaltate (III)
4	Preparation and characterization (UV-Vis, FT-IR, etc.) of hexa(amine) cobalt (III)

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5	Preparation and characterization (UV-Vis, FT-IR, etc.) of tetrapyridine copper (II)persulphate
6	Preparation and characterization (UV-Vis, FT-IR, etc.) of dinitrotetrapyridine nickel (II)
7	Preparation and characterization (UV-Vis, FT-IR, etc.) of hexamine nickel (II) chloride
8	Preparation and characterization (UV-Vis, FT-IR, etc.) of bis(acetylacetonato) copper (II)
9	Preparation and characterization (UV-Vis, FT-IR, etc.) of tris(acetylacetonato) iron (III)
10	Preparation and characterization (UV-Vis, FT-IR, etc.) of tris(acetylacetonato) manganese (III)

<b>4.</b>	<b>Books Recommended</b>
1	J. E. Huheey, E. A. Keiter, R. L. Keiter, O. K. Medhi, Inorganic Chemistry - Principles of Structure and Reactivity, 5 <sup>th</sup> Edition, Pearson Education, India, 2022.
2	J. D. Lee, Concise Inorganic Chemistry, 5 <sup>th</sup> Edition, Oxford University Press, India, 2014.
3	B.R. Puri, L.R. Sharma, K.C. Kalia, Principles of Inorganic Chemistry, 33 <sup>rd</sup> Edition, Vishal Publishing Co., India, 2022.
4.	W. W. Porterfield, Inorganic chemistry: A Unified Approach, 2 <sup>nd</sup> Edition, Elsevier India Pvt. Ltd., New Delhi, 2013.
5.	R. B. Jordan, 'Inorganic Photochemistry', Reaction Mechanisms of Inorganic and Organometallic Systems, 3 <sup>rd</sup> Edition, Oxford Academic, New York, 2020.

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M.Sc. - IV (Chem), Semester – VII SYNTHETIC APPROACHES IN ORGANIC CHEMISTRY CY403	Scheme	L	T	P	Credit
		3	0	4	05

<b>1.</b>	<b>Course Outcomes (COs):</b> <b>At the end of the course, the students will be able to</b>
CO1	Define the role of protecting groups in organic synthesis.
CO2	Extend the knowledge in the mechanisms of various named reactions and their significance in synthesis of drugs.
CO3	Learn the mechanistic and stereo chemical aspects in the reactions of carbon-carbon and carbon-hetero multiple bonds molecules.
CO4	Investigate the mechanistic details of various rearrangement reactions in organic molecules.
CO5	Learn the mechanistic pathways of various name reactions.

<b>2.</b>	<b>Syllabus</b>	
	<b>PROTECTING GROUPS</b>	<b>(05 Hours)</b>
	Protection and deprotection methodology for functional groups. Synthetic applications in peptide synthesis, biology and medicine.	
	<b>REARRANGEMENTS IN CARBON SKELETON</b>	<b>(08 Hours)</b>
	Classification and general mechanistic treatment of nucleophilic, free radical and electrophilic rearrangements, Pinacol-Pinacolone, Semipinacol, Wagner Meerwein, Favorskii, Curtius, Hoffmann, Schmidt, Beckmann's, Wittig, Benzil-Benzilic acid, Demjanov, Claisen-Johnson-Ireland and Oxy-Cope rearrangements.	
	<b>REMODELING OF CARBON SKELETON</b>	<b>(07 Hours)</b>
	Cleavage of C-C bonds. Decarboxylation, Baeyer-Villiger oxidation, and 1,2-diol cleavage in a total synthesis, synthetic utilization of the double bond cleavage reactions.	
	<b>ASYMMETRIC SYNTHESIS</b>	<b>(07 Hours)</b>
	Synthesis of Taxol and strychnine, Sharpless asymmetric epoxidation, Jacobsen epoxidation, Shi epoxidation. Alkenes to diols, Sharpless asymmetric dihydroxylation, metathesis reactions.	
	<b>ADDITION TO CARBON-CARBON &amp; CARBON-HETEROATOM MULTIPLE BONDS</b>	<b>(18 Hours)</b>
	Mechanistic and stereochemical aspects of addition reactions involving electrophiles, nucleophiles and free radicals, regio- and chemoselectivity, orientation and reactivity, addition to cyclopropane ring, hydrogenation of double and triple bonds, hydrogenation of aromatic rings, hydroboration, Michael reaction, ene reaction, Wittig reaction, Perkin reaction, Claisen – Schmidt condensation, Peterson's synthesis. Cannizzaro and cross Cannizzaro reactions, Benzoin condensation, Wolff-Kishner reduction, Clemmenson reduction, MPV reduction, Birch reduction. Riemer-Tiemann reaction, Gatterman reaction, Chichibabin reaction. Uses of organoboron compounds in organic synthesis. Addition of Grignard reagent, organo zinc, organo copper, and organo lithium reagents to carbonyl and unsaturated carbonyl compounds. Mechanism of condensation reactions involving enolates- Knoevenagel, Mannich and Stobbe reactions. Sakurai reaction, Nozarov reaction, Achmotowitz reaction, McMurry reaction, Julia olefination, Prins reaction, Baylis-Hillmann reaction, Corey-Fuch's reaction, Nozaki-Hiyama-Kishi reaction.	
	<b>Practical will be based on the coverage of the above topics separately</b>	<b>(60 Hours)</b>

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	(Total Contact Time: 45 Hours + 60 Hours = 105 Hours)
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<b>3.</b>	<b>Practical will be based on</b>
1	Backmann's rearrangement. #
2	Wolff-Kishner reduction. #
3	Cannizzaro reaction. #
4	Sandmayer's reaction. #
5	Asymmetric synthesis (ketone reduction). #
6	Asymmetric synthesis (epoxidation). #
7	Diazocoupling. #
8	Nitration. #
9	Reimer-Tiemann reaction. #
10	Diels-Alder Reaction. #

#Identification of formed compounds by spectroscopic methods.

<b>4.</b>	<b>Books Recommended</b>
1	W. Carruthers, I. Coldham, Modern Methods of Organic Synthesis, 4 <sup>th</sup> Edition, Cambridge University, 2005.
2	F. A. Carey, R. J. Sundberg, Advanced Organic Chemistry: Structure and Mechanism (Part A), 5 <sup>th</sup> Edition, Springer, 2007.
3	Michael B. Smith, March's Advanced Organic Chemistry: Reactions, Mechanisms and Structure, 8 <sup>th</sup> Edition, John Wiley & Sons, Inc, USA, 2019.
4	R. O. C. Norman, J. M. Coxon, Principles of Organic Synthesis, 3 <sup>rd</sup> Edition, Nelson Thornes, 2005.
5	G. S. Zweifel, M. H. Nantz, P. Somfai, Modern Organic Synthesis: An Introduction, 2 <sup>nd</sup> Edition, John Wiley & Sons, Inc, USA, 2017.

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M.Sc. - IV (Chem), Semester – VII ATOMIC SPECTROSCOPY AND ELECTRON MICROSCOPIC TECHNIQUES CY405	Scheme	L	T	P	Credit
		3	1	0	04

<b>1.</b>	<b>Course Outcomes (COs):</b> <b>At the end of the course, the students will be able to</b>
CO1	Define basic principles and instrumental aspects for atomic spectroscopic techniques.
CO2	Explain theory and applications of photoelectron spectroscopy.
CO3	Predict elemental composition by atomic spectroscopic techniques.
CO4	Distinguish morphology and structures of various materials by electron microscopic techniques.
CO5	Interpret spectral data of atomic spectroscopic and electron microscopic techniques for chemical analysis.

<b>2.</b>	<b>Syllabus</b>	
	<b>ATOMIC SPECTROSCOPIC TECHNIQUES</b>	<b>(16 Hours)</b>
	Atomic mass spectrometry – general features of atomic mass spectrometry, mass spectrometer, inductively coupled plasma mass spectrometry (MS), instrumentation, atomic mass spectra and interferences, spark source MS, glow-discharge MS, elemental surface analysis. Atomic X-ray spectrometry – Fundamental principles. X-ray fluorescence. X-ray absorption. X-ray emission and diffraction. Instrumentation, quantitative and semiquantitative analysis, advantages and disadvantages of X-ray fluorescence methods.	
	<b>PHOTOELECTRON SPECTROSCOPY</b>	<b>(14 Hours)</b>
	Photoexcitation and photoionization, principle of Ultraviolet photoelectron spectroscopy (UPS) and X-ray photoelectron spectroscopy (XPS), types of peaks, chemical shifts, Instrumentation, XPS and UPS of simple molecules, applications. Auger electron microscopy-principle, instrumentation and applications, similarities and differences in ESCA and AES, advantages and disadvantages.	
	<b>ELECTRON MICROSCOPY</b>	<b>(15 Hours)</b>
	Introduction to study of surface, Electron stimulated microanalysis methods- (electron microprobe, Transmission Electron Microscope, Scanning Electron Microscope, Scanning Transmission Electron Microscope, Analytical Electron Microscopy, Scanning-Probe Microscopes) and atomic force microscope – principle, instrumentation and applications.	
	<b>Tutorials will be based on the coverage of the above topics separately</b>	<b>(15 Hours)</b>
	<b>(Total Contact Time: 45 Hours + 15 Hours = 60 Hours)</b>	

<b>3.</b>	<b>Tutorials will be based on</b>
1	Describe the basic differences among atomic emission, atomic absorption, and atomic fluorescence spectroscopy.
2	Type of interferences encountered in atomic mass spectrometry
3	Why is atomic emission more sensitive to flame instability than atomic absorption?
4	Discuss the differences that result in ICP atomic emission when the plasma is viewed axially rather than radially.

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5	Atomic spectral problems for determination of element 1
6	Atomic spectral problems for determination of element 2
7	Atomic spectral problems for determination of element 3
8	Atomic spectral problems for determination of element 4
9	Atomic spectral problems for quantitative analysis 1
10	Atomic spectral problems for quantitative analysis 2
11	Atomic spectral problems for quantitative analysis 3
12	Atomic spectral problems for quantitative analysis 4
13	Atomic spectral problems for chromium determination in steel
14	Atomic spectral problems for copper determination in water
15	Atomic spectral problems for manganese in geological sample

<b>4.</b>	<b>Books Recommended</b>
1	D. A. Skoog, D. M. West, Holler, Crouch, Fundamentals of Analytical Chemistry, 8 <sup>th</sup> Edition, Cengage Learning, USA, 2013
2	G. D. Christian, P. K. Dasgupta, K.A. Schug, Analytical Chemistry, 7 <sup>th</sup> Edition, John Wiley & Sons, New York, 2013.
3	J. I. Goldstein, D. E. Newbury, J. R. Michael, N. W.M. Ritchie, J. H. J. Scott, D. C. Joy, Scanning Electron Microscopy and X-Ray Microanalysis, 4 <sup>th</sup> Edition, Springer New York, NY, 2018
4	D. B. Williams and C. B. Carter. "Transmission Electron Microscopy: A Textbook for Materials Science" 2 <sup>nd</sup> Edition, Springer, 2009
5	Paul van der Heide, X-Ray Photoelectron Spectroscopy: An Introduction to Principles and Practices, 1 <sup>st</sup> Edition, John Wiley & Sons, Inc., USA, 2012.

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M.Sc. - IV (Chem), Semester – VII COMPUTATIONAL CHEMISTRY CY407	Scheme	L	T	P	Credit
		3	0	4	05

<b>1.</b>	<b>Course Outcomes (COs):</b> <b>At the end of the course, the students will be able to</b>
CO1	Describe the theoretical concepts of molecular mechanics and geometry optimizations.
CO2	Predict excited state geometry and properties in order to calculate molecular spectroscopy-based parameters.
CO3	Compare the theoretical data with experimental spectra.
CO4	Explore molecular dynamic simulations.
CO5	Explain and perform molecular docking with suitable examples.

<b>2.</b>	<b>Syllabus</b>	
	<b>AB INITIO CALCULATIONS</b>	<b>(12 Hours)</b>
	Principles of ab initio method, Hartree SCF method, Hartree–Fock equations, basis sets, Gaussian functions; basis set preliminaries; direct SCF, types of basis sets and their uses, post-Hartree–Fock calculations, electron correlation, Møller–Plesset approach to electron correlation, configuration interaction approach to electron correlation - coupled cluster method, applications of ab initio method – geometries, energies, frequencies and vibrational spectra, bond orders, Atoms-in-Molecules (AIM), other important properties -, ionization energies, and electron affinities, strengths and weaknesses of ab initio calculations.	
	<b>SEMIEMPIRICAL AND DFT CALCULATIONS</b>	<b>(12 Hours)</b>
	Principles of SCF semiempirical methods, Pariser-Parr-Pople (PPP) method, Complete Neglect of Differential Overlap (CNDO) method, Intermediate Neglect of Differential Overlap (INDO) method, Neglect of Diatomic Differential Overlap (NDDO) method, Principles of density functional theory (DFT), previous DFT methods, Kohn–Sham approach, Kohn–Sham Approach, applications of semiempirical and DFT methods – geometries, energies, frequencies and vibrational spectra, properties arising out of electron distribution – dipole moments, charges, bond orders, other important properties - UV and NMR spectra, ionization energies, and electron affinities, strengths and weaknesses of semiempirical and DFT methods.	
	<b>SOLVATION, DIRADICALS AND HEAVY ATOMS</b>	<b>(06 Hours)</b>
	Solvation, ways of treating solvation, singlet diradicals - model chemistries and beyond model chemistries, Complete Active Space (CAS) calculations, heavy atoms and relativistic corrections, heavy atom calculations, transition metals.	
	<b>MOLECULAR MECHANICS</b>	<b>(08 Hours)</b>
	History and fundamental assumptions, potential energy functional forms, bond stretching, valence angle bending, torsions, van der Waals interactions, electrostatic interactions, cross terms and additional non-bonded terms, parameterization strategies, force-field energies and thermodynamics, geometry optimization, optimization algorithms, optimization aspects specific to force fields, menagerie of modern force fields, available force fields, validation, force fields.	
	<b>MOLECULAR DOCKING</b>	<b>(07 Hours)</b>

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	Docking, basic theories and algorithms used on docking, rigid docking, flexible docking, manual docking, applications of docking – receptor –ligand binding, virtual screening, drug discovery, protein – protein interaction, enzymatic studies, software available for docking and their uses.
	<b>Practical will be based on the coverage of the above topics separately (60 Hours)</b>
	<b>(Total Contact Time: 45 Hours + 60 Hours = 105 Hours)</b>

<b>3.</b>	<b>Practical will be based on</b>
1	Demonstration of chemical structure drawing program ChemDraw and molecular modelling counterpart Chem3D to draw and manipulate different organic chemistry structures.
2	Drawing chemical structure with ChemDraw and Chem3D.
3	Geometry optimization techniques and their effect on geometry, energy and frequencies with butane as an example using Gaussian 09W.
4	Location of different conformations and transition states in 1,2 – dichloroethane using Gaussian 09W.
5	Calculation of IR, Raman and polarizability using the Gaussian 09W and to demonstrate the other importance of frequency calculations.
6	Calculation of the UV Vis spectrum and emission spectra of acrolein/phenol using CIS/TDDFT method.
7	Theoretical prediction of <sup>1</sup> H and <sup>13</sup> C NMR spectra and spin-spin coupling constants of ethanol.
8	Calculation of vibrational circular dichroism (VCD) Electronic circular dichroism (ECD), and Optical rotary dispersion (ORD) using the Gaussian 09W.
9	Demonstration of molecular dynamic simulation with Gromacs/Amber.
10	Demonstration of molecular docking with Autodock.

<b>4.</b>	<b>Books Recommended</b>
1	F. Jensen, Introduction to Computational Chemistry, 3 <sup>rd</sup> Edition, John Wiley & Sons, Ltd, Chichester, UK, 2017.
2	E.G. Lewars, Computational Chemistry, 3 <sup>rd</sup> Edition, Springer, Switzerland, 2016.
3	T. Chakraborty, P. Ranjan, A. Pandey, Computational Chemistry Methodology in Structural Biology and Materials Sciences, 1 <sup>st</sup> Edition, Apple Academic Press, New York, 2017.
4	J. Schrier, Introduction to Computational Physical Chemistry, University Science Books, Mill Valley, California, 2017.
5	J. Leszczynski, Handbook of Computational Chemistry, 2 <sup>nd</sup> Edition, Springer, New York, 2017.

<b>5.</b>	<b>Additional Reading Material</b>
1	D. Bove, Computational Chemistry: Theories, Methods and Applications, Nova Science Publishers, Inc., New York, 2014.
2	A. Kukol, Molecular Modelling of Proteins, 2 <sup>nd</sup> Edition, Springer, New York, 2015.

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**Department of Chemistry**  
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M.Sc. - IV (Chem), Semester – VII SURFACTANT CHEMISTRY CY451	Scheme	L	T	P	Credit
		3	0	0	03

<b>1.</b>	<b>Course Outcomes (COs):</b> <b>At the end of the course, the students will be able to</b>
CO1	Learn the basics of Surfactants and their importance in various fields of engineering.
CO2	Appraise a deep knowledge on their phase study and micellization process.
CO3	Correlate the solution behaviour surfactants.
CO4	Evaluate various models defining surfactant solutions.
CO5	Collaborate the skill to apply the advances of surfactants.

<b>2.</b>	<b>Syllabus</b>	
	<b>INTRODUCTION</b>	<b>(07 Hours)</b>
	Molecular structure of surfactants, Classification of surfactants, Properties and other criteria influencing surfactant choice, Surface activity, Surface tension, Interfacial and dynamic surface tension, Reduction of Surface, interfacial and dynamic tension by Surfactants, Efficiency and Effectiveness in surface tension Reduction: Kraft point (KP). Test methods for surface and interfacial tension measurements: Wilhelmy Plate, Pendant Drop, Du Nouy's Ring, Drop Volume (Weight), and Spinning Drop. The Economic Importance of Surfactants, Surfactants in the Environment, Biodegradation of Surfactants.	
	<b>ADSORPTION OF SURFACTANTS</b>	<b>(07 Hours)</b>
	Gibbs Monolayers, Surface Pressure, Surface Potential, Surface Rheology, Gibbs Surface Excess, Electrical Double layer, Gibbs Adsorption Isotherm, Equation of State Approach, Classification of Solid–Vapor Adsorption Isotherms: Langmuir, Freundlich, Brunauer–Emmett–Teller (BET) Isotherm for Surface Area calculation.	
	<b>PHASE BEHAVIOR OF SURFACTANT SYSTEMS</b>	<b>(06 Hours)</b>
	Solubility–Temperature relationship for Ionic surfactants, surfactant self-assembly, structure of Liquid Crystalline Phases: Hexagonal, Micellar Cubic, Lamellar, Bicontinuous Cubic. Phase Diagrams of Ionic and Nonionic Surfactants.	
	<b>MICELLE FORMATION BY SURFACTANTS</b>	<b>(09 Hours)</b>
	The Critical Micelle Concentration (CMC), Packing Parameter, Micellar structure and shape, Aggregation number ( $N_{agg}$ ), Factors Affecting the CMC in aqueous media: Structure of the Surfactant, the Hydrophobic and Hydrophilic group, the Counterion in Ionic surfactants, Degree of Binding to the Micelle, Electrolyte (inorganic/ organic), and Temperature.	
	<b>SOLUTION PROPERTIES OF SURFACTANT</b>	<b>(09 Hours)</b>
	Solubility–Temperature relationship for Surfactants, Thermodynamics of Micellization, Kinetic aspects, Equilibrium aspects, Phase Separation Model, Mass Action Model, Enthalpy and Entropy of Micellization, Driving force for micelle formation, Micellization in Polar and Non-Polar solvents, synergistic or antagonistic micellization in surfactant mixtures (Mixed Micelles). Rheology of surfactant solutions: Introduction to various rheological terms, Rheological behaviour of monomeric solutions and non-interacting micelles, Entanglement networks of rod-like micelles, the rheological behavior of bilayer phases.	
	<b>MULTIDISCIPLINARY APPLICATIONS OF SURFACTANTS</b>	<b>(07 Hours)</b>

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	Surfactants as Foaming and Antifoaming agents, as Dispersants, in Wetting (Contact angle), Spreading and Adhesion, in Nano-emulsions and Micro-emulsification, in Stabilization of suspensions, in Detergency, in Aerosols, in Personal Care and Cosmetics, in Pharmaceutical Formulations, in Agrochemicals, in the Food Industry.
	<b>(Total Contact Time: 45 Hours)</b>

<b>3.</b>	<b>Books Recommended</b>
1	T. F. Tadros, Applied Surfactants - Principles and Applications, 2 <sup>nd</sup> Edition, Wiley VCH, Verlag GmbH & Co., Germany, 2005.
2	M. R. Porter, Handbook of Surfactants, Reprint, Springer; Softcover reprint of the original 2 <sup>nd</sup> Edition, 2012.
3	J. Falbe, Surfactants in Consumer Products Theory, Technology and Applications, Softcover reprint of the original 1 <sup>st</sup> Edition, 2011.
4	D. Myers, Surfaces, Interfaces, and Colloids - Principles and Applications, John Wiley & Sons, Inc., New York, 2002.
5	M. J. Rosen, J. T. Kunjappu, Surfactants and Interfacial Phenomena, 4 <sup>th</sup> Edition, John Wiley & Sons, Inc., Hoboken, New Jersey, 2012.

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M.Sc. - IV (Chem), Semester – VIII CHEMISTRY OF NANOMATERIALS CY452	Scheme	L	T	P	Credit
		3	0	0	03

1.	<b>Course Outcomes (COs):</b> <b>At the end of the course, the students will be able to</b>
CO1	Identify synthetic procedure for processing of nanomaterials as per needs and specifications.
CO2	Acquire knowledge about the electronic, mechanical and thermal properties of nanomaterials.
CO3	Illustrate the structure and morphology of nanomaterials.
CO4	Classify the applications of nanomaterials in sustainable developments and technology.
CO5	Extend the knowledge on the synthetic routes for synthesis of nanomaterials

2.	<b>Syllabus</b>	
	<b>STRUCTURES &amp; CLASSIFICATION OF NANOMATERIALS</b>	<b>(10 Hours)</b>
	Definition of Nano, Atomic Structure and atomic size, emergence and challenges of nanoscience and nanotechnology, carbon age-new form of carbon nanostructures, influence of nano over micro/macro, size effects and crystals, large surface to volume ration, surface effects on the properties. Types of nanostructure and properties of nanomaterials: One dimensional, Two dimensional and three-dimensional nanostructured materials, Quantum Dots shell structures, metal oxides, semiconductors, composites, mechanical-physical-chemical properties.	
	<b>SYNTHETIC ROUTES OF NANOMATERIALS</b>	<b>(18 Hours)</b>
	Principle and relative merits of each technique for production of Nano-structures including ultra-thin films and multilayer by: (a) Laser Ablation technique, (b) Arc Discharge technique and (c) Mechanical Milling. Physico-chemical methods such as Chemical Vapor Deposition (CVD), Plasma, Sputtering, Hot-Wire Plasma Enhanced CVD method, and Self-assembly technique. Chemical methods: Synthesis of nanomaterials by precipitation and co-precipitation methods, Sol-Gel synthesis, Microemulsions synthesis, Hydrothermal and Solvothermal methods. Microwave assisted synthesis, Sonochemical assisted synthesis. Metal nanocrystals synthesis by polyol, and borohydrate reduction methods, Photochemical synthesis, Synthesis in supercritical fluids and Electrochemical synthesis, Synthesis of Core-Shell nanostructure, Organic –Inorganic Hybrids, Quantum dots (QDs), Carbon Nanotubes, Graphenenanosheets. Biological methods: Use of bacteria, and fungi.	
	<b>PROPERTIES, CHARACTERIZATION AND APPLICATIONS OF NANOMATERIALS</b>	<b>(17 Hours)</b>
	Properties and size effect of nanomaterials, electrical, Mechanical, Magnetic, Optical and catalytic properties, Analytical techniques for the characterization of nanostructure materials, Applications of nanomaterials in analytical chemistry, organic chemistry, biomedical sciences and sustainable development and technology.	
	<b>(Total Contact Time: 45 Hours)</b>	

3.	<b>Books Recommended</b>
1	G. A. Ozin, A. C. Arsenault, L. Cademartiri, Nanochemistry: A Chemical Approach to Nanomaterials, 2 <sup>nd</sup> Edition, The Royal Society of Chemistry, Cambridge, 2009.
2	C. N. R Rao, A. Muller, A. K Cheetham, Nanomaterials Chemistry, 1 <sup>st</sup> Edition, Wiley-VCH, 2007.

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3	G. Cao, Y. Wang, Nanostructures & Nanomaterials: Synthesis, Properties, and Applications, 2 <sup>nd</sup> Edition, World Scientific Publishing Co Pvt. Ltd; Singapore, 2011.
4	M. Naito, T. Yokoyama, K. Hosokawa, K. Nogi, Nanoparticle Technology Handbook, 3 <sup>rd</sup> Edition, Elsevier, Amsterdam, Netherlands, 2018.
5	T. Pradeep, Nano the Essentials: Understanding Nanoscience and Nanotechnology, 1 <sup>st</sup> Edition, Tata McGraw-Hill Publishing Company Ltd., New Delhi, 2007.

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**(M. Sc. IV) (Sem. – VIII)**

Sr. No.	Subject	Code	Scheme L-T-P	Credits (Min.)	Notional hours of Learning (Approx.)
<b>Eight Semester (4<sup>th</sup> Year of M. Sc.)</b>					
1	Symmetry, Spectra and Magnetism	CY402	3-1-0	4	70
2	Chemistry of Natural Products	CY404	3-0-4	5	115
3	Physical Aspects of Molecular Spectroscopy	CY406	3-1-0	4	70
4	Purification and Separation Techniques	CY408	3-0-4	5	115
5	Core Elective-2	CY4BB	3-0-0	3	55
6	MOOC Course*	CY456	3-0-0/ 3-1-0	3/4	
			<b>Total</b>	<b>24-25</b>	<b>425</b>
7	Skill Development on GMP and GLP Vocational Training / Professional Experience (Optional) (mandatory for exit)	CYV08/ CYP08	0-0-10	5	200 (20x10)

Sr. No.	Core Elective	Code	Scheme L-T-P
1	Green Chemical Processing	CY454	3-0-0
2	C-H Functionalization	CY455	3-0-0

\*Students will be required to opt any one Massive Open Online Courses (MOOC) course through NPTEL / SWAYAM platform in Semester- VII or Semester VIII excluding the courses of the existing curriculum of five years integrated programme in chemistry. Necessary approval from the department is required before the registration of the courses on above platform. The credit of the courses through above platform will be considered as per the norms of the institute.

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M.Sc. - IV (Chem), Semester – VIII SYMMETRY, SPECTRA AND MAGNETISM CY402	Scheme	L	T	P	Credit
		3	1	0	4

<b>1.</b>	<b>Course Outcomes (COs):</b> <b>At the end of the course, the students will be able to</b>
CO1	Demonstrate the principles and concepts of symmetry and group theory.
CO2	Explore the use of character tables and projection operator techniques.
CO3	Interpret molecular symmetry, symmetry operations, and molecular point groups.
CO4	Analyze electronic spectra of coordination compounds.
CO5	Describe inorganic magnetism.

<b>2.</b>	<b>Syllabus</b>	
	<b>SYMMETRY AND GROUP THEORY</b>	<b>(25 Hours)</b>
	Symmetry Operations and Elements of Symmetry: Rotational Axis of Symmetry, Plane of Symmetry, Improper Rotational Axis of Symmetry (Alternate Axis of Symmetry), Centre of Symmetry, Identity Element, Cartesian Coordinate System and Symmetry Elements, More about Symmetry Elements, Mathematical requirements for a point group, Group multiplication tables, Group generating elements, Subgroups and Classes-exercises, Point groups, Identification of Molecular point groups, Notation of Point Groups, Systematic assignment of point groups to molecules, Descent in Symmetry of Molecules with substitution, Exercises on Point Groups, Matrix Representations of Symmetry Elements, Reducible and Irreducible Representations, Properties of Irreducible Representations. Great Orthogonality Theorem (G.O.T.), Construction of character tables for $C_{2v}$ , $C_{3v}$ , $C_{2h}$ , and $C_{4v}$ point groups using G.O.T., Standard reduction formula, IR and Raman active modes of the water molecule, Symmetry restrictions of dipole moment, Symmetry criteria of optical activity, Applications of group theory to chemical bonding.	
	<b>SPECTRA &amp; MAGNETISM OF TRANSITION METAL COMPLEXES</b>	<b>(20 Hours)</b>
	The energy terms, coupling schemes, spin-spin coupling, orbital coupling, spin-orbital coupling, R-S coupling, J-J coupling scheme, selection rules, and relaxation of selection rules. Energy levels in an atom, Calculation of the number of the microstates Determining the Ground State, Term Symbols, Terms-Hunds Rule, Hole formulation (derivation of the Term Symbol for a closed sub-shell, derivation of the terms for a $d^2$ configuration), Orgel diagrams for $d^1$ to $d^9$ systems, Electronic spectra of $[Ti(H_2O)_6]^{3+}$ , $[Cu(H_2O)_6]^{2+}$ , $[V(H_2O)_6]^{3+}$ , $[Ni(H_2O)_6]^{2+}$ , $[CoF_6]^{3-}$ , $[CoCl_4]^{2-}$ and $[NiCl_4]^{2-}$ complexes, Charge transfer spectra, electronic absorption spectra of spin paired complexes, Jahn-Teller effect and electronic spectra of complexes; properties of paramagnetic complexes, magnetic moment, antiferromagnetism and ferromagnetism.	
	<b>Tutorials will be based on the coverage of the above topics separately</b>	<b>(15 Hours)</b>
	<b>(Total Contact Time: 45 Hours + 15 Hours = 60 Hours)</b>	

<b>3.</b>	<b>Tutorials will be based on</b>
1	Discussion of problems on symmetry operations and elements of symmetry.
2	Discussion of examples on lower-order point groups.
3	Discussion of examples on higher-order point groups.
4	Discussion of problems on matrix representation of symmetry elements.

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5	Discussion of problems on reducible representations.
6	Discussion of problems on irreducible representations.
7	Discussion of problems on great orthogonality theorem.
8	Discussion of problems on standard reduction formula.
9	Discussion of problems on dipole moment.
10	Discussion of problems with the calculation of the number of microstates.
11	Discussion of problems on ground state term symbols.
12	Discussion of examples of electronic spectra of metal complexes.
13	Discussion of examples of charge transfer spectra.
14	Discussion of examples of the Jahn-Teller effect.
15	Discussion of examples of magnetic properties of metal complexes.

<b>4.</b>	<b>Books Recommended</b>
1	J. E. Huheey, E. A. Keiter, R. L. Keiter, O. K. Medhi, Inorganic Chemistry: Principles of Structure and Reactivity, 4 <sup>th</sup> Edition, Pearson Education, London, 2006.
2	F. A. Cotton, Chemical Applications of Group Theory, 3 <sup>rd</sup> Edition, Wiley, Germany, 2008.
3	H. H. Jaffe, M. Orchin, Symmetry in Chemistry, Dover Publications, New York, 2012.
4	K. Veera Reddy, Symmetry and Spectroscopy of Molecules, New Age International, 2 <sup>nd</sup> Edition, India, 2020.
5	D. F. Shriver and P. W. Atkins, Inorganic Chemistry, Oxford University Press, 4 <sup>th</sup> Edition, London, 2006.

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M.Sc. - IV (Chem), Semester – VIII CHEMISTRY OF NATURAL PRODUCTS CY404	Scheme	L	T	P	Credit
		3	0	4	5

1.	<b>Course Outcomes (COs):</b> <b>At the end of the course, the students will be able to</b>
CO1	Identify and characterize various classes of natural products.
CO2	Learn the biogenesis of various important natural products.
CO3	Apply the skill to isolate and purify the natural plant products.
CO4	Demonstrate the knowledge on the role of biomolecules and their importance.
CO5	Illustrate the properties, composition, biosynthesis and synthesis of the natural products.

2.	<b>Syllabus</b>	
	<b>NATURAL PRODUCT CHEMISTRY</b>	<b>(25 Hours)</b>
	Primary and secondary metabolites, general methods for isolation and structural determination of natural products, <b>Terpenoids:</b> Classification, occurrence, isoprene rule, structure determination, stereochemistry, biosynthesis and synthesis of Citral, Geraniol, $\alpha$ -terpineol, Menthol. Vitamins A, D and E. <b>Steroids:</b> Classification, occurrence, basic skeleton, Diel's hydrocarbon and stereochemistry, synthesis of Cholesterol, Progesterone and Testosterone. <b>Alkaloids:</b> Structure determination, stereochemistry, biosynthesis and synthesis of Nicotine, Quinine and Morphine.	
	<b>NATURAL PIGMENTS</b>	<b>(06 Hours)</b>
	Classification of natural pigments, structure determination of Porphine, Porphyrin, Hb, Chl, flavones, and flavonoids.	
	<b>AMINO ACIDS, PEPTIDES AND PROTEINS</b>	<b>(07 Hours)</b>
	Classification, acid-base behaviour, Isoelectric point and electrophoresis. Structure and confirmation of peptides and proteins, Determination of structure of peptide, classical peptide synthesis solid phase peptide synthesis, Structure of peptide and proteins, Classification and function of proteins, denaturation of proteins.	
	<b>BIO-ORGANIC CHEMISTRY</b>	<b>(07 Hours)</b>
	Organic reactions in laboratory and in biological systems. Weak interactions in organic and biological systems; proximity effect in organic chemistry. Nature of biomolecular interactions. Stereo-specificity and rate enhancement in enzyme catalyzed reactions. Mechanism of hydrolysis of esters, amides in biological systems; C-C and C=C bond formation, oxidation, reduction and decarboxylation.	
	<b>Practical will be based on the coverage of the above topics separately</b>	<b>(60 Hours)</b>
	<b>(Total Contact Time: 45 Hours + 60 Hours = 105 Hours)</b>	

3.	<b>Practical will be based on</b>
1	Separation of amino acids by paper chromatography
2	Synthesis of bioactive compound
3	Extraction of essential oil from Cinnamon

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4	Isolation of Lycopene from Tomato
5	Phytochemical screening of plant extract.
6	To find the percentage of casein in milk.
7	Estimation of phenol.
8	Estimation of aniline.
9	Extraction of caffeine from tea leaves.
10.	Separation of amino acids by thin layer chromatography

<b>4.</b>	<b>Books Recommended</b>
1	I. L. Finar, Organic Chemistry: Stereochemistry and the Chemistry of Natural Products, Volume 2, 8 <sup>th</sup> Edition, Pearson Education India, 2011.
2	M. Cox, D. L. Nelson, Lehninger Principles of Biochemistry, 6 <sup>th</sup> Edition, W. H. Freeman and Company, 2013.
3	John M. Beale Jr, John H. Block, Wilson and Gisvold's Textbook of Organic, Medicinal and Pharmaceutical Chemistry, 12 <sup>th</sup> Edition, India, 2010.
4	V. Alagarsamy, Textbook of medicinal Chemistry Vol.2, 2 <sup>nd</sup> Edition, Elsevier, India, 2013.
5	S. K. Talapatra, B. Talapatra, Chemistry of Natural products: Stereochemistry, Conformation, Synthesis, Biology and Medicine, Springer-Verlag Berlin Heidelberg, 2015.

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M.Sc. - IV (Chem), Semester – VIII PHYSICAL ASPECTS OF MOLECULAR SPECTROSCOPY CY406	Scheme	L	T	P	Credit
		3	1	0	04

1.	<b>Course Outcomes (COs):</b> <b>At the end of the course, the students will be able to</b>
CO1	Gain fundamental knowledge of electromagnetic spectrum.
CO2	Employ concepts of molecular spectroscopy and selection rules.
CO3	Learn the structural elucidation by molecular spectroscopy.
CO4	Demonstrate structural characterization of a molecule through spectroscopy.
CO5	Apply selection rules in rotational, IR and Raman spectroscopy.

2.	<b>Syllabus</b>	
	<b>THE WAVE PHENOMENA</b>	<b>(15 Hours)</b>
	The Electromagnetic spectrum. General nature of electromagnetic waves; wave parameters, radiant power (Intensity), superposition of waves, diffraction, transmission, dispersion, refraction, reflection, scattering and polarization of radiation. Interaction of light and matter. Born-Oppenheimer approximation, Signal to noise ratio, Width and intensity of transition, line broadening.	
	<b>MICROWAVE SPECTROSCOPY</b>	<b>(15 Hours)</b>
	Pure Rotational Spectra – Microwave Spectroscopy. Rotational constant, moment of inertia and rotational energy levels of diatomic molecules. Rigid rotor (diatomic only), Selection rule, Spectrum: position and intensity of spectral lines. Non-rigid rotor and its effect on energy levels, Selection rule and spectrum, Isotope effect, Rotational spectra of polyatomic molecules. Numericals.	
	<b>VIBRATIONAL (IR AND RAMAN) SPECTROSCOPY</b>	<b>(15 Hours)</b>
	Polarizability, dipole moment, Rotational Raman spectra. Vibrational Spectroscopy (IR and Raman) – Diatomic Molecules. The vibrations of diatomic molecules. The harmonic oscillator. Selection rules and infrared spectra of diatomic molecules. Anharmonicity. Vibration-rotation spectra. Vibrational Raman spectra, Isotope effect, the rule of Mutual Exclusion, vibrational modes of functional groups. Structure elucidation. Numericals.	
	<b>Tutorials will be based on the coverage of the above topics separately</b>	<b>(15 Hours)</b>
	<b>(Total Contact Time: 45 Hours + 15 Hours = 60 Hours)</b>	

3.	<b>Tutorials will be based on</b>
1	Problem based on Electromagnetic spectrum.
2	Problems based on superposition of waves, diffraction, transmission, dispersion, refraction, reflection, scattering and polarization of radiation.
3	Problem based on Interaction of light and matter. Born-Oppenheimer approximation.
4	Problems based on signal to noise ratio, Width and intensity of transition, line broadening.
5	Problems based on moment of inertia.
6	Problems based on Rotational constant.

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7	Problem based on Rigid rotor (diatomic only), Selection rule, Spectrum: position and intensity of spectral lines.
8	Problems based on Isotope effect, Rotational spectra of polyatomic molecules.
9	Problems based on Vibrational Spectroscopy (IR and Raman).
10	The harmonic oscillator. Selection rules and infrared spectra of diatomic molecules.
11	Problems based on anharmonicity. Vibration-rotation spectra. Vibrational Raman spectra, Isotope effect.
12	Vibrational modes of functional groups.
13	Structure elucidation-I based on microwave, IR and RAMAN.
14	Structure elucidation-II based on microwave, IR and RAMAN.
15	Structure elucidation-III based on microwave, IR and RAMAN.

<b>4.</b>	<b>Books Recommended</b>
1	J. M. Hollas, Modern Spectroscopy, 4 <sup>th</sup> Edition, Wiley, New Jersey, United States, 2013.
2	C. N. Banwell, Elaine M. Mc Cash, Fundamentals for Molecular Spectroscopy, 4 <sup>th</sup> Edition, McGraw-Hill, New York, United States, 2017.
3	N. Levine, Quantum Chemistry, 7 <sup>th</sup> Edition, Pearson Education India, Chennai, 2016.
4	B. R. Puri, L. R. Sharma, Principles of Physical Chemistry, 49 <sup>th</sup> Edition, Vishal Publications, New Delhi, India, 2020.
5	S. Maity, N. Ghosh, Physical Chemistry Practical, 1 <sup>st</sup> Edition, New Central Book Agency (P) Ltd., India, 2012.

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M.Sc. - IV (Chem), Semester – VIII PURIFICATION AND SEPARATION TECHNIQUES CY408	Scheme	L	T	P	Credit
		3	0	4	05

<b>1.</b>	<b>Course Outcomes (COs):</b> <b>At the end of the course, the students will be able to</b>
CO1	Interpret the role of analytical techniques in separation and identification of various chemical species.
CO2	Acquire a deep knowledge on chromatography.
CO3	Apply the basics of the separation and chromatographic techniques in multidisciplinary areas
CO4	Develop the skill to apply the advances in chromatography in separation.
CO5	Propose the importance of purity of product in industrial use.

<b>2.</b>	<b>Syllabus</b>	
	<b>SEPARATION TECHNIQUES</b>	<b>(10 Hours)</b>
	Distribution law, thermodynamic derivation, application, process of extraction, factors affecting extraction, techniques for solvent extraction, conventional, liquid membranes, bulk, supported and emulsified; solid phase extraction (SPE), ion-exchange, conventional membranes. quantitative treatment of solvent extraction equilibria, classification of solvent extraction system, types of extraction system, advantages of solvent extraction system, applications of liquid extraction, solvent. extraction methods in metallurgy, solid liquid extraction.	
	<b>CHROMATOGRAPHY</b>	<b>(09 Hours)</b>
	Principle, methods of elution, ideal and non-ideal chromatography, plate theory, rate theory, reasons for broadening of lands, Van-Deemter equation and significance of terms involved, optimum velocity, resolution, methods to improve resolution. introduction to chromatographic techniques: paper chromatography, Thin Layer Chromatography (TLC) and Column Chromatography.	
	<b>GAS CHROMATOGRAPHY (GC)</b>	<b>(10 Hours)</b>
	Principle, different types of GC, mobile phase and criteria for its selection, stationary phase, sample introduction system, columns, Stationary phases used in GSC and GLC, difference between GSC and GLC, supports for liquid stationary phases, Selection of columns, packed, WCOT, SCOT, FSOT, Detectors: FID, TCD, FPB, ECD, TID - merits and demerits, temperature programming in GC, derivatisation in GC, Qualitative analysis from retention parameters, Quantitative analysis. GC-Mass Spectroscopy, Waston-Biemann Separator, Ryhage Separator, Llewellyn Separator, Instrumentation, Applications.	
	<b>LIQUID CHROMATOGRAPHY</b>	<b>(09 Hours)</b>
	Principle of LC, instrument and significance of each component, Pumps, Guard column, Stationary phases (solid, liquid), Mobile Phases, Bonded phase supports, Detectors - Fluorescence detector, RI detector, electrochemical detector, Normal phase and Reversed phase. Introduction to HPLC and UPLC, LC Mass Spectroscopy, LC/MS interfaces, solvent removal and ionization, atmospheric-pressure interfaces, electro spray interface, ion spray interface, secondary detectors.	
	<b>ION-EXCHANGE CHROMATOGRAPHY</b>	<b>(07 Hours)</b>

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	Introduction: Principle of exchange resins, swelling capacity of resin and its determination, effect of different parameters on exchange behavior, techniques of IEC, eluent suppressor column. Applications.	
	<b>Practical will be based on the coverage of the above topics separately</b>	<b>(60 Hours)</b>
	<b>(Total Contact Time: 45 Hours+ 60 Hours= 105 Hours)</b>	

<b>3.</b>	<b>Practical will be based on</b>
1	The Analysis of Artificial Sweeteners and Additives in Beverages by HPLC.
2	Determination of Caffeine in Beverages by High Performance Liquid Chromatography.
3	High Performance Liquid Chromatography of Some Analgesic Compounds.
4	Quantitative HPLC Analysis of a Psychotherapeutic Medication: Simultaneous Determination of Amitriptyline Hydrochloride and Perphenazine.
5	Determination of Sodium, Potassium, and Chloride concentration using Ion Chromatography.
6	Determine the caffeine content in various beverages (e.g., coffee, tea, energy drinks) using GC.
7	Gas Chromatographic Determination of Environmentally Significant Pesticides.
8	Analyze and compare the composition of essential oils extracted from different plants using GC.
9	Separate and identify isomers of dichlorobenzenes using GC.
10	Separate and identify isomers of xylenes using GC.

<b>4.</b>	<b>Books Recommended</b>
1	G. D. Christian, P. K. Dasgupta, K. A. Schug, Analytical Chemistry, 7 <sup>th</sup> Edition, Wiley-Interscience, New Jersey, 2013.
2	R. M. Verma, Analytical Chemistry - Theory and Practice, 3 <sup>rd</sup> Edition, CBS Publication, New Delhi, 2018.
3	J. M. Miller, Chromatography Concepts and Contrasts, 2 <sup>nd</sup> Edition, Wiley-Interscience, New Jersey, 2005.
4.	D. A. Skoog, F. J. Holler, S. R. Crouch, Principles of Instrumental Analysis, 7 <sup>th</sup> Edition, Cengage Learning, Massachusetts, 2017.
5.	H. M. McNair, J. M. Miller, N. H. Snow, Basic Gas Chromatography, 3 <sup>rd</sup> Edition, John Wiley Interscience, 2019.

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M.Sc. - IV (Chem), Semester – VII GREEN CHEMICAL PROCESSING CY454	Scheme	L	T	P	Credit
		3	0	0	03

<b>1.</b>	<b>Course Outcomes (COs):</b> <b>At the end of the course, the students will be able to:</b>
CO1	Explain green chemistry concepts and its significance for environment sustainability.
CO2	Differentiate between conventional and green raw materials.
CO3	Design green process and analyze sustainability of materials.
CO4	Analyze sustainability of chemical processes.
CO5	Establish various applications of green processes.

<b>2.</b>	<b>Syllabus</b>	
	<b>ENVIRONMENT SUSTAINABILITY OF CHEMICAL PROCESSES</b>	<b>(10 Hours)</b>
	Introduction to Green Chemistry, Green Chemistry Principles, Sustainable Solvents (Supercritical fluids, Liquid polymers, Renewable solvents, Ionic liquids and Deep eutectic solvents), Waste minimization and design for degradation, Use of renewable feed stocks.	
	<b>GREEN SYNTHETIC ROUTES</b>	<b>(12 Hours)</b>
	ChemieDouce approach of material synthesis, Sol-gel method, Intercalation, Anchoring, Pillaring, Sonochemical method, Microwave synthesis, Mechanochemical synthesis, Electrochemical synthesis and Photochemical synthesis.	
	<b>GREEN MATERIALS</b>	<b>(08 Hours)</b>
	Zeolites, Heteropoly acids, Metal organic frameworks and Sulfated zirconia as Catalysts.	
	<b>APPLICATIONS OF GREEN PROCESSES</b>	<b>(15 Hours)</b>
	For active pharma ingredients (API), polymers, green fuel production and polymer membrane fuel cells, CO <sub>2</sub> utilization and carbon credit and biomass to value added products.	
	<b>(Total Contact Time: 45 Hours)</b>	

<b>3.</b>	<b>Books Recommended</b>
1	M. Lancaster, Green Chemistry: An Introductory Text, 4 <sup>th</sup> Edition, Royal Society of Chemistry, 2025.
2	E. Lichtfouse, J. Schwarzbauer, Green Materials for Energy, Products and Depollution (Environmental Chemistry for a Sustainable World), Softcover reprint of the original 1 <sup>st</sup> Edition, 2016.
3	G. Rothenberg, Catalysis: Concepts and Green Applications, 2 <sup>nd</sup> Edition, Wiley-VCH Verlag GmbH & Co. KGaA, Weinheim, UK, 2017.
4	V. K. Ahluwalia, Green Chemistry: Environmentally Benign Reactions, 3 <sup>rd</sup> Edition, Ane Books Pvt. Ltd., India, 2021.
5	R. Xu, W. Pang, O. Huo, Modern Inorganic Synthetic Chemistry, 2 <sup>nd</sup> Edition, Amsterdam, 2011.

<b>4.</b>	<b>Additional Reading Material</b>
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1	P. T. Anastas, J. C. Warner, Green Chemistry: Theory and Practice, 1 <sup>st</sup> Edition, Oxford University Press, 2000.
2	P. Wasserscheid, A. Stark, Green Solvents, Volume 6, Ionic liquids, in P. Anastas, Handbook of Green Chemistry, 1 <sup>st</sup> Edition, Wiley-VCH Verlag GmbH & Co. KGaA, Weinheim, 2014.

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M.Sc. - IV (Chem), Semester – VIII C-H FUNCTIONALIZATION CY455	Scheme	L	T	P	Credit
		3	0	0	

<b>1.</b>	<b>Course Outcomes (COs):</b> <b>At the end of the course, the students will be able to</b>
CO1	Acquire deep knowledge of advanced organometallic chemistry
CO2	Identify how these individual reactions make up a catalytic cycle
CO3	Examine C-H interactions with transition metals and how C-H activation can occur at a transition metal center.
CO4	Explain the role of photocatalysis in modern synthetic methodology.
CO5	Study the importance of catalysis in industrial processes.

<b>2.</b>	<b>Syllabus</b>	
	<b>Advanced Organometallic Chemistry of Transition Elements</b>	<b>(18 Hours)</b>
	Introduction to the fundamentals of homogeneous catalysis and the mechanisms in organometallic chemistry: Oxidative addition, sigma bond metathesis, reductive elimination, insertion and elimination. Metal mediated C-C and C-X coupling reactions Heck, Negishi, Suzuki, and Stille, Sonogashira, Nozaki-Hiyama, Kumada, Buchwald-Hartwig, Catellani, Fujiwara-Moritani reactions and their synthetic utility in drug synthesis. Directed orthometalation, Metal (Pd, Rh) catalyzed C-H activation reactions and their synthetic utility, Copper and rhodium based carbene and nitrene complexes, Cyclopropanation, Rh catalyzed C-H insertion and aziridination reactions including asymmetric version, Noyori asymmetric hydrogenation. Introduction to N-heterocyclic carbene metal complexes. Tebbe's reagent, Pauson-Khand reaction, Hydroformylation, and Carbonylation reactions.	
	<b>C-H Bond Activation and Functionalization</b>	<b>(15 Hours)</b>
	Interaction of metal centers with C-H bonds, agostic interactions and C-H activation, electrophilic and metalloradical activation. Organic synthesis involves chelation-assisted C-H activation, ortho-C-H activation, and Distal C-H activation in heterocycles synthesis. C-H, C=C and C≡C activated annulation reactions. Important synthetic approaches via C-X (X= C, N, O, S etc.) bond activation. Role of non-metallic activation of bonds in organic synthesis.	
	<b>Visible Light Photocatalysis in Organic Chemistry</b>	<b>(12 Hours)</b>
	Introduction, Basics of the photocatalytic cycle, Generation of radicals, C—X (X = N, O, S etc.) bond formation, C-C bond formation, Atom transfer radical addition reactions, Cycloaddition reactions, Arene functionalization, Application of visible-light-mediated reactions to the synthesis of pharmaceutical compounds.	
	<b>(Total Contact Time: 45 Hours)</b>	

<b>3.</b>	<b>Books Recommended</b>
1	R. H. Crabtree, The Organometallic Chemistry of the Transition Metals, 6 <sup>th</sup> Edition, John Wiley & Sons, Germany, 2014.
2	D. W. C. MacMillan, Visible light photocatalysis in organic chemistry, 1 <sup>st</sup> Edition, John Wiley, Germany, 2018.

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3	J. Yu Z. Shi, C-H Activation (Topics in Current Chemistry Book 292), 1 <sup>st</sup> Edition, Springer, London, 2010.
4	J. Yu, Science of Synthesis: Catalytic Transformations via C-H Activation, Volume 1, 1 <sup>st</sup> Edition, Thieme, Germany, 2016.
5	B. D. Gupta and A. J. Elias, Basic Organometallic Chemistry- Concepts, Synthesis, and Applications, Universities Press Private Limited, India, 2011.

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**(M. Sc. V) (Sem. – IX)**

Sr. No.	Subject	Code	Scheme L-T-P	Credits (Min.)	Notional hours of Learning (Approx.)
<b>Ninth Semester (5<sup>th</sup> Year of M. Sc.)</b>					
1	Quantum Chemistry	CY501	3-0-0	3	55
2	Heterocycles and Organic Synthesis	CY503	3-0-0	3	55
3	Research Methodology in Chemistry	CY505	3-0-0	3	55
4	Core Elective-3	CY5AA	3-0-0	3	55
5	Core Elective-4	CY5BB	3-0-0	3	55
6	Research Training in Chemical Sciences	CYP09	0-0-10	5	200 (20x 10)
			<b>Total</b>	<b>20</b>	<b>475</b>

Sr. No.	Core Elective	Code	Scheme L-T-P
1	Catalysis	CY551	3-0-0
2	Medicinal Chemistry	CY552	3-0-0
3	Supramolecular Chemistry	CY553	3-0-0
4	Nuclear Chemistry	CY554	3-0-0

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M.Sc. - V (Chem), Semester – IX QUANTUM CHEMISTRY CY501	Scheme	L	T	P	Credit
		3	0	0	3

<b>1.</b>	<b>Course Outcomes (COs):</b> <b>At the end of the course, the students will be able to</b>
CO1	Memorize the fundamentals of classical quantum chemistry.
CO2	Gain knowledge about the basics of various operators with their applications.
CO3	Develop skill to calculate eigen values and eigen functions for various systems.
CO4	Interpret the mathematical problems based on quantum mechanics.
CO5	Learn advanced quantum mechanics for multi-electron systems

<b>2.</b>	<b>Syllabus</b>	
	<b>BASICS OF QUANTUM</b>	<b>(10 Hours)</b>
	Rutherford atomic model, Bohr theory of hydrogen atom, Black body radiation, Classical Theory of Rayleigh-Jean, and Planck's theory, Photoelectric effect, Einstein's Quanta, Compton effect, Dual nature of electromagnetic radiation, de Broglie's hypothesis, Wave particle duality, Matter wave, Concept of wave packets, Uncertainty principle, its various mathematical forms and its justifications. Numericals.	
	<b>OPERATORS AND EIGEN FUNCTIONS</b>	<b>(12 Hours)</b>
	Operators, Linear operators, Hermitian operators, Postulates of Quantum Mechanics, Schrödinger wave equation (Time dependent and time independent), Solution of Schrödinger equation as wave function and energy (eigen values and eigen functions), Commutators and their implication with respect to $x$ , $p_x$ , Expectation values, Properties of eigen functions, Energy quantization for hydrogen atom. Numericals.	
	<b>SOLUTION OF SCHRÖDINGER EQUATION</b>	<b>(14Hours)</b>
	Simple systems: 1-D and 3-D box (eigen values, eigen functions, expectation values, quantum numbers, degeneracy, probability density), Simple Harmonic Oscillator: Setting the Schrödinger equation, derivation, eigen values and eigen functions, zero-point energy, Basics of hydrogen atom and rigid rotar.	
	<b>MOLECULAR QUANTUM MECHANICS</b>	<b>(09 Hours)</b>
	Molecular orbital theory (MOT), Valence bond theory (VBT), Hybridization, Calculation of the coefficients of AOs used in hybridization, Huckel molecular orbital theory (HMOT) of conjugated systems.	
	<b>(Total Contact Time: 45 Hours)</b>	

<b>3.</b>	<b>Books Recommended</b>
1	B. R. Puri, L. R. Sharma, Principles of Physical Chemistry, 49 <sup>th</sup> Edition, Vishal Publications, New Delhi, India, 2020.
2	Donald A. McQuarrie, Quantum Chemistry, Viva Student Edition, Viva, New Delhi, India 2016.
3	M. Reiher, Relativistic Quantum Chemistry: The Fundamental Theory of Molecular Science, 2 <sup>nd</sup> Edition, John Wiley, Hoboken, New Jersey, US, 2014.
4	N. Levine, Quantum Chemistry, 7 <sup>th</sup> Edition, Pearson Education India, Chennai, 2016.

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5	S. Maity, N. Ghosh, Physical Chemistry Practical, 1 <sup>st</sup> Edition, New Central Book Agency (P) Ltd., India, 2012.
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M.Sc. - V (Chem), Semester – IX HETEROCYCLES AND ORGANIC SYNTHESIS CY503	Scheme	L	T	P	Credit
		3	0	0	03

1.	<b>Course Outcomes (COs):</b> <b>At the end of the course, the students will be able to</b>
CO1	Discuss synthesis, reactivity and significance of various types of heterocycles.
CO2	Demonstrate the importance of microwave assisted synthesis over conventional methods.
CO3	Utilize synthetic strategies.
CO4	Analyze multicomponent reactions and discuss its advantage over traditional approach.
CO5	Learn synthesis, reactivity and significance of various types of heterocycles.

2.	<b>Syllabus</b>	
	<b>THREE AND FOUR MEMBERED HETEROCYCLES</b>	<b>(08 Hours)</b>
	Synthesis, reactivity, aromatic character and importance of following three membered heterocyclic rings: Azirines, Oxiranes, Diaziridines, Oxaziridines, Azetidines, Oxetanes.	
	<b>FIVE AND SIX MEMBERED HETEROCYCLES WITH ONE AND TWO HETEROATOMS</b>	<b>(07 Hours)</b>
	Synthesis, reactivity, aromatic character and importance of following heterocyclic rings: Pyrazole, Imidazole, Oxazole, Thiazole, Isoxazole, Pyrimidine, Pyrazine.	
	<b>CONDENSED FIVE AND SIX MEMBERED HETEROCYCLES</b>	<b>(07 Hours)</b>
	Synthesis, reactivity, aromatic character and importance of Benzofuran, Benzothiophene, Coumarins and Chromones, Condensed five membered heterocycles- Benzoxazole, Benzothiazole, Benzimidazole.	
	<b>FIVE AND SIX MEMBERED HETEROCYCLES WITH MORE THAN TWO HETEROATOMS</b>	<b>(09 Hours)</b>
	Synthesis, reactivity, aromatic character and importance of following heterocycles: 1,2,3-triazole, 1,2,4-triazole, 1,2,4-oxadiazole, 1,3,4-oxadiazole, 1,2,5-oxadiazole, tetrazole, 1,2,3-triazine, 1,2,4-triazine, 1,3,5-triazine, tetrazine, purines, pyrimidines and pteridines.	
	<b>MICROWAVE ASSISTED ORGANIC SYNTHESIS</b>	<b>(07 Hours)</b>
	Microwave effect vs. thermal effect, microwave reactors, reactions in homogeneous media and solvent, reactions of reagent supported on mineral acids, solvent free phase transfer catalysis.	
	<b>MULTI-COMPONENT REACTIONS</b>	<b>(07 Hours)</b>
	Relative reactivities of functional group to MCR, selected reactive functionalities in MCR like carbonyl, isocyanide; types of MCR, Diversity in MCR: Ugi, Passerini, Biginelli and Mannich reactions.	
	<b>(Total Contact Time: 45 Hours)</b>	

Subject Code: ##nXX; ##: Department Identity, n: Year, XX: Subject Sequence number XX: last digit 0 (subject offered in both ODD and EVEN semesters, XX: 01 to 30 – last digit ODD and EVEN for ODD and EVEN semesters (Mandatory Core), XX: 31 to 50 (Optional Core), XX: 51 to 99 (Elective), Subjects list for Minor and Honor (M/H#1-4), Subjects list for Specialization track (#1-4) EG: Engineering Subject, SC: Science Subject (offered combinedly by departments) (SVNIT Surat)

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<b>3.</b>	<b>Books Recommended</b>
1	J. A. Joule, K. Mills, Heterocyclic Chemistry, 5 <sup>th</sup> Edition, Wiley Blackwell, West Sussex, 2010.
2	A.R. Katritzky, C.A. Ramsden, J.A. Joule, V.V. Zhdankin, Handbook of Heterocyclic Chemistry, 3 <sup>rd</sup> Edition, Elsevier, Oxford, 2010.
3	R. R. Gupta, M. Kumar, V. Gupta, Heterocyclic Chemistry, Volume 1 and 2, 3 <sup>rd</sup> Edition, Springer, New York, 2013.
4	T. J. J. Muller, Science of Synthesis: Multicomponent Reactions, Volume 1, 1 <sup>st</sup> Edition, Thieme publishers, Stuttgart, 2014.
5	S. C. Ameta, P. B. Punjabi, R. Ameta, C. Ameta, Microwave-Assisted Organic Synthesis: A Green Chemical Approach, Apple Academic Press, Toronto, 2015.

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M.Sc. - V (Chem), Semester – IX RESEARCH METHODOLOGY IN CHEMISTRY CY505	Scheme	L	T	P	Credit
		3	0	0	03

1.	<b>Course Outcomes (COs):</b> <b>At the end of the course, the students will be able to</b>
CO1	Impart knowledge of introduction and purpose of research.
CO2	Explore the importance of literature review to identify research problem.
CO3	Practice research paper writing and present research data.
CO4	Interpret data obtained from characterization techniques using various software.
CO5	Learn chemical safety and research ethics.

2.	<b>Syllabus</b>	
	<b>RESEARCH BASICS</b>	<b>(05 Hours)</b>
	Basics of scientific research, research process and steps involved, Hypothesis, Research proposals and aspects, literature survey, sources of information, review.	
	<b>SCIENTIFIC REPORT WRITING AND PUBLICATION PROCESS</b>	<b>(08 Hours)</b>
	Writing of research report and synopsis (steps involved), paper writing (steps involved), review writing, report preparation, publication process, selection of journals, citation index, impact factor, <i>h</i> -index.	
	<b>DATA AND SAMPLE COLLECTION</b>	<b>(12 Hours)</b>
	Datatypes and collection: qualitative and quantitative, data processing, data analysis. Sampling: Concepts of Statistical Population, Sample, Sampling Frame, Sampling Error, Sample Size, Non-Response. Characteristics of a good sample. Probability Sample – Simple Random Sample, Systematic Sample, Stratified Random Sample and Multi-stage sampling. Determining size of the sample– Practical considerations in sampling and sample size.	
	<b>DATA ANALYSIS</b>	<b>(05 Hours)</b>
	Data Preparation – Univariate analysis (frequency tables, bar charts, pie charts, percentages), Bivariate analysis – Cross tabulations and Chi-square test including testing hypothesis of association.	
	<b>SOFTWARES FOR CHEMISTRY RESEARCH</b>	<b>(12 Hours)</b>
	General awareness of software packages and other scientific applications. Application and uses of common software in chemistry-SciFinder, Origin, ChemSketch, Chemdraw, softwares for NMR: Mestronova and Topspin, XPS Peak 41 and Image for micrographs.	
	<b>CHEMICAL SAFETY AND ETHICS OF RESEARCH</b>	<b>(03 Hours)</b>
	Safety rules of laboratory acquaintance of experimental set up, importance of safety and security of data. Research ethical issues, Intellectual property right, Copy right, royalty, citation and acknowledgement, Reproducibility, plagiarism.	
	<b>(Total Contact Time: 45 Hours)</b>	

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<b>3.</b>	<b>Books Recommended</b>
1	Kumar, R., Research Methodology-A Step by Step Guide for Beginners, 3 <sup>rd</sup> Edition, Pearson Education, Delhi, 2011.
2	Montgomery, D.C, Design and Analysis of Experiments, 10 <sup>th</sup> Edition, Wiley India, 2019.
3	Kothari, C. K, Research Methodology-Methods and Techniques, 2 <sup>nd</sup> Edition., New Age International, New Delhi, 2019.
4.	Chakraborty, T., Ledwani, L. Research Methodology in Chemical Sciences, 1 <sup>st</sup> Edition, Apple Academic Press, New York, 2016.
5.	Mendham, J. et al., Vogel's Textbook of Quantitative Chemical Analysis, 6 <sup>th</sup> Edition, Pearson Education 2009.

Subject Code: ##nXX; ##: Department Identity, n: Year, XX: Subject Sequence number XX: last digit 0 (subject offered in both ODD and EVEN semesters, XX: 01 to 30 – last digit ODD and EVEN for ODD and EVEN semesters (Mandatory Core), XX: 31 to 50 (Optional Core), XX: 51 to 99 (Elective), Subjects list for Minor and Honor (M/H#1-4), Subjects list for Specialization track (#1-4) EG: Engineering Subject, SC: Science Subject (offered combinedly by departments) (SVNIT Surat)

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M.Sc. - V (Chem), Semester – IX CATALYSIS CY551	Scheme	L	T	P	Credit
		3	0	0	03

<b>1.</b>	<b>Course Outcomes (COs):</b> <b>At the end of the course, the students will be able to:</b>
CO1	Analyse basics and principle of catalysis and their potential to be used for range of applications.
CO2	Obtain knowledge on catalyst preparation and its evaluation.
CO3	Interpret characterization data of catalysts, correlate structure and properties of catalysts and learn how this insight can be used to design new catalysts.
CO4	Obtain knowledge on various microscopic, spectral and thermal techniques for catalyst characterization.
CO5	Compile and propose new applications of catalysis in multidisciplinary areas.

<b>2.</b>	<b>Syllabus</b>	
	<b>INTRODUCTION TO CATALYSIS CONCEPTS</b>	<b>(06 Hours)</b>
	Activation energy, activity, selectivity, stability, enantioselectivity, promoter, concept of TON and TOF, catalyst deactivation, homogeneous catalysis, heterogeneous catalysis, homogenized heterogeneous catalysis, environmental catalysis, phase transfer catalysis and bio-catalysis.	
	<b>CATALYST TYPES</b>	<b>(05 Hours)</b>
	Metal based catalysts, metal oxides, metal nanoparticles, supported catalysts, solid acid catalysts and shape selective catalysts.	
	<b>CATALYST PREPARATION METHODS</b>	<b>(06 Hours)</b>
	Precipitation, impregnation, sol-gel, dry-gel, template method, hydrothermal method, vapour phase method, microwave method, solid state crystallization method, ion exchange and catalyst preparation by functionalization, and an overview of commercial manufacturing of catalysts.	
	<b>CATALYST CHARACTERIZATION CONCEPTS</b>	<b>(10 Hours)</b>
	Catalyst characterization by thermal methods, by spectral methods (X-Ray, IR, NMR), by electron microscopic methods (SEM and TEM), N <sub>2</sub> sorption isotherms studies for surface area and pore size distribution determination of catalysts, Acidity and basicity measurements of catalysts by NH <sub>3</sub> -TPD and CO <sub>2</sub> adsorption methods.	
	<b>ENVIRONMENTAL AND INDUSTRIAL APPLICATIONS OF HETEROGENOUS CATALYSIS</b>	<b>(18 Hours)</b>
	Application in H <sub>2</sub> production (via dry reforming or steam reforming or electrolysis), fertilizer industries (e. g. NH <sub>3</sub> synthesis), hydrogenation reaction, shape selective catalysis in organic and petrochemical transformations, biomass conversion, plastic waste conversion to value added products.	
	<b>(Total Contact Time: 45 Hours)</b>	

<b>3.</b>	<b>Books Recommended</b>
1	G. C. Bond, Catalysis by Metals, 2 <sup>nd</sup> Edition, Academic Press: London, 1962.

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2	Jiří Čejka, Russell E Morris, Petr Nachtigall; Zeolites in Catalysis: Properties and Applications, Royal Society of Chemistry, 2017.
3	J. Cejka, A. Corma, S. Zones, Zeolites and Catalysis Synthesis, Reactions and Applications, 1 <sup>st</sup> Edition, Wiley-VCH Verlag GmbH & Co. KGaA, Weinheim, 2009.
4	W Delgass; Spectroscopy in Heterogeneous Catalysis, Elsevier, 2012.
5	G. Rothenberg, Catalysis: Concepts and Green Applications, 2 <sup>nd</sup> Revised and Enlarged Edition, John Wiley & Sons, 2017.

<b>4.</b>	<b>Additional Reading Material</b>
1	C. N. R. Rao and K. Biswas, Essentials of Inorganic Materials Synthesis, 1 <sup>st</sup> Edition, John Wiley & Sons, Inc., India, 2015.
2	Y. B. Pottathara, S. Thomas, N. Kalarikkal, Y. Grohens, V. Kokol, Nanomaterials Synthesis: Design, Fabrication and Applications, 1 <sup>st</sup> Edition, A volume in Micro and Nano Technologies, Elsevier, India, 2019.

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M.Sc. - V (Chem), Semester – IX MEDICINAL CHEMISTRY CY552	Scheme	L	T	P	Credit
		3	0	0	03

<b>1.</b>	<b>Course Outcomes (COs):</b> <b>At the end of the course, the students will be able to</b>
CO1	Recognise the drug metabolic pathways, adverse effect and therapeutic value of drugs.
CO2	Gain knowledge of structural activity relationship of different class of drugs.
CO3	Compute ligand and structure-based drug design.
CO4	Learn the mechanism pathways of different class of medicinal compounds.
CO5	Develop skill regarding the chemistry of drugs with respect to their pharmacological activity.

<b>2.</b>	<b>Syllabus</b>	
	<b>INTRODUCTION TO DRUG DISCOVERY AND DEVELOPMENT</b>	<b>(07 Hours)</b>
	Process of drug discovery, Stages of drug discovery and development, Methods of Lead discovery, Random screening, Non-random screening, serendipitous drug discovery. Rational and modern drug discovery.	
	<b>DRUG-RECEPTOR INTERACTION</b>	<b>(07 Hours)</b>
	Types of receptors, Drug-Receptor interaction, agonist, antagonist, partial agonist, enzyme inhibition: competitive, non-competitive and allosteric inhibition.	
	<b>PHYSICOCHEMICAL PROPERTIES IN RELATION TO BIOLOGICAL ACTION</b>	<b>(08 Hours)</b>
	Ionization, Solubility, Partition Coefficient, Hydrogen bonding, Protein binding, Chelation, Bio-isosterism, Optical and Geometrical isomerism. Drug metabolism: principles- Phase I and Phase II metabolic reactions. Factors affecting drug metabolism including stereo chemical aspects.	
	<b>SAR AND QSAR</b>	<b>(07 Hours)</b>
	SAR of some important chemical scaffold including barbiturates, quinolone, antihistaminic, estrogen etc. Introduction to QSAR and its application in drug design.	
	<b>DRUG DESIGN APPROACHES</b>	<b>(08 Hours)</b>
	Ligand and structure-based drug design. Understanding of virtual screening, Molecular Docking, Pharmacophore modelling, Protein data bank (PDB), overview of chemical databases like NCI, zinc, PubChem etc. overview of different software used for drug design.	
	<b>MECHANISMS AND THERAPEUTIC APPLICATIONS OF SOME IMPORTANT DRUGS</b>	<b>(08 Hours)</b>
	Antacid, oral contraceptive, anticancer, antihypertensive, antidiabetic, anxiolytics, anti-allergic.	
	<b>(Total Contact Time: 45 Hours)</b>	

<b>3.</b>	<b>Books Recommended</b>
1	M.E. Wolf, ed, The Basis of Medicinal Chemistry, Burger's Medicinal Chemistry John Wiley and Sons, 8 <sup>th</sup> Edition, New York 2021.
2	Y. C. Martin, Quantitative Drug Design, Dekker, 2 <sup>nd</sup> 8 <sup>th</sup> Edition, New York 2010.
3	J.M. Beale, J.H. Block, Wilson and Gisvolds's Text Book of Organic Medicinal & Pharmaceutical Chemistry, Lippincott Williams & Wilkins, 12 <sup>th</sup> Edition, New York 2011.

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4.	T. L. Lemke, D. A. Williams, V. F. Roche, S. W. Zito, Foye's Principles of Medicinal Chemistry, Lippincott, Williams Wilkins, 7 <sup>th</sup> Edition, Baltimore 2013.
5	G.L. Patrick, An Introduction to Medicinal Chemistry, Oxford University Press, 7 <sup>th</sup> Edition, Oxford 2023.

<b>4.</b>	<b>Additional Reading Material</b>
1	A. Korolkovas, Essentials of Medicinal Chemistry, Wiley Interscience, 2 <sup>nd</sup> Edition, New York, 2008.
2	H.J. Smith, H. Williams, Introduction to the principles of Drug Design, 4 <sup>th</sup> Edition, Wright Boston 2005.
3	R. B. Silverman, The Organic chemistry of drug design and drug action, Academic Press New York 3 <sup>rd</sup> Edition, 2014.

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M.Sc. - V (Chem), Semester – IX SUPRAMOLECULAR CHEMISTRY CY553	Scheme	L	T	P	Credit
		3	0	0	03

<b>1.</b>	<b>Course Outcomes (COs):</b> <b>At the end of the course, the students will be able to</b>
CO1	Acquire basic and need of supramolecular chemistry.
CO2	Study on thermodynamic and kinetic aspects of host-guest chemistry.
CO3	Gain advance knowledge on artificial host molecules.
CO4	Learn basic and applications of molecular self-assembly.
CO5	Explore the application of supramolecular chemistry in device fabrication.

<b>2.</b>	<b>Syllabus</b>	
	<b>FUNDAMENTALS OF SUPRAMOLECULAR CHEMISTRY</b>	<b>(09 Hours)</b>
	Molecules, super molecules and supramolecular Chemistry, non-covalent interactions, complementarity and cooperativity, supramolecular chemistry of life.	
	<b>HOST-GUEST CHEMISTRY</b>	<b>(14 Hours)</b>
	Host-guest complexation, Thermodynamics of host-guest complexation, Molecular recognition – factors involved, Molecular receptors/ Ionophores – design principles; Molecular receptors for cations, anions and neutral molecules, Crown ethers, cryptands, spherands, cyclodextrins, cucurbituril, and calixarenes, cavitands, molecular clips, clefts and tweezers, Threading of a linear molecule through a cyclic molecule, Creation of rotaxanes and catenanes.	
	<b>SELF-ASSEMBLY</b>	<b>(12 Hours)</b>
	Biological self-assembly, self-assembly in synthetic systems, self-assembling coordination compounds, capsules, helicates and molecular knots, organic and inorganic nanomaterials, Crystal nucleation and growth, understanding crystal structures, supramolecular gels, supramolecular polymers, Amphiphiles and their aggregation, Aggregation induced emission and quenching.	
	<b>MOLECULAR DEVICES</b>	<b>(10 Hours)</b>
	Supramolecular photochemistry and devices, chemosensors, molecule-based electronics: Molecular wires, molecular switches, molecular logic, molecular rectifiers and molecular electronic devices.	
	<b>(Total Contact Time: 45 Hours)</b>	

<b>3.</b>	<b>Books Recommended</b>
1	J. W. Steed and J. L. Atwood, Supramolecular Chemistry, 3 <sup>rd</sup> Edition, John Wiley, New York, 2022.
2	K. Ariga and T. Kunitake, Supramolecular chemistry-fundamentals and applications, 1 <sup>st</sup> edition, Springer, Heidelberg, 2006.
3	J.W. Steed, D.R. Turner, K.J. Wallace, Core concepts in supramolecular chemistry and nanochemistry, 1 <sup>st</sup> Edition, Wiley, USA, 2007.
4	H. Dodziuk, Introduction to supramolecular chemistry, 1 <sup>st</sup> Edition, Springer (India) Pvt. Ltd., New Delhi, 2002.
5	J. M. Lehn, Supramolecular chemistry, 1 <sup>st</sup> Edition, Wiley-VCH, Germany, 1995.

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<b>M.Sc. - V (Chem), Semester – IX</b> <b>NUCLEAR CHEMISTRY</b> <b>CY554</b>	<b>Scheme</b>	<b>L</b>	<b>T</b>	<b>P</b>	<b>Credit</b>
		<b>3</b>	<b>0</b>	<b>0</b>	<b>03</b>

<b>1.</b>	<b>Course Outcomes (COs):</b> <b>At the end of the course, the students will be able to</b>
CO1	Acquire knowledge and understanding on some nuclear models for calculating nuclear properties.
CO2	Interpret the theoretical background for the synthesis and separation of man-made radio isotopes as well elements.
CO3	Correlate fundamental knowledge of mechanism and functioning of nuclear detectors based on interaction radiation on matter.
CO4	Prioritize the knowledge of different types of nuclear reactions, mechanism of nuclear reactions, and calculation of fission probability.
CO5	Justify the relationship between the statistics and radiation detection methods.

<b>2.</b>	<b>Syllabus</b>	
	<b>FUNDAMENTALS OF NUCLEAR CHEMISTRY</b>	<b>(10 Hours)</b>
	Nuclear angular momentum, magnetic dipole moment and electronic quadruple moment, parity of nuclear energy states, binding energy, nuclear size, root mean square radius of atomic nucleus, nuclear models – nuclear forces, liquid drop model, formulation of semi-empirical binding energy equation, mass parabola, application of binding energy equation, compound nucleus theory (qualitative approach), optical model, , shell model, nuclear magic number and its derivation from nuclear potential well, calculation of nuclear spin, nuclear isomerism.	
	<b>NUCLEAR REACTIONS</b>	<b>(10 Hours)</b>
	nuclear reactions – energetics, mechanism, models, nuclear fission and nuclear fusion, Q-value and cross section of nuclear reaction, calculation of fission probability, nuclear reactions in stars, solar neutrino hypothesis, alpha decay paradox - explanation in terms of tunnel effect, explanation of beta and gamma transition, selection rules synthetic elements: theoretical background, production and separation of super heavy elements, production and nuclear properties of transactinide elements, fundamental and experimental aspects of one-atom-at a time chemistry.	
	<b>NUCLEAR EQUILIBRIUM</b>	<b>(07 Hours)</b>
	Successive disintegration, Bateman equation, secular and transient equilibrium, no equilibrium; special successive disintegrations, formation of radioelement in a nuclear reaction, hot-atom, positron annihilation, probability of positronium formation, reactions of positronium ion, chemistry of muonium and pionium ions, Szilard-Chalmer reaction, retention of activity, primary and secondary retention, synthesis of labelled compounds, overview of activation analyses.	
	<b>RADIATION AND MATTER</b>	<b>(08 Hours)</b>
	Different radiations, quarks, interactions of heavy charged particles, energy loss, collisional and radiative stopping power - related semi-empirical calculations, Bethe formula, mean excitation energy, range, slowing down time, Cerenkov radiation, attenuation coefficient, interaction between electrons & matter, synchrotron radiation, Mu-meson, range-energy relation for	

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	mono-energetic electrons, pair production, interaction of neutrons with matter, radiative capture, types of reactors & accelerators, carbides and nitrides as nuclear fuel substrate, four-factor formula, nuclear hazards and nuclear waste.
	<b>STATISTICAL METHODS IN RADIOACTIVITY</b> <span style="float: right;"><b>(10 Hours)</b></span>
	Counting statistics, radioactivity as a statistical phenomenon, optimization of counting experiments, types of scintillators – inorganic, organic, liquid scintillators and their applications, scintillation mechanism, semiconductor detectors, gas-filled detectors-principle of operation and applications, Geiger–Müller and proportional counters, classification of nuclear detectors, variation of amplitude vs. voltage - characterization of different zones, role of quench gases - limitations of proportional detectors: proportional counter performance, flow-type proportional counter, gas multiplication factor, space charge effects.
	<b>(Total Contact Time: 45 Hours)</b>

<b>3.</b>	<b>Books Recommended</b>
1	P. A. C. Mcpherson, Principles of Nuclear Chemistry, World Scientific Publishing Europe Ltd, London, UK, 2016.
2	J. V. Kratz, Nuclear and Radiochemistry: Fundamentals and Applications, WILEY-VCH, NJ, USA, 2022.
3	J. Hofstader, Nuclear Chemistry, Larsen and Keller Education, New York, USA, 2022.
4	M. N. Devi, Elements of Nuclear Chemistry, Anmol Publisher, Delhi, 2011.
5	J. Kónya and N. M. Nagy, Nuclear and Radiochemistry, 2 <sup>nd</sup> Edition, Elsevier Inc., Amsterdam, Netherlands, 2018.

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**(M. Sc. V) (Sem. – X)**

Sr. No.	Subject	Code	Scheme L-T-P	Credits (Min.)	Notional hours of Learning (Approx.)
<b>Tenth Semester (5<sup>th</sup> Year of M. Sc.)</b>					
1	M.Sc. Dissertation** Industrial Internship/Professional Experience (Mandatory)	CYP10	0-0-40	20	800 (40X20)
			<b>Total</b>	<b>20</b>	800

\*\* Students can continue their dissertation work along with the internship / placement, if offered by the companies through Carrer Development Cell (CDC), SVNIT Surat. However, student will be required to complete their dissertation work and viva voce examination as per the academic calendar of the institute.

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