MALAVIYA NATIONAL INSTITUTE OF TECHNOLOGY JAIPUR

DEPARTMENT OF CHEMISTRY

COURSE STRUCTURE
FOR

M.Sc. CHEMISTRY

M.Sc. First Year (First Semester)				
Sl. No.	**Code**	**Subject**	**L-T-P**	**Credits**
1	21CYT505	Advanced Inorganic Chemistry	3-1-0	4
2	21CYT506	Analytical Chemistry	3-1-0	4
3	21CYT507	Organic Chemistry	3-1-0	4
4	21CYT508	Quantum Chemistry	3-1-0	4
5	21CYP501	Inorganic Chemistry Lab-I	0-0-4	2
6	21CYP502	Organic Chemistry Lab-I	0-0-4	2
7	21CYP503	Physical Chemistry Lab-I	0-0-4	2
8	21CYP504	Analytical Chemistry Lab-I	0-0-4	2
			Total	**24**

M.Sc. First Year (Second Semester)				
Sl. No.	**Code**	**Subject**	**L-T-P**	**Credits**
1	21CYT513	Advanced Organic Chemistry	3-1-0	4
2	21CYT514	Bonding in Main Group Elements and Transition Metal Organometallic Chemistry	3-1-0	4
3	21CYT515	Classical and Statistical Thermodynamics	3-1-0	4
4	21CYT516	Spectroscopy and its Applications	3-1-0	4
5	21CYP509	Inorganic Chemistry Lab-II	0-0-4	2
6	21CYP510	Organic Chemistry Lab-II	0-0-4	2
7	21CYP511	Physical Chemistry Lab-II	0-0-4	2
8	21CYP512	Analytical Chemistry Lab-II	0-0-4	2
			Total	**24**

M.Sc. Second Year (Third Semester)				
Sl. No.	**Code**	**Subject**	**L-T-P**	**Credits**
1	21CYT807-21CYT829	Program Elective-I	3-0-0	3
2	21CYT807-21CYT829	Program Elective-II	3-0-0	3
3	21CYT807-21CYT829	Program Elective-III	3-0-0	3
4	21CYT807-21CYT829	Program Elective-IV	3-0-0	3
5	21CYT807-21CYT829	Program Elective-V	3-0-0	3
6	21CYD601	Dissertation – I	0-0-12	6
			Total	**21**

M.Sc. Second Year (Fourth Semester)				
Sl. No.	**Code**	**Subject**	**L-T-P**	**Credits**
1	21CYT807-21CYT829	Program Elective-VI	3-0-0	3
2	-	Open Elective-I	3-0-0	3
3	21CYD 602	Dissertation – II	0-0-20	10
			Total	**16**

List of Program Electives				
Sl. No	**Code**	**Program Electives**	**L-T-P**	**Credits**
1	21CYT807	Photo-Inorganic Chemistry	3-0-0	3
2	21CYT808	Organometallics and Catalysis	3-0-0	3
3	21CYT809	Supramolecular Chemistry	3-0-0	3
4	21CYT810	Polymer Chemistry	3-0-0	3
5	21CYT811	Organometallic Chemistry of Main Group Elements	3-0-0	3
6	21CYT812	Bio-Inorganic Chemistry	3-0-0	3
7	21CYT813	Symmetry and Group Theory	3-0-0	3
8	21CYT814	Organic Synthesis	3-0-0	3
9	21CYT815	Applied Biocatalysis (Enzymes)	3-0-0	3
10	21CYT816	Heterocyclic Chemistry	3-0-0	3
11	21CYT817	Chemistry of Natural Products	3-0-0	3
12	21CYT818	Pharmaceutical Chemistry	3-0-0	3
13	21CYT819	Cell Structure & Biomolecules	3-0-0	3
14	21CYT820	Biochemistry	3-0-0	3
15	21CYT821	Physical Organic Chemistry	3-0-0	3
16	21CYT822	Electrochemistry: Ionics and Electrodics	3-0-0	3
17	21CYT823	Solid State Chemistry - Fundamentals and Applications	3-0-0	3
18	21CYT824	Laser Spectroscopy: Theory and Applications	3-0-0	3
19	21CYT825	Advanced Analytical Chemistry	3-0-0	3
20	21CYT826	Dyes and Pigments	3-0-0	3

21	21CYT827	Molecular Spectroscopy	3-0-0	3
22	21CYT828	Concepts in Chemical Kinetics and Dynamics	3-0-0	3
23	21CYT829	Green and Industrial Organic Chemistry	3-0-0	3
List of Open Electives				
Sl. No	**Code**	**Open Electives**	**L-T-P**	**Credits**
1	21CYT801	Chemistry for Renewable Energy	3-0-0	3
2	21CYT802	Environmental Chemistry	3-0-0	3
3	21CYT803	Introduction to Density Functional Theory	3-0-0	3
4	21CYT804	Atmospheric Chemistry	3-0-0	3
5	21CYT805	Introduction to Astrochemistry	3-0-0	3
6	21CYT806	Electrochemical Energy Storage Systems	3-0-0	3

<table>
<tr><th colspan="4">Advanced Inorganic Chemistry (21CYT505)</th></tr>
<tr><td>Prerequisite: General knowledge on chemical bonding, structure and geometry. Periodic properties of elements</td><td>L</td><td>T</td><td>P</td></tr>
<tr><td>Type: Core Course</td><td>3</td><td>1</td><td>0</td></tr>
<tr><td colspan="4">Course Description:
To enable the students to understand the stereochemistry and bonding in transition metal complexes
To enable students to understand the reaction mechanism in transition metal complexes
To enable students to understand the basic properties and use of inorganic complexes/materials in daily life</td></tr>
<tr><td colspan="4">Course Content</td></tr>
<tr><td>Module1 (12L)</td><td colspan="3">Stereochemistry and Bonding
Bonding models in d block elements, Walsh diagrams, dπ-dπ bonds, stereochemistry, distortions and electronic spectra of coordination compounds</td></tr>
<tr><td>Module 2 (12L)</td><td colspan="3">Reaction Mechanism
Inert and labile complexes, thermodynamic and kinetic aspects, kinetics of octahedral substitution reactions, substitution reactions in square planar complexes, trans effects, mechanism of substitution reaction, redox reactions, outer sphere reactions, cross reactions and Marcus-Hush theory, inner sphere reactions, the experiments of Taube</td></tr>
<tr><td>Module 3 (6L)</td><td colspan="3">Chemistry of f-block Elements
General discussion on the properties of the f-block elements, spectral and magnetic properties, use of lanthanide compounds as shift reagents, photophysical properties of lanthanide complexes</td></tr>
<tr><td>Module 6 (10L)</td><td colspan="3">Applicative aspects of inorganic chemistry
Electron transfer in biological system, inorganic complexes as cancer drugs, as renewable energy, and electroluminescent complexes, oxidative and reductive reactions.</td></tr>
<tr><td>Reference Books</td><td colspan="3">1. Advanced Inorganic Chemistry, F.A. Cotton & Wilkinson, John Wiley.
2. Inorganic Chemistry (Fourth Edition), J.E. Huheey, E. A. Keiter, R. L. Keiter (Pearson publishers).
3. Chemistry of the elements (Second Edition), N.N. Greenwood and A. Earnshaw (Elsevier publishers).</td></tr>
<tr><td>Course Outcomes</td><td colspan="3">CO1. The students will be able to understand the stereochemistry and bonding in transition metal complexes
CO2. Students will be able to understand reaction mechanism in transition metal complexes</td></tr>
</table>

	CO3. Students will be familiar with the various transition metal-based inorganic materials

Analytical Chemistry (21CYT506)			
Prerequisite: Knowledge of basic topics in analytical chemistry	**L**	**T**	**P**
Type: Core Course	**3**	**1**	**0**

Course Objectives:

- To enable the students to acquire fundamental knowledge of the principles of analytical chemistry for various applications
- To bring adaptability to new developments in analytical chemistry and a knowledge of contemporary issues
- To make them apply the knowledge of analytical chemistry for identification, solution and analysis of complex problems and design system components or processes that meet the specified needs with appropriate consideration for the public health and safety, and the cultural, societal, and environmental considerations

Course Content

Module 1 (7L)	**Basic tools and operations:** Role of analytical chemistry, Classification of analytical methods, Types of instrumental analysis, Selecting an analytical method, Neatness and cleanliness, Laboratory operations and practices, errors, Sample preparation-dissolution and decompositions, Selecting and handling of reagents, Laboratory notebooks, Safety in the analytical laboratory
Module 2 (7L)	**Data handling:** Accuracy and precision, types of error, statistical data treatment, significant figures and propagation of errors, use of spreadsheet and data treatment software, control chart, confidence limit, test of significance, outliers, calibration methods, linear and non-linear data fitting
Module 3 (7L)	**Thermal methods:** Thermogravimetry analysis (TGA), Differential Thermogravimetry (DTG), instrumentation, applications with some examples, Differential Thermal analysis (DTA) and DSC with applications **Spectroscopic techniques:** Absorption, emission, fluorescence and phosphorescence
Module 4 (10L)	**Electroanalytical methods:** Polarography, voltammetry, cyclic voltammetry, amperometry, coulometry and conductometry. Annodic sttripping voltammetry; – principle, instrumentation, limitations, applications to qualitative and quantitative analysis, Amperometric and Bioamperometric titrations, Potentiometry, Fundamentals of potentiometry, different types of electrodes
Module 5 (9L)	**Separation methods:** Solvent extraction: Partition law and its limitations, distribution ratio, separation factor, factor influencing extraction, multiple extractions, solid phase extraction, cloud point extraction, Chromatography: classification, theory of column

	chromatography, concept of plate and rate theory, Ion exchangers , Resolution, Van Deemter equation, paper and TLC, Liquid chromatographic techniques
Reference Books	1. Christian G.D., Dasgupta P.K., Schug K.A., "Analytical Chemistry" 7th Ed., Wiley 2013 2. Mendham J., Denny R.C., Barnes J.D. and Thomas M.J.K., "Vogel's Text Book of Quantitative Chemical Analysis" 6th Ed., Pearson Education 2004 3. Skoog D.A., West D.M., Holler F.J. and Crouch S.R., "Fundamentals of Analytical Chemistry" 8th Ed., Thomson Brooks/Cole.2004 4. Fifield F.W., and Kealey D., "Principles and Practice of Analytical Chemistry", 5th Ed., Blackwell Science. 2000 5. Ewing G.W., "Instrumental Methods of Chemical Analysis", 5th Ed., McGraw Hill. 2004
Course Outcomes	CO1. Students will be able to understand various aspects and importance of analytical chemistry. They can identify, formulate, and analyze complex analytical problems reaching substantiated conclusions using various principles of analytic chemistry CO2. Students will be able to design/development of various methods based on analytical tools for the public health and safety. CO3. Students will be able to conduct investigations of complex problems by the use research-based knowledge and research methods including design of experiments, analysis and interpretation of data, and synthesis of the information to provide valid conclusions. CO4. Students will learn about environment and sustainability of analytical tools and their impact on societal and environmental contexts, and demonstrate the knowledge of, and need for sustainable development.

Organic Chemistry (21CYT507)			
Prerequisite: Basic knowledge of biomolecules, photochemistry and pericyclic reactions	**L**	**T**	**P**
Type: Core Course	**3**	**1**	**0**

Course Description: To impart knowledge of advance organic chemistry including carbohydrates, pericyclic reactions and photochemical reactions.	
Course Content	
Module 1 (12L)	**Carbohydrates and importance** Classification, structure, uses, isolation and importance of Carbohydrates with special reference to Nucleotides, glycosides and glycoproteins, Separation of carbohydrates, Structure and biological importance of synthetic and natural occurring carbohydrate-based molecules
Module 2 (14L)	**Pericyclic Reactions** Classification of periycyclic reactions, Woodward-Hoffmann correlation diagrams. FMO and PMO approach, Electrocyclic reactions-conrotatory and disrotatory motions, 4n, 4n+2 and allyl systems, Cycoladditions-antrafacial and suprafacial addition, 4n and 4n+2 systems, 2+2 addition of ketenes, 1,3 dipolar Cycoladditions and cheleotropic reaction Sigmatropic rearrangements-suprafacial and atrafacial shifts of H, sigmatropic shifts involving carbon moieties, 3,3-and 5,5- Sigmatropic rearrangements, Claisen, Cope Ene reaction.
Module 3 (14L)	**Photochemistry** Principles and mechanistic background in Photochemistry, Photochemical Processes; Jablonski diagram, Internal conversion, Intersystem crossing, and associated phenomenon, Fluorescence & Phosphorescence Photochemical reactions involving organic molecules, cis-trans Isomerization, Paterno Buchi reaction, Norrish type reactions, photoreduction of ketones, Dienone-photochemistry & photochemistry of aromatics (addition & isomerization), Photosensitization, Photo-Fries rearrangement, Barton reaction, Di-π-methane rearrangement.
Reference Books	1. Principles of Organic Synthesis, R.O.C. Norman and J.M. Coxon, Blackie Academic & Professional. 2. Reaction Mechanism in Organic Chemistry, S.M. Mukherji and S.P. Singh, Macmillan. 3. Pericyclic Reactions, S.M. Mukherji, Macmillan, India 4. Chemistry of Natural Products, S. V. Bhat, B. A. Nagasampagi, M. Sivakumar, Narosa Publishing House, New Delhi. 5. Introduction to Medicinal chemistry A. Gringuage, Wiley VCH.

	6. Fundamental of Photochemistry, K.R. Rohtagi-Mukherji, Wiley-Eastern 7. Introductory Photochemistry, A. Cox & T. Camp, McGraw-Hill 8. Photochemistry, R.P. Kundall & A. Gilbert, Thomson Nelson. 9. Molecular Reactions & Photochemistry, C.H. Depuy & O.S. Chapman, Prentice-Hall. 10. Pericyclic Reactions - A Textbook: Reactions, Applications and Theory, S. Sankararaman, Wiley-VCH. 11. Carbohydrate Chemistry, Antony J. Fairbanks and B. G. Davis, Oxford University Press.
Course Outcomes	CO1. Understand basics of carbohydrates, their structure, types and importance in biological system. CO2. Explain the theoretical basis pericyclic reaction and also helps them to find a way to carry out these types of reaction CO3. Explain theory and practice of common photochemical and photophysical methods CO4. Explain and discuss theories for photoinduced electron transfer and excitation energy transfer CO5. Explain photochemical reactions in organic molecules

Quantum Chemistry (21CYT508)			
Prerequisite: Knowledge of basic mathematics	**L**	**T**	**P**
Type: Core Course	**3**	**1**	**0**

Course Objectives: This course will serve as a basic foundation course for any other course or concept which require quantum mechanics like spectroscopy, bonding, statistical and thermodynamics, Reaction rate theories etc.

Course Content

Module 1 (5L)	**Introduction:** Historic background, Wave particle duality, uncertainty principle
Module 2 (4L)	**Schrodinger equation:** wave function and interpretation, time-dependent and time-independent Schrodinger equation, Eigen value problem
Module 3 (7L)	**Quantum mechanics of some simple systems:** free particle, particle in a box, harmonic oscillator, Rectangular barrier crossing, Tunneling
Module 4 (5L)	**Angular Momentum:** Ladder operator methods, rigid rotor, orbital and spin angular momentum, addition of angular momentum
Module 5 (4L)	Hydrogen and hydrogen like atoms
Module 6 (6L)	**Approximate methods:** perturbation theory, variation method, some simple examples
Module 7 (4L)	**Many electron atom:** Pauli antisymmetry principle, Slater determinant, He atom, Hartree-Fock Theory
Module 8 (4L)	H_2^+ system, Heitler-London treatment of H_2 molecule, Huckel Theory, Extended Huckel Theory
Module 9 (3L)	Term Symbols, Introduction to Band theory, Quantum Dots
References	Text Books: 1. D. A. McQuarrie, J. D. Simon; Physical Chemistry- A Molecular Approach, Viva Books, First Edition 2. L. Pauling, E. B. Wilson; Introduction to Quantum Mechanics, Dover Books on Physics, First Edition 3. Ira N. Levine; Quantum Chemistry, Pearson Education India, First Edition 4. Donald A. McQuarrie, Quantum Chemistry, Viva Books, First Edition Reference Books 1. J. J. Sakurai; Modern Quantum Mechanics, Cambridge University Press, Third Edition 2. Feynman Lectures in Physics vol III, Pearson Education, First Edition

	3. Quantum Mechanics: L. D. Landau and E. M. Liefshitz, Pergamon Press, Second Edition 4. Quantum Mechanics: E. Merzbacher, Wiley, Third Edition 5. Lectures On Quantum Mechanics, Ashok Das, World Scientific Publishing, Second Edition
Course Outcome	CO1. They learn how a chemical bond is formed. CO2. Basic quantization of matter which become key in spectroscopy CO3. Simple models to illustrate the role of quantization in chemistryproblems

Inorganic Chemistry Lab-I (21CYP501)

Prerequisite: Understanding of qualitative and quantitative reactions	**L**	**T**	**P**
Type: Core Course	**0**	**0**	**4**

Course Description: To impart knowledge on the process of performing inorganic laboratory experiment

Course Content

Experiment Number	**Title of the Experiment**
1	Preparation of Co-SALEN complex and its oxygen binding properties
2	Preparation of di(chloro)-bis-(tri-phenylphosphine)Nickel(II)
3	Preparation of tetra-amine cupric-sulphate $[Cu(NH_3)_4]SO_4 .H_2O]$
4	Preparation of tris-acetylacetonato iron(III)
5	Synthesis and characterization of potassium tris-oxalato chromate(III) tri-hydrate
6	Synthesis of hexa-ammine cobalt(III) chloride
7	Synthesize the bis-(N, N'-di-salicyl-ethylene-diamine)-µ-aqua-dicobalt (II)
8	Color effects due to ligand-exchange in nickel complexes: the experiment describes the simpler demonstration of ligand-field strength in the spectrochemical series
9	Acidic and basic salts: the experiment describes the hydrolysis of salts and its consequences
10	Color effects in aqueous systems containing divalent 3d metal ions: the experiment describes the demonstration of crystal-field splitting parameters of 3d metal ions
References	1. Handouts of all the experiments in full details shall be provided 2. A Collection of Interesting General Chemistry Experiments, A.J. Elias, Universities Press, 2002
Course Outcomes	CO1. Student will be exposed to advance inorganic synthetic methods that may include the use of Schlenk line, solvent drying procedures. CO2. Student will understand the commercial importance of inorganic catalysts that are used to propel various organic reactions. CO3. Student will get to prepare the inorganic complexes that they study in their inorganic chemistry, photo-inorganic chemistry courses. A hands-

	on experience in preparing standard dyes will allow them to familiarize with solar energy conversion.

Organic Chemistry Lab-I (21CYP502)			
Prerequisite: Basic understanding of practical handling of chemicals and basic chemistry.	**L**	**T**	**P**
Type: Core Course	**0**	**0**	**4**

Course Description: To provide practical training on qualitative analysis of binary mixtures of organic compounds and synthesis of various organic compounds involving two steps.

Course Content

Module 1 (P)	**Qualitative Analysis** Separation, purification and identification of binary mixture of Organic compounds using chemical methods. Wherever possible a suitable derivative is to be prepared.
Module 2 (P)	**Organic Synthesis involving two steps**. (Synthesis of Organic Compounds) 1. Acetylation of salicylic acid, aniline, and other organic molecules. 2. Benzoylatinon of aniline and phenol. 3. Preparation of Iodoform from ethanol and acetone. 4. Nitration Preparation of m-dinitrobenzene Preparation of p-nitroacetanilide 5. Halogenation Preparation of p-bromoacetanilide Preparation of 2,4,6-tribromophenol. 6. Diazotization/coupling Preparation of methyl orange and methyl red. 7. Oxidation: Preparation of benzoic acid from toulene. 8. Reduction: Preparation of aniline from nitrobenzene Preparation of m-nitroaniline from m-dinitrobenzene.
Reference Books	1. Experiments and Techniques in Organic Chemistry, D.P. Pasto, C. Johnson and M. Miller, Prentice Hall. 2. Macroscale and Microscale Organic Experiments, K.L. Williamson, D.C. Health. 3. Systematic Qualitative Organic Analysis, H. Middleton, Adward Arnold. 4. Handbook of Organic Analysis-qualitative and quantitative. H. Clark, Adward Arnold. 5. Vogel's Textbook of Practical Organic Chemistry, A.R. Tatchell, John Wiley
Course Outcome	CO1. Separate and identify different organic compounds from mixture CO2. Synthesize organic compounds and gain hands on practice of handling laboratory equipment

<table>
<tr><th colspan="4">Physical Chemistry Lab-I (21CYP503)</th></tr>
<tr><td>Prerequisite: Basic understanding of fundamental Physical Chemistry</td><td>L</td><td>T</td><td>P</td></tr>
<tr><td>Type: Core Course</td><td>0</td><td>0</td><td>4</td></tr>
<tr><td colspan="4">Course Objective: To familiarize the students with the practice of experimental physical chemistry</td></tr>
<tr><td colspan="4">Course Content</td></tr>
</table>

Experiment 1	Determination of the molecular formula of copper-ammonia complex by the partition coefficient method
Experiment 2	Catalytic constant of an acid
Experiment 3	Effect of ionic strength on the rate of persulphate-iodide reaction
Experiment 4	Complex ion composition by job's method
Experiment 5	Kinetics of the iodide-hydrogen peroxide clock reaction
Experiment 6	Velocity constant of the base-catalyzed hydrolysis (saponification) of ethyl acetate
Experiment 7	Determination of the heat of solution of oxalic acid from its solubility at different temperatures
Experiment 8	Association constant of benzoic acid
Experiment 9	Study of influence of ionic strength on the solubility of $CaSO_4$ and determination of its thermodynamic solubility product and mean ionic activity
Experiment 10	Conductometric determination of critical micellar concentration
Experiment 11	Kinetics of crystal violet hydrolysis by colorimetric methods
Experiment 12	Study of a model antibiotic reaction using colorimetry (crystal violet as model antibody)
Experiment 13	Determination of E^o of ferricyanide-forrocyanide system
Experiment 14	pKa determination of a weak acid by pH-metric method
Experiment 15	Numerical Experiment: Least square method, Correlation coefficient, Newton-Raphson method
Reference Books	1. C.Garland, J. Nibler and D.Shoemaker, Experiments in Physical Chemistry, McGrawHill Education; 8th Edn., 2008 2. B. Viswanathan and P. S. Raghavan, Practical Physical Chemistry, Viva Books Pvt. Ltd.

	3. Halpern, A. M. McBane, G. C., Experimental Physical Chemistry: A Laboratory Text Book, W. H. Freeman.
Course Outcomes	CO1. Design and conduct experiments CO2. Apply the principles of thermodynamics, kinetics, spectroscopy and various other topics presented in the physical chemistry courses, in experiments CO3. Use different instrumental methods of analysis and estimation CO4. Analyze and interpret experimental data

Analytical Chemistry Lab-I (21CYP504)			
Prerequisite: To impart practical knowledge of analysing samples by analytical techniques	L	T	P
Type: Core course	0	0	4

Course Description:

- To enable the students to acquire advance knowledge of analytical techniques for various applications
- Handling of Flame photometer, UV-Vis spectrophometer, HPLC, GC, Ion chromatograph and spectrofluorometer

Course Content

Experiment 1	Estimation of Na and K in natural water and ORS by flame photometer
Experiment 2	Determination of organochlorine pesticides in food by gas chromatography
Experiment 3	Determination of Nickel in environmental samples by AAS
Experiment 4	Estimation of Calcium in cement solution by spectrophotometer
Experiment 5	Determination of ion exchange capacity of a cation exchange resin (Dowex-50) anion exchange resin (Amberlite-IRA 400).
Experiment 6	Colorimetric determination of Iron in unknown water sample
Experiment 7	Thermal decompositions of calcium oxalate monohydrate
Experiment 8	Separation of organic mixture by Thin layer Chromatography
Experiment 9	Estimations of fluoride ions in drinking water by spectrophotometer
Experiment 10	Polarographic estimation of Pb, Sn, Ni and Zn in a copper alloy
Experiment 11	Estimation of power of LED light using chemical actinometry
Experiment 12	Determination of ascorbic acid in vitamin-C tablet
Reference Books	1. Christian G.D., Dasgupta P.K., Schug K.A., “Analytical Chemistry” 7th Ed., Wiley 2013 2. Mendham J., Denny R.C., Barnes J.D. and Thomas M.J.K., “Vogel’s Text Book of Quantitative Chemical Analysis” 6th Ed., Pearson Education 2004 3. Skoog D.A., West D.M., Holler F.J. and Crouch S.R., “Fundamentals of Analytical Chemistry” 8th Ed., Thomson Brooks/Cole.2004 4. Fifield F.W., and Kealey D., “Principles and Practice of Analytical Chemistry”, 5th Ed., Blackwell Science. 2000 5. Ewing G.W., “Instrumental Methods of Chemical Analysis”, 5th Ed., McGraw Hill. 2004

Course outcomes	CO1. Students will be able to understand importance of analytical tools in industry as well as in day by day applications CO2. Students will be able to learn about working of various analytical equipment's and their uses CO3. Students will learn basics as well advanced knowledge about use of analytical tools CO4. Hands on training will make students more carrier oriented

Advanced Organic Chemistry (21CYT513)			
Prerequisite: Basic organic chemistry	**L**	**T**	**P**
Type: Core Course	**3**	**1**	**0**
Course Description: To impart knowledge of stereochemistry, structure reactivity relationship, reactive intermediates, mechanism of general organic reactions and Aromaticity.			
Course Content			

Module 1 (10L)	**Stereochemistry and Conformation** Basic concepts and principles in Stereochemistry. Chirality, Isomerism, Methods of resolution of isomers. Conformation analysis of acyclic and cyclic compounds, Neighbouring group participation.
Module 2 (12L)	**Reaction Mechanism: Structure and Reactivity** Reactive intermediates; Generation, structure, stability and reactivity of carbocation, carbanions, free radicals, carbenes, nitrenes, and benzyne. Mechanistic aspects of Thermodynamic and kinetic control, Hammond's postulate, Curtin-Hammett principle, potential energy diagrams, transition state and intermediates, methods of determining mechanisms, isotopic labeling.
Module 3 (8L)	**Reaction mechanism: Structural Effects on Stability and Reactivity** Effects of structure on reactivity, resonance and field effects, steric effects, quantitative treatment. The Hammett equation and linear free energy relationship, substituent and reaction constants, Taft equation, Hard Soft Acid Base concept
Module 4 (10L)	**Nature of Bonding in Organic Molecules** Aromaticity; Hückel's rule, Benzenoids and non-benzonoids, annulenes, anti-aromaticity and homo-aromaticity Bonds weaker than covalent-addition compounds and crown ether complexes and cryptands, inclusion compounds and catenanes and rotaxanes
Reference Books	1. Advanced Organic Chemistry, Reactions Mechanisms and Structure, J. March. John Wiley. 2. Advanced Organic Chemistry, F.A. Carey and R.J. Sunderg, Plenum. 3. A Guide Book to Mechanism in Organic Chemistry, Peter Sykes, Longman. 4. Structure and Mechanism in Organic Chemistry, C.K. Ingold, Cornell University Press. 5. Organic Chemistry, Paula Yukanis Bruice, Pearson. 6. Organic Chemistry, J. Clayden, N. Greeves and S. Warren, Oxford University Press.
Course Outcomes	CO1. Identify and differentiate prochirality and chirality at centers, axis, planes and helices and determine the absolute configuration

	CO2. Evaluate the stability of various conformers of acyclic and cyclic systems using steric, electronic and stereoelectronic effects and correlate them to reactivity. CO3. Analyze the role of reactive intermediates such as carbocations, carbanions, nonclassical carbocation in the chemical reactions. CO4. Demonstrate effect of structure on reactivity. CO5. Explain nature of bonding in organic molecules with understanding of aromaticity, antiaromaticity and homoaromaticity.

<table>
<tr><th colspan="4">Bonding in Main Group Elements and Transition Metal Organometallic Chemistry (21CYT514)</th></tr>
<tr><td colspan="1">Prerequisite: General knowledge on chemical bonding, structure and geometry. Periodic properties of elements</td><td>L</td><td>T</td><td>P</td></tr>
<tr><td>Type: Core Course</td><td>3</td><td>1</td><td>0</td></tr>
<tr><td colspan="4">Course Description:
To enable students to understand the bonding in main group elements compounds
Introduce students to the organometallic chemistry of the transition metal
Introduce students to the chemistry of f-block elements</td></tr>
<tr><td colspan="4">Course Content</td></tr>
<tr><td>Module 1 (20L)</td><td colspan="3">Bonding in Main Group Element
Inorganic chains, rings, cages and clusters in main group element chemistry, element-element bonds, Synthesis, Properties and Structure of halides and oxides, Phosphorus and Sulfur. Synthesis, properties and structure of boranes, carboranes, borazines, silicates carbides, Silicones, phosphazenes, sulphur-nitrogen, phosphorous-nitrogen compounds, peroxo compounds of boron, carbon and sulphur, oxy-acids of Nitrogen, phosphorus, sulphur and halogens, inter-halogens, pseudo-halides and noble gas compounds</td></tr>
<tr><td>Module 2 (5L)</td><td colspan="3">Concept of Acid base
Lewis acid – Lewis base adducts, Frustrated Lewis Pairs (FLPs) – concepts and mechanism, heterolytic cleavage of molecular hydrogen, activation of other inert small molecules, and uses in symmetric and asymmetric catalysis</td></tr>
<tr><td>Module 3 (18L)</td><td colspan="3">Transitionmetal organometallic Chemistry
σ– Bonded molecules: metal-alkyls, -aryls and –hydrides; synthesis, reactivity and stability of metal-carbonyls, metal-phosphines, metal-nitrosyls and metal-isocyanides, structures, reactivity and bonding in metal-carbenes, metal-carbynes - Fischer carbenes and Schrock carbenes, complexes with N-heterocyclic carbenes - application in olefin metathesis reactions
π– Bonded molecules: metal-olefins, -alkyls, -alkynes, -dienes - structure, bonding and reactivity</td></tr>
<tr><td>References</td><td colspan="3">1. Advanced Inorganic Chemistry, F.A. Cotton & Wilkinson, John Wiley
2. Inorganic Chemistry (Fourth Edition), J.E. Huheey, E. A. Keiter, R. L. Keiter (Pearson publishers)
3. Chemistry of the elements (Second Edition), N.N. Greenwood and A. Earnshaw (Elsevier publishers)
4. Robert H. Crabtree, The Organometallic Chemistry of the Transition Metals, John Wiley and Sons, 4th edition. John Wiley and sons 2005.</td></tr>
<tr><td>Course Outcomes</td><td colspan="3">CO1. Compare the bonding in main group elements and discuss the chemistry of Si, B, C based compounds</td></tr>
</table>

	CO2. Know the different definitions of acids/bases and predict the reactions between acids and bases CO3. Understand the principles of electronic structure, bonding and reactivity of organometallic complexes CO4. Recognize the concept of synthesis and stability of transition metal organometallic complexes CO5. Apply the principles of transition metal complexes in understanding the magnetic properties of coordination complexes and solid state energetics

Classical and Statistical Thermodynamics (21CYT515)			
Prerequisite: Basic understanding of thermodynamics and Quantum Mechanics	**L**	**T**	**P**
Type: Core Course	**3**	**1**	**0**
Course Objectives: In this course student will learn the basic principles of thermodynamics and statistical mechanics. This is absolutely essential for a proper understanding of systems ranging from atoms and molecules to black holes and galaxies.			
Course Content			

Module 1 (9L)	**Classical Thermodynamics:** Review of laws of thermodynamics, Legendre Transformation, Theormodynamic potentials and there role in chemical equilibrium, Partial molar quantities and chemical potential, Fundamental equations for open systems, Phase behaviour of one and two component systems, Thermodynamics of electrochemical cells and applications
Module 2 (13L)	**Statistical Thermodynamics**: Concept of ensembles, partition functions and distributions, microcanonical, canonical and grand canonical ensembles, canonical and grand canonical partition functions, Boltzmann, Fermi-Dirac and Bose-Einstein distributions, Canonical partition function for interacting particles, intermolecular potential (Lennard-Jones, Hard-sphere and Square-well) and virial coefficients, Einstein and Debye models for Heat capacity of Solids
Module 3 (12L)	**Molecular Reaction dynamics**: Integrated rate laws, Photochemical and Radiation-Chemical Reaction, Composite Reactions, Reactions on Surfaces, Homogeneous Catalysis, Activation energy, Collision Theory, Transition state Theory, RRKM theory
Module 4 (6L)	**Transport Phenomena**: Phenomenological description of transport processes, Ionic conductivity, Debye-Hückel Theory, Nernst-Einstein Relation, Stoke-Einstein Relation
References	Text Books 1. D.A. McQuarrie, Statistical Thermodynamics, Harper & Row, 1976 2. B. Widom, Statistical Mechanics: A Concise Introduction for Chemists, Cambridge, 2002 3. S. Glasstone, An Introduction to Electrochemistry, Maurice Press, 2011 4. K. J. Laidler, Chemical Kinetics, Pearson, 1997 5. J. Rajaram, J. C. Kuriacose, Chemical Thermodynamics, Pearson, 2013 Reference Books 1. D. Chandler, Introduction to Modern Statistical Mechanics, OUP USA, 1987

Course Outcome	CO1. Learn basic concepts of thermodynamics and statistical mechanics CO2. Understand the fundamental concepts of reactions in molecular level CO3. Learn how to use the thermodynamics concepts in various important chemical processes.

Spectroscopy and its Applications (21CYT516)			
Prerequisite: To impart knowledge for spectral analysis based on multiple spectroscopic data	**L**	**T**	**P**
Type: Core Course	**3**	**1**	**0**

Course Description:

- To enable the students to understand the applications of various spectroscopic techniques
- To facilitate the student to interpret the unknown organic and inorganic compounds based on the spectral analysis
- A small portion enables to understand the application of several spectroscopic techniques to understand the biological processes and materials

Course Content	
Module 1 (4L)	**Ultraviolet and Visible spectroscopy:** Introduction and identification of possible transition associated to conjugated and extended conjugated systems etc. Woodward rules. Electronic spectra of transition metal complexes.
Module 2 (4L)	**Infrared-Spectroscopy:** Introduction and identification of functional groups, hydrogen bonding etc., metal ligand vibrations
Module 3 (3L)	**Raman Spectroscopy:** Introduction and identification of chemical compounds, materials, nano-materials and in imaging applications.
Module 4 (9L)	**Nuclear Magnetic Resonance Spectroscopy**: General introduction, definition and applications of ^{1}H and ^{13}C NMR spectroscopy including two dimensional NMR COSY, NOESY, NOE, DEPT, INEPT techniques in the structural determination of complex organic systems. Application in conformational analysis. Multinuclear NMR of various inorganic, bioinorganic, and industrial organometallic compounds.
Module 5 (8L)	**Mass Spectrometry:** Introduction, ion production- EI, CI, FD and FAB, ion analysis, ion abundance, molecular ion peak, metastable peak. McLafferty rearrangement, Examples of mass spectral fragmentation of organic compounds, HRMS technique
Module 6 (3L)	**Structural elucidation** of unknown organic and inorganic compounds by joint application of UV, IR, NMR and mass spectrometry
Module 7 (3L)	**X-Ray Photo-Electron Spectroscopy:** Physical concepts. Application to determine atomic charges, oxidation numbers, catalyst surface structures and in some cases molecular structures
Module 8 (3L)	**Mossbauer Spectroscopy:** Basic physical concepts and interpretation of Mossbauer parameters of 57Fe, 99Ru, 101Ru, 195Pt, 193Ir and 110Sn. Some special applications: Solid state reactions, thermal decomposition, ligand exchange, electron transfer, isomerism, surface studies and biological applications

Module 9 (3L)	**Electron Spin Resonance spectroscopy:** Introduction, analysis of ESR spectra of systems in liquid phase, radicals containing single set, multiple sets of protons, triplet ground states. Transition metal ions. Rare earth ions, ion in solid state, in Biological applications
References	1. Physical Methods in Chemistry, RS Drago, 2nd edn., Saunders, 1992 2. Carbon-13 Nuclear Magnetic Resonance Spectroscopy, G. C. Levy, R. L. Lichter and G. L. Nelson, Wiley, 1980 3. NMR Spectroscopy - An Introduction, H. Gunther, John Wiley, 1980. 4. Basic One- and Two-Dimensional NMR Spectroscopy, H. Friebolin, VCH, 1991 5. Spectroscopic Methods in Organic Chemistry, D. H. Williams and I. Fleming, 4th ed., 1988 6. Spectrometric Identification of Organic Compounds, R.M. Silverstein, G.C. Bassler and T.C. Morrill, John Wiley & Sons, New York, 5th Ed. 1991. 7. Interpretation of Mass Spectra, F. W. McLafferty, 1980 8. Electron Paramagnetic Resonance, Elementary Theory and Practical Applications, Weil, John A, J. R. Bolton, and Wertz, J. E, Wiley-Interscience, New York, (1994) 9. Structural Methods in Inorganic Chemistry, E. A. V. Ebsworth, D. W. H. Rankin, & S. Cradock, 2nd Ed. 1991, CRC Press, Boca Raton, Florida
Course Outcomes	CO1. Interpret the unknown compounds and molecules CO2. Understand the transformation in materials and nanostructures CO3. Differentiate between similar compounds and materials

Inorganic Chemistry Lab-II (21CYP509)			
Prerequisite: Understanding of qualitative and quantitative reactions	**L**	**T**	**P**
Type: Core Course	**0**	**0**	**4**
Course Description: Using advanced methods to prepare inorganic complexes and introduce state-of-the art methods like NMR, IR, UV-VIS, HRMS, electrochemical methods to characterize them			
Course Content			

Experiment Number	**Tiles of the Experiment**
1	Preparation of Chromium (III) SALEN complex.
2	Preparation of Mn(III)(acac)$_3$ complex
3	Synthesis and characterization of tris-triphenylphosphine copper(I) nitrate
4	Synthesis of Cp*Co(CO)$_2$/(CpMo(CO)$_3$diamer
5	Synthesis and characterization of [Ru(p-cymene)(Cl)$_2$]$_2$
6	Synthesis of [Pd(PPh$_3$)]$_4$ and performing a Suzuki-Miyaura coupling reactions between aryl boronic acid and aryl halides
7	Preparation of standard inorganic dyes namely: N3 and N719 dyes. (These are ruthenium complexes with bipyridine/terpyridine ligands.)
8	Preparation of miniature- DSSC using from fruit pulp and comparing its I-V characteristics with any one standard inorganic dye (N3 or N719)
9	Synthesis of Fe(bpy)$_3$ Complex
10	Preparation and characterization of sodium hexanitrocobalt (III)
11	Inorganic Nanomaterials: Synthesis and Applications
Reference	Complete manual shall be provided for the experiments
Course Outcomes	CO1. Student will be exposed to advance inorganic synthetic methods that may include the use of Schlenk line, solvent drying procedures. CO2. Student will understand the commercial importance of inorganic catalysts that are used to propel various organic reactions. CO3. Student will get to prepare the inorganic complexes that they study in their inorganic chemistry, photo-inorganic chemistry courses. A hands-on experience in preparing standard dyes will allow them to familiarize with solar

	energy conversion.

<table>
<tr><th colspan="5">Organic Chemistry Lab-II (21CYP510)</th></tr>
<tr><td colspan="2">Prerequisite: Basic understanding of practical handling of chemicals and basic chemistry</td><td>L</td><td>T</td><td>P</td></tr>
<tr><td colspan="2">Type: Core Course</td><td>0</td><td>0</td><td>4</td></tr>
<tr><td colspan="5">Course Description: To provide practical training on quantitative analysis of various functional groups in organic compounds and extraction of organic compounds from natural sources.</td></tr>
<tr><td colspan="5">Course Content</td></tr>
<tr><td>Module 1 (P)</td><td colspan="4">Quantitative Analysis
• Determination of the percentage or number of hydroxyl groups in an organic compound by acetylation method.
• Estimation of amines/phenols using bromate bromide solution/or acetylation method.
• Determination of Iodine and Saponification values of an oil sample.</td></tr>
<tr><td>Module 2 (P)</td><td colspan="4">II. Extraction of organic compounds from natural sources:
1. Isolation of caffeine from tea leaves.
2. Isolation of casein from milk.
3. Isolation of lactose from milk.
4. Isolation of nicotine dipicrate from tobacco.
5. Isolation of piperine from black pepper.
6. Isolation of lycopene from tomatoes.
7. Isolation of fructose from sugar.</td></tr>
<tr><td>Reference Books</td><td colspan="4">1. Experiments and Techniques in Organic Chemistry, D.P. Pasto, C. Johnson and M. Miller,Prentice Hall.
2. Macroscale and Microscale Organic Experiments, K.L. Williamson, D.C. Health.
3. Systematic Qualitative Organic Analysis, H. Middleton, Adward Arnold.
4. Handbook of Organic Analysis-qualitative and quantitative. H. Clark, Adward Arnold.
5. Vogel's Textbook of Practical Organic Chemistry, A.R. Tatchell, John Wiley</td></tr>
<tr><td>Course Outcome</td><td colspan="4">CO1. Able to determine hydroxyl group and amino groups in organic compounds.
CO2. Able to determine saponification value of fats/oils.
CO3. Gain hands on practice for isolation of organic compounds from natural resources.</td></tr>
</table>

Physical Chemistry Lab-II (21CYP511)			
Prerequisite: Basic understanding of Mathematics and fundamental Physical Chemistry	**L**	**T**	**P**
Type: Core Course	**0**	**0**	**4**
Course Objective: To familiarize the students with the practice of experimental and theoretical physical chemistry			
Course Content			

Experiment 1	Conductometric titration of mixture of acids and precipitation titration (KCl Vs $AgNO_3$) using conductivity bridge
Experiment 2	Kinetic study of iodination of aniline (analytical and colorimetric method)
Experiment 3	Verification of Walden's rule
Experiment 4	Determination of specific rotation of tartaric acid by polarimetric method
Experiment 5	Determination of isoelectric point of gelatin by viscosity measurement
Experiment 6	Phase diagram of two component simple eutectic system
Experiment 7	Determination of Planck's constant and work function of metals using photoelectric method
Experiment 8	A computational experiment of the endo versus exo preference in a Diels–Alder reaction
Experiment 9	A mechanistic study of the Wittig reaction
Experiment 10	Dissociation of the ethyl radical.
Experiment 11	Theoretical Hammett Plot for the gas-phase ionization of benzoic acid versus phenol.
Experiment 12	Computing the fundamental rotational-vibrational band of CO and NO.
Experiment 13	Calculating the tunneling splitting of ammonia inversion.
Experiment 14	Determination of Pauling's electronegativity
Experiment 15	Verification of Trouton's rule, determination of correlation coefficient
Experiment 16	Verification of Stirling approximation

References	1. C.Garland, J. Nibler and D.Shoemaker, Experiments in Physical Chemistry, McGrawHill Education; 8th Edn., 2008. 2. B. Viswanathan and P. S. Raghavan, Practical Physical Chemistry, Viva Books Pvt. Ltd. 3. Halpern, A. M. McBane, G. C., Experimental Physical Chemistry: A Laboratory Text Book, W. H. Freeman. 4. Journal of Chemical Education, ACS Publication.
Course Outcomes	CO1. Design and conduct experiments CO2. Use different instrumental methods of analysis and estimation CO3. Analyze and interpret experimental data CO4. Understand theoretical concepts of chemical reactions

Analytical Chemistry Lab-II (21CYP512)			
Prerequisite: To impart practical knowledge of analysing samples by analytical techniques	**L**	**T**	**P**
Type: Core Course	**0**	**0**	**4**

Course Description:

- To enable the students to acquire advance knowledge of analytical techniques for various applications
- Handling of Flame photometer, UV-Vis spectrophometer, HPLC, GC, Ion chromatograph and spectrofluorometer

Course Content	
Experiment 1	Flame emission spectrometric determination of Sodium
Experiment 2	Determination of carbamate pesticides in food by high performance liquid chromatography
Experiment 3	Estimation of Ca in hardwater and drugs by flame photometer
Experiment 4	Ion exchanger determination of Ca+2 and Mg+2 (hardness causing ions)
Experiment 5	Determination of metals by Atomic absorption spectrophotometry
Experiment 6	Fluorometric determination of Riboflavin (Vit B2)
Experiment 7	Qualitative and quantitative analysis of fruit juices for vitamin C using high performance liquid chromatography
Experiment 8	Determination of phenylenediamines and quinones by Polarography
Experiment 9	Determination of toxic metals by ion chromatograph
Experiment 10	Estimation of copper in brass
Experiment 11	Column chromatographic separation of organic/inorganic mixtures
Experiment 12	Analysis of Analgesic using high performance liquid chromatography
Reference Books	1. Christian G.D., Dasgupta P.K., Schug K.A., “Analytical Chemistry” 7th Ed., Wiley 2013 2. Mendham J., Denny R.C., Barnes J.D. and Thomas M.J.K., “Vogel’s Text Book of Quantitative Chemical Analysis” 6th Ed., Pearson Education 2004 3. Skoog D.A., West D.M., Holler F.J. and Crouch S.R., “Fundamentals of Analytical Chemistry” 8th Ed., Thomson Brooks/Cole.2004 4. Fifield F.W., and Kealey D., “Principles and Practice of Analytical Chemistry”, 5th Ed., Blackwell Science. 2000

	5. Ewing G.W., “Instrumental Methods of Chemical Analysis”, 5th Ed., McGraw Hill. 2004
Course outcomes	CO1. Students will be able to understand importance of analytical tools in industry as well as in day by day applications CO2. Students will be able to learn about working of various analytical equipment’s and their uses CO3. Students will learn basics as well advanced knowledge about use of analytical tools CO4. Hands on training will make students more carrier oriented

Chemistry for Renewable Energy (21CYT801)			
Prerequisite: Understanding of basic chemistry and physics at undergraduate level.	**L**	**T**	**P**
Type: Open Elective	**3**	**0**	**0**
Course Description: To study the basic principles that govern the light induced chemical processes that can be utilized to the benefit of society (power generation or newer materials)			
Course Content			

Module 1 (10 L)	**Basic Photochemistry** Molecular ground and excited states, radiative and non-radiative deexcitation, Jablonski diagram, potentialenergy surfaces, reaction dynamics, electron and energy transfer, absorption and emission characteristics, excited state lifetime, electroluminescent molecules, and their use in photonic devices, experimental techniques, Franck-Condon Principle, Energy transfer, Excimer, Exciplex, quenching and sensitization.
Module 2 (10 L)	**Electrochemical Methods and Devices** Chronoamperometry, cyclic voltammetry (interpretation using transition metal complexes), and spectro-electrochemistry; electrodes and electrochemical processes of relevance to energy conversion, photo-electrochemical cells, light sources, photodetectors and device design and measurements.
Module 3 (10 L)	**Solar Cell Technology** Principles for conversion of solar energy to electricity, Shockley-Queisser limit, tandemsolar cells. Different solar cell technologies (inorganic, organic, hybrid) with specific reference to dye sensitized solar cells and perovskite technology. Recombination processes in solar cells. Basic and advanced characterization methods for solar cells and solar cell materials. Integration of solar cells into modules.
Module 4 (12 L)	**Molecular Systems for Renewable Energy** Molecular approaches to solar fuel production, structures and mechanisms of biocatalysts and artificial catalysts for water oxidation, carbon dioxide fixation, nitrogen fixation, oxygen reduction and hydrogen formation, principles governing design of molecular catalysts in oxidative and reductive reactions, structural aspects, thermodynamics, kinetics, proton coupled electron transfer and over-potentials for catalytic reactions, strategies to optimize catalytic activity, robustness and efficiency of catalysts made of earth-abundant elements, how to define and measure solar-to-fuel energy efficiencies and the stabilities of catalytic systems.

Reference Books	1. Principles of Fluorescence Spectroscopy, Lakowicz, III-Edition, Springer. 2. Highly Efficient OLEDs with Phosphorescent Materials, Wiley- VCH Verlag GmbH & Co., 2007 3. Organic Photochemistry and Photophysics, V. Ramamurthy, Kirk S. Schanze, CRC Press. 4. Photochemistry and Photophysics: Concepts, Research, Applications, VincenzoBalzani,Paola Ceroni,Alberto Juris, 2014. 5. Molecular Fluorescence: Principles and Applications, Bernard Valeur, Mário NunoBerberan-Santos 6. Photochemistry and Photophysics: Concepts, Research, Applications, Vincenzo Balzani,Paola Ceroni,Alberto Juris, 2014. 7. Electrochemical Methods: Fundamentals and Applications, 2nd Edition, Allen J. Bard, LarryR. Faulkner, 2000\ 8. Photochemistry of Organic Compounds from concepts to practice, Petr Klan and Jakob Wirz, Wiley, 2009.
Course Outcomes	CO1. Describe and explain photochemical and photo-physical processes and mechanisms with suitable theoretical models and apply established experimental methods for the investigation of these processes CO2. Describe the interaction of excited states with their surroundings and analyses photo-induced electron transfer and excitation energy transfer with quantitative models CO3. Apply knowledge about photochemical and photo-physical processes and the reactivity of excited states to explain applications in photochemical energy conversion and other selected issues

Environmental Chemistry (21CYT802)				
Prerequisite: To impart knowledge of environmental chemistry		**L**	**T**	**P**
Type: Open Elective		**3**	**0**	**0**
Course Description: Students will acquire knowledge of importance of environmental chemistry, an interdisciplinary science that involve physics, chemistry, life science and agriculture etc. They will understand importance of protection and conservation of our environment and need to restrain anthropogenic activities responsible for extensive release of pollutants in environment.				
Course Content				
Module 1 (5L)	**Introduction:** concept and importance of environmental chemistry. Environmental segments, Natural and Man-made Disasters, green chemistry, Environmental sampling			
Module 2 (10L)	**Atmosphere:** Composition and structures of Atmosphere, Vertical temperature profile, Properties of troposphere, Temperature inversion. Particles, ions and radicals in atmosphere, chemical and photochemical reactions in atmosphere, Mechanism of Ozone formation and catalytic Ozone depletion, Control Strategies			
Module 3 (10L)	**Water Pollution:** Water pollutants, Eutrophication, dye, Pesticides, phenols, toxic metals as Pollutants, chemical speciation, water quality parameters and standards, sampling and preservation, Monitoring techniques and methodology, Fluorosis			
Module 4 (10L)	**Air Pollution:** Air pollutants and their classifications. Carbon mono-oxides, Nitrogen oxides, Hydrocarbons and photochemical smog, Aerosols-sources, size distribution and effect on visibility, climate and health. Major greenhouse gases and their sources and Global warming potentials. Climate change and consequences. Acid rain precursors and their aqueous and gas phase atmospheric Oxidation reactions. Damaging effects on aquatic life, plants, buildings and health. Monitoring of SO2 and NOx. Acid rain control strategies.			
Module 5 (5L)	**Chemical toxicology:** Toxic chemicals in the environment, Impact of toxic chemicals on enzymes, biochemical effects: CO, NOx, SO_x, Ozone and PAN, Cyanides and pesticides; Carcinogens, Bio-warfare Agents, Environment and public health			

Reference Books	1. Environmental Chemistry, Colin Baird, W.H. Freeman Co. New York, 1998. 2. Chemistry of Atmospheres, R.P. Wayne, Oxford. 3. Environment Chemistry, A.K. De, Wiley Eastern, 2004. 4. Environmental Chemistry, S.E. Manahan, Lewis Publishers.
Course Outcomes	CO1. Students will be able to understand that environmental chemistry is a part of environmental educations CO2. They will get the knowledge of chemistry involved in atmosphere, air pollution, and water pollution CO3. Information about the various environmental episodes

<table>
<tr><th colspan="4">Introduction to Density Functional Theory (21CYT803)</th></tr>
<tr><td colspan="1">Prerequisite: Basic understanding of Quantum Chemistry</td><td>L</td><td>T</td><td>P</td></tr>
<tr><td>Type: Open Elective</td><td>3</td><td>0</td><td>0</td></tr>
<tr><td colspan="4">Course Description: Density-functional theory (DFT) is a modern computational quantum mechanical modelling method which is used in almost every branch of sciences and engineering. In this course student will learn basic principles of DFT with emphasis on in hand experience of DFT calculations.</td></tr>
<tr><td colspan="4">Course Content</td></tr>
<tr><td>Module 1 (4L)</td><td colspan="3">Review of Quantum Mechanics: Time independent Schrodinger Equation, Eigen value problem, exactly solvable one electron systems.</td></tr>
<tr><td>Module 2 (14L)</td><td colspan="3">Many electron problem: Pauli antisymmetry principle, Slater determinant, Hartree-Fock Theory, Configuration Interaction, Coupled Cluster theory.</td></tr>
<tr><td>Module 3 (14L)</td><td colspan="3">Density based approach: Thomas-Fermi model, Hohenberg-Kohn theorems, Kohn-Sham equations, Exchange and correlation functionals, Local density approximation, Generalized gradient approximation, Adiabatic connection, Hybrids functionals.</td></tr>
<tr><td>Module 4 (8L)</td><td colspan="3">Popular Functionals: B3LYP, PBE, B3LYP-D, Minnesota Functionlas etc.</td></tr>
<tr><td>Module 5 (8L)</td><td colspan="3">Solid state calculations: Bloch Theorem, Periodic boundary condition , Fourier Transformation, Band calculation.</td></tr>
<tr><td>References</td><td colspan="3">Text Books:
1. Koch and Max C. Holthausen; A Chemist’s Guide to Density Functional Theory (Wiley)
2. David S. Sholl and J. A. Steckel ; Density Functional Theory: A Practical Introduction (Wiley-Interscience)
3. C. Fiolhais, F. Nogueira, Miguel A.L. Marques; A Primer in Density Functional Theory (Springer)
Reference Books:
1. Robert Parr; Density-functional theory of atoms and molecules (OUP USA)
2. A. Szabo and N. S. Ostlund; Modern quantum chemistry (Dover Publications)</td></tr>
<tr><td>Course Outcome</td><td colspan="3">CO1. It will give a broad idea about how a multi-electron electronic structure problem can be solved.
CO2. This course will also give some in hand experience for performing DFT calculations along with introduction of many modern DFT functional.</td></tr>
</table>

Atmospheric Chemistry (21CYT804)			
Prerequisite: High School Chemistry, Physics and Mathematics	**L**	**T**	**P**
Type: Open Elective	**3**	**0**	**0**
Course description: This course is designed to provide an overview of the chemical processes that controls the composition, behaviour and evolution of Earth's atmosphere and discuss their societal implications			
Course content			

Module 1 (5L)	**Composition, Structure, and Transport in the Atmosphere** Composition: Units, Table of Composition, Pressure Structure: Barometric Law for gases at equilibrium, Scale height for actual atmosphere Temperature Structure Transport mechanisms and timescales: Vertical and Horizontal
Module 2 (4L)	**Photochemistry** Factors affecting light flux: Common Factors, Solar Zenith Angle, absorption, Rayleigh scattering, Graphs illustrating light flux Rates of Photolysis: Rate Law, Calculating a photolysis rate constant, NO2 as example. Calculation of SZA and photolysis rate constant, photolysis of O3 as a source of O(1D) and O(3P)
Module 3 (6L)	**Kinetics** First and Second Order, elementary vs. composite, pseudo-first order approximation, Steady State Approximation, Arrhenius expression, Transition state theory: canonical and variational, RRKM theory, master equation, quantum mechanical tunneling
Module 4 (10L)	**Stratospheric Ozone** Chapman Cycle, Ozone-Destroying Catalytic Cycles, Sources of Radicals, Propagation, Termination, Null Cycles, Coupling radical families, CFCs and their replacements, Effectiveness of Initiation and Termination: Cl versus other halogens, Thermodynamics and kinetics of HX formation, Photolysis of HO_X and $XONO_2$ Decadal Ozone Loss, Night and Day/Summer and Winter Observations of the Ozone Hole: [O_3] vs time and altitude, the polar vortex and competing hypotheses, The smoking gun Meteorology and Chemistry Needed for Ozone Hole: Polar Stratospheric Cloud (PSC) formation, Reactions on PSCs, Gas phase reactions and cycles, Arctic vs. Antarctic, Closing the hole Heterogeneous Chemistry Outside the Polar Vortices: Stratospheric Sulfate (Junge) Layer (SSL), Reaction of N2O5 on SSL, Deducing the effects on Ozone

Module 5 (4L)	**Tropospheric Ozone** Catalytic Cycles Producing Ozone: Photostationary State, Cycles consuming CO, Cycles consuming hydrocarbons Propagation vs. Termination, Radical Sources and Concentrations, Kinetics of barrierless reactions, Photochemistry, Meteorology of Ozone, NOx- vs. VOC-limited Ozone Formation, Modeling, Dry Deposition
Module 6 (4L)	**Atmosphere as an oxidizing medium:** Fate of Alkanes, Kinetic overview, Reactions initiated by OH Fate of Alkenes: Kinetic overview, Reactions initiated by OH, NO_3 and O_3, Night versus Day, Fate of Aromatic Hydrocarbons, Oxygenates: Alcohols, Aldehdyes
Module 7 (4L)	**Aqueous Aerosols in the Troposphere** Liquid Water in the Atmosphere, Henry's Law, Introduction, Monoprotic acids, Aldehydes, SO_2 Oxidation, S(IV) equilibria, HSO_4^- oxidation by HOOH, S(IV) oxidation by ozone Kinetics of Gas-Surface Interactions Aerosol Size Distributions: Size Classes, Discrete, Continuous (Normal, Semi-log, Log-log)
Module 8 (5L)	**Global Climate Change** Black Body Model of Earth's temperature, Greenhouse Effect, Clouds, Temperature Record, Radiative Forcing and Absolute and Relative Global Warming Potential, Feedbacks, Aerosol Effects, Flow of heat energy in atmosphere and its effects
References	Text Books: 1. J. H. Seinfeld, S. N. Pandis, Atmospheric Chemistry and Physics: From Air Pollution to Climate Change, Wiley, 2016 2. D. J. Jacob, Introduction to Atmospheric Chemistry, Princeton University Press, 1999 3. B. J. Finlayson-Pitts, J. N. Pitts Jr., Chemistry of the Upper and Lower Atmosphere: Theory, Experiments and Applications, Academic Press, 2000 4. K. J. Laidler, Chemical Kinetics, Pearson, 1997 Reference Books: 1. P. Fabian, M. Dameris, Ozone in the Atmosphere: Basic Principles, Natural and Human Impacts, Springer, 2014 2. S. Ramachandran, Atmospheric Aerosols: Characteristics and Radiative Effects, CRC Press, 2018
Course Outcome	CO1. Predict fate of molecules and radicals under typical atmospheric conditions. CO2. Qualitatively explain and quantitatively compute trends in photolysis rate constants with altitude, season, and time of day for molecules whose photochemistry is known. CO3. Compute rates of heterogeneous and homogeneous oxidation of S(IV).

	CO4. Qualitatively predict effects of chemical perturbations on catalytic cycles producing and destroying ozone. CO5. Explain basic principles of greenhouse effect and compute global warming potentials. CO6. Predict major atmospheric degradation pathways of natural and anthropogenic trace gases

Introduction to Astrochemistry (21CYT805)			
Prerequisite: High School Chemistry, Physics and Mathematics, Basic quantum mechanics	**L**	**T**	**P**
Type: Open Elective	**3**	**0**	**0**
Course description: The course would cover topics like interstellar medium, atomic and molecular physics, interstellar chemistry, molecular astronomy and unresolved problems.			
Course Content			

Module 1 (6L)	**The Interstellar Medium** Introduction to the Interstellar Medium, Conditions, time and length scales, constituents (elemental abundances, isotopic ratios, grains, radiation field, cosmic rays, shocks, magnetic fields). Structure and Evolution of the Interstellar Medium, Three-phase interstellar medium. Heating and cooling. Life cycle of interstellar matter (astration). Types of interstellar environments (diffuse clouds, dense clouds, star forming cores, photodissociation regions)
Module 2 (12L)	**Atomic & Molecular Physics** Interaction of Radiation with Matter: Semi-classical approach, oscillator strengths and Einstein coefficients, introduction to spectroscopy. Atomic structure (principal, angular momentum, magnetic, and spin quantum numbers; fine structure; hyperfine structure), atomic spectroscopy. Structure and Spectra of Diatomic Molecules: Energy level structure (electronic, vibrational and rotational). Electronic, vibrational spectra and rotational spectra. Application to H_2, C_2, CH, CO. Structure and Spectra of Polyatomic Molecules: Energy level structure of spherical, linear, symmetric, and asymmetric tops. Rotation-vibration interaction. Application to H_3^+, C_3, H_2O, HCO^+. Radiative and collisional excitation processes: Radiative excitation and selection rules. Collisional excitation and de-excitation. Rotational excitation of C_2 and CO. Radiative transfer
Module 3 (10L)	**Interstellar Chemistry:** H_2 Formation and Destruction, Formation of H_2 on interstellar grains. Chemical Kinetics and Rate Equations, Ion-Neutral Reaction Dynamics, Types of chemical reactions, endo/exothermicities, activation energies, rate expressions. Langevin cross-sections and temperature independence. Importance of ion-neutral reactions for interstellar chemistry. Chemical Modelling, Calculation of molecular abundances using chemical reaction networks: steady state and time-dependent. Identification of primary formation/destruction pathways for individual molecules. Dependence on laboratory data. Isotopic Fractionation, Quantum mechanical effects leading to fractionation of rare isotopes in molecules, and observational evidence.

Module 4 (14L)	**Molecular Astronomy** Detecting interstellar molecules in the optical spectra, Principles of optical spectrographs, and echelles. Basics of Radioastronomy, Fourier transforms, single dish studies, mapping, backends for spectroscopy, Radio Interferometry, Principles of interferometry (aperture synthesis). Interstellar molecules (with special reference to CO, CH^+, HCO^+, H_2CO, NH, N_2H^+, NH_3, OH, H_2O, H_3O^+, C_2H, C_2H_2, C_3H, C_3H_2, CN, HCN, HNC, $HCNH^+$)
References	Text Books: 1. A. M. Shaw, Astrochemistry: From astronomy to astrobiology, Wiley, 2006 2. S. Yamamoto, Introduction to Astrochemistry, Springer, 2017 3. D. A. Williams and S. Vitti, Observational Molecular Astronomy, Cambridge University Press, 2013 4. P. Bernath, Spectra of Atoms and Molecules, OUP, 1995 5. K. J. Laidler, Chemical Kinetics, Pearson, 2008 Reference Materials: Related primary and review articles from literature, especially from Annual Review of Astronomy and Astrophysics
Course Outcomes	CO1. Gain basic idea about the nature of interstellar medium, classification, physical conditions and their importance in the evolution of universe. CO2. Understand the various spectroscopic features important for identifying interstellar molecules and assessing the physical conditions of the medium CO3. Understand the different chemical processes, their energetic and kinetic behaviour and importance and utilities of chemical reactions network CO4. Learn about various aspects of interstellar molecules, including their energy level structures, their spectra, their chemistry, where they have been detected, and what they tell us as astronomical probes

Electrochemical Energy Storage Systems (21CYT806)			
Prerequisite: Basic understanding of Physical Chemistry	**L**	**T**	**P**
Type: Open Elective	**3**	**0**	**0**

Course Objectives: The objective of this course is to understand the fundamentals and increase the knowledge regarding electrochemical energy conversion and storage methods.

Course Content	
Module 1 (6L)	**Electrochemical Power Sources**: Introduction to electrochemical energy storage, Major types of reaction mechanisms in electrochemical cells, General equivalent circuit of an electrochemical cell, Voltage and capacity of an electrochemical cell, Steady state and potential step techniques (polarography, cyclic voltammetry, Chrono methods), Electrode types for electrochemical energy storage devices
Module 2 (9L)	**Batteries:** Lead-Acid Batteries, Negative and positive electrodes in lithium systems, Primary non-rechargeable batteries, Zn/MnO_2 "alkaline" cells, Li/FeS_2 cells, Li/I_2 batteries, Zn/Air cells, Magnesium and aluminum based cells, Sodium/sulfur batteries, Flow batteries, ZEBRA batteries
Module 3 (9L)	**Fuel Cells:** Types of fuel cells, Chemistry in different fuel cells, Single fuel cell setup, Cell potential, Cell potential-current density behaviour, Power density and efficiency of fuel cells, Methodology for analysis, Tafel slope, Electrocatalysis of fuel cell reactions, Experimental methods in low temperature fuel cells
Module 4 (9L)	**Electrochemical Supercapacitors:** Capacity vs capacitance, Introduction to various types of capacitors, Electrochemical double layer capacitors, Pseudocapacitors, Electrochemical flow capacitors, Supercapacitor components and materials, Instrumentation and measurement, Characterization, Performance evaluation and diagnostics of supercapacitors, Fabrication and performance evaluation of all-solid-state and wearable supercapacitors, Supercapacitor/battery hybrid systems
Module 5 (6L)	**Nanostructured Materials in Electrochemical Energy Storage Systems:** Nanostructured materials for electrochemical energy systems, Nanostructured electrodes and interfaces for the electrochemical storage of energy, Nanostructuring of current collectors/active film interface, Nano-architectured current collectors, Nano-structuring of active material/electrolyte interfaces, Nanofabrication techniques for electrochemical energy storage devices
Reference Books	1. D. Linden, Hand book of batteries and Fuel cells, McGraw Hill Book Company, 1984.

	2. Ali Eftekhari, Nanostructured Materials in Electrochemistry, Wiley-VCH, 2008 3. Allen J. Bard, Larry R. Faulkner, ELECTROCHEMICAL METHODS: Fundamentals and Applications, JOHN WILEY & SONS, INC., 2001 4. B.E. Conway, Electrochemical Supercapacitors, Kluwer Academic/Plenum Publisher, 1999 5. Supramaniam Srinivasan, Fuel Cells: From Fundamentals to Applications, Springer Science Publisher, 2006 6. Robert A. Huggins, Advanced Batteries, Materials Science Aspects, Springer Science Publisher, 2009 7. Javier Garcia-Martinez, Nanotechnology for the Energy Challenge, Wiley-VCH, 2010
Course Outcome	CO1. Understand the basics and complex nature of electrochemical systems CO2. Learn the interface of transport phenomena, materials characterization, basic electrochemistry and system engineering CO3. Understand the interdisciplinary nature of electrochemical systems for energy. CO4. Understanding of electrochemical energy systems relevant to modern energy technologies.

Photo-Inorganic Chemistry (21CYT807)			
Prerequisite: Understanding of basic chemistry and physics at undergraduate level.	**L**	**T**	**P**
Type: Program Elective	**3**	**0**	**0**

Course Description:
To study the basic principles that govern the light induced chemical processes that can be utilized to the benefit of society (power generation or newer materials)

Course Content

Module 1 (10L)	**Introduction** State Diagrams-Beer Lambert law-calculation of fluorescence rate constants from absorption spectra-Dipole and transition moments, selection rules-Rate constants of internal conversion; the energy gap law-Rate constants of inter system crossing, Sayed rules-Kasha and Vavilov rules-Franck-condon principle-Energy transfer, Excimer, Exciplex, quenching and sensitization.
Module 2 (10 L)	**Techniques and Methods** Light sources, filters, monochromator and detectors-Preparative Irradiation-Absorption Spectra-Steady state emission spectra-Time resolved luminescence-Quantum yields: Differential quantum yield- Actinometry-Spectrophotometric determination of the reaction progress-Reversible Photoreactions-Luminescence quantum yields-Stern-Volmer analysis-Quantum yields of triplet formation-Experimental arrangements for quantum yield measurements.
Module 3 (10 L)	**Applications** Transition Metal Complexes as sensitizers, Dye-Sensitized solar cells, Pervoskite solar cells, Factors affecting the efficiency, Device Fabrication, Incident to Photon Conversion efficiency (IPCE), Sunlight to chemical feedstocks, Hydrogen and methanol alternative energy, Photo-electrochemical cells,fabrication aspects, efficiency studies, Drawbacks of using 1st row transition metals in P-V devices, resolving efficiency issues through ligand design, inorganic nano particles-based water oxidation catalysts, Transition metal complexes in flexible displays, device structure of OLEDs, thermally activated delayed fluorescence, color tuning, aggregation induced emission, organometallic complexes in sensing applications.

Module 4 (10 L)	Properties of Excited States Structure, dipole moment, acid-base strengths, reactivity. Excited States of Metal Complexes Excited states of metal complexes: Comparison with organic compounds, electronically excited states of metal complexes, charge transfer spectra, charge transfer excitations. Redox Reactions by Excited Metal Complexes Energy transfer under conditions of weak interaction and strong interaction-examples formation; condition of the excited states to be useful as redox reactants, excited electron transfer, metal complexes as attractive candidates, (2,2-bipyridine and 1,10-phenanthroline complexes), illustration of reducing and oxidizing character of ruthenium (bipyridal complex, comparison with Fe (bipy); role of spin-orbit coupling-life time of these complexes. Application of redox processes of electronically excited states for catalytic purposes, transformation of low energy reactants into high energy products, chemical energy into light.
Reference Books	1. Principles of Fluorescence Spectroscopy, Lakowicz, III-Edition, Springer. 2. Highly Efficient OLEDs with Phosphorescent Materials, Hartmut Yersin, 2007, Wiley- VCH. 3. Organic Photochemistry and Photophysics, V. Ramamurthy, Kirk S.Schanze, CRC Press. 4. Photochemistry and Photophysics: Concepts, Research, Applications, Vincenzo Balzani, Paola Ceroni, Alberto Juris, 2014.
Course Outcomes	CO1. Understand the underlining physical principles that govern the light emitting devises. CO2. Understand the role of inorganic and organometallic complexes in the step towards clean energy devices. CO3. To familiarize with techniques and methods that have direct implication in developing new materials.

Organometallics and Catalysis (21CYT808)			
Prerequisite: Basic knowledge of inorganic/organic and coordination chemistry	**L**	**T**	**P**
Type: Program Elective	**3**	**0**	**0**
Course Description: To impart the knowledge and applications of advance organometallic chemistry in catalysis and other various metal catalyzed organic transformations			
Course Content			

Module 1 (4L)	Fundamental and basics of organometallic chemistry in catalysis
Module 2(4L)	Elementary organometallic reactions, Ligand substitutions; Oxidative addition; Reductive elimination; Intramolecular insertions/eliminations; Nucleophilic/Electrophilic attacks on coordinated ligands and migration reactions
Module 3(8L)	Bimetallic complexes and metal Clusters, metal-metal bond, isolobal analogy
Module 4(20L)	Fundamental of catalysis, homogeneous, heterogeneous catalysis, concept of TS state, TOF, TON, regio- and chemo- selectivity
Module 5 (2L)	**Homogeneous catalysis** Alkene isomerization, Hydrogenation, hydro-formylation, monsanto acetic acid process, alkene polymerization, cross coupling reactions; C-C, C-N, C-O and C-S bond coupling reactions (Heck, Sonogashira, Suzuki), olefin metathesis, oxidation of olefins, C-H activation and functionalization
Module 6 (3L)	Metal clusters and catalysis, reduction using transition metal hydrides, asymmetric hydrogenation.
Reference Books	1. Robert H. Crabtree, The Organometallic Chemistry of the Transition Metals, John Wiley and Sons, 4th edition. John Wiley and sons 2005**.** 2. Elschenbroich, C.; Salzer, A.; Organometallics: A Concise Introduction 3rd Edition. John Wiley and sons 2005 3. J. Tsuji, “Transition metal reagents and catalyst innovations in organic synthesis” John-Wiley- & Sons, Ltd, New York, 2000
Course Outcome	CO1. Develop the understand of fundamentals of catalysis CO2. Strategy to design and synthesis the target oriented catalyst CO3. Metal based organic reactions, mechanism and role of metal in catalysis. CO4. New advancement in the industrial catalysis and the chemistry involved.

Supramolecular Chemistry (21CYT809)

Prerequisite: Basic knowledge of different coordination bonds	**L**	**T**	**P**
Type: Program Elective	**3**	**0**	**0**

Course Description:
To impart knowledge of types of supramolecular Chemistry, structures-bonding and their applications as Organic materials, sensors, and devices

Course Content

Module 1(10 L)	**Introduction** Concepts and development, Nature of binding interactions in supramolecular structures: ion-ion, ion-dipole, dipole-dipole, H-bonding, cation-π, anion-π, π-π and van der Waal interactions, Supramolecular Chemistry in Life, Ionophores, Porphyrin and other tetra-pyrrole macrocycles
Module 2(10 L)	**Host–guest Chemistry** Synthesis and structures of crown ethers, Lariat ethers, Podands, Cryptands, Spherands, Calixarene, Cyclodextrins, Cyclophanes, Cryptophanes, Carcerands and hemicarcerands, Host-guest interactions, Preorganization and complementarity, Lock and key analogy, binding of cationic, Anionic, Ion pair and neutral guest molecules
Module 3(12 L)	**Supramolecular Polymers** Self-assembly molecules: Design, Synthesis and Properties of the molecules, Self-assembly by H-bonding, Catenanes, Rotaxanes, Dendrimers and Supramolecular gels. Relevance of supramolecular chemistry to mimic biological system
Module 4 (4 L)	**Molecular Devices** Molecular Electronic devices, Molecular wires, Molecular rectifiers, Molecular Switches and Molecular logic gates. Examples of recent developments in supramolecular chemistry from current literature
References	1. Lehn, J. M., Supramolecular Chemistry-Concepts and Perspectives, Wiley – VCH (1995). 2. Beer, P.D., Gale, P. A., and Smith, D. K., Supramolecular Chemistry, Oxford University Press (1999). 3. Steed, J. W., and Atwood, J. L., Supramolecular Chemistry, Wiley (2000). 4. Recent Literature
Course Outcomes	CO1. Molecular recognition and nature of bindings involved in biological systems CO2. Structures of various supramolecular structure in solution and solid state CO3. Applications of supramolecular compounds in miniaturization of molecular devices

Polymer Chemistry (21CYT810)			
Prerequisite: Basic knowledge of chemistry	**L**	**T**	**P**
Type: Program Elective	**3**	**0**	**0**

Course Description:

- To impart the knowledge of basic concepts of the polymers.
- To provide the knowledge of polymer chemistry based on synthesis, characterization and applications.

Course Content

Module 1 (10L)	**Introduction** Introductory concepts, definition, monomers, repeat units, degree of polymerization, linear, branched and network polymers, characterization: molecular weight studies and molecular weight distribution, determination of thermal parameters, importance of polymers, Mechanistic aspects: addition, ionic, emulsion, suspension, aqueous, coordination, condensation polymerization.
Module 2 (12L)	**Classification and Polymerization** Classification of polymers, polymerization in homogeneous and heterogeneous systems, step-growth syntheses, chain polymerizations, ring-opening polymerizations, reductive coupling and other redox polymerization reactions
Module 3 (12L)	**Inorganic polymer elastomers** Bridge between small and finite molecules, homopolar inorganic polymers, heteropolar inorganic polymers, Phosphorous based polymer: Polyphosphazenes, Sulphur containing polymer: Polysiloxanes, Polysilanes and Boron based polymer, Metal coordinated polymers
Module 4 (8L)	**Applications of inorganic polymers** Catalysis, medical purposes, flame retardants, high-temperature fluids and lubricants
Reference Books	1. Textbook of Polymers Science, F.W. Billmeyer Jr. Wiley. 2. Contemporary Polymer Chemistry, H.R. Allcock and F.W. Lambe, Prentice Hall. 3. Ronald D. Archer, Inorganic and Organometallic Polymers, Wiley-VCH, Inc. 4. James E. Mark, Harry R. Allcock, Robert West, Inorganic polymers, Oxford University Press, USA 5. Inorganic Chemistry, Keith F. Purcell, John C. Kotz, Cengage, India.

Course Outcomes	CO1. Explain the classification of various types of polymers. CO2. Understand the different methods for the synthesis and characterization of the polymers. CO3. Demonstrate the ability to quickly acquire the knowledge of new polymer-related applications and development of new polymer materials and related processes with respect to sustainability considerations.

Organometallic Chemistry of Main Group Elements (21CYT811)

	L	T	P
Prerequisite: Basic knowledge of covalent and Ionic bonds. Knowledge on the periodic properties of the elements			
Type: Program Elective	**3**	**0**	**0**

Course Description:
To impart knowledge on the bonding and structure in Main Group Organometallic compounds and recent development in their potential applications

Course Content

Module 1 (4 L)	**Introduction** Milestones in organometallic chemistry, organo-element compounds: classification and electronegativity consideration, energy, polarity and reactivity of M-C bond
Module 2 (8 L)	**Organometallic compounds of Alkali and Alkaline-Earth Metal** Organo-lithium compounds, Li NMR Spectroscopy, organometallic compounds of the heavier alkali metals, organo-beryllium, -magnesium, - calcium, -strontium and -barium compounds, examples of some organo-zinc compounds, some catalytic applications of organo-magnesium and organo-zinc compounds
Module 3 (12 L)	**Organometallic Compounds of Boron group** Organo-Boron, -aluminium, -gallium and -indium compounds, Al^{III}, Ga^{III} and In^{III} organyls and their Lewis base adducts, sub-valent organo-aluminium compounds, $Ga^{II,I}$, $In^{II,I}$ and $Tl^{II,I}$ organyls, thallium in organic synthesis
Module 4 (6 L)	**Organo-element Compounds of Carbon Group** Organosilicon compounds, sub-valent organosilicon compounds, organo-germanium and organo-tin compounds, sub-valent organo-germanium and –tin compounds
Module 5 (4 L)	**Organo-element Compounds of the Nitrogen group and Oxygen group** E^{V} (P, As, Sb) organyls, E^{III} (P, As, Sb) organyls, E-C double and triple bonds, E-E double and triple bonds; examples, structure, bonding and reactivity of organo-selenium and organo-tellurium compounds
References	1. Christoph Elschenbroich, Orgaometallics (Third Edition), Wiley-VCH. 2. B.D. Gupta and A. J. Elias, Basic Organometallic Chemistry (Concept, Syntheses and Applications) (Second Edition) (University Press) 3. Recent Literature
Course Outcomes	CO1. Bonding and structure in main group organo-element compounds CO2. Unusual structure and bonding in main group elements CO3. Stability of main group elements in different oxidation number and coordination number in their organo-element compounds

	CO4. Applications of earth abundant main group organo-elements in catalysis

Bio-Inorganic Chemistry (21CYT812)			
Prerequisite: To impart knowledge of basic topics in Inorganic chemistry	L	T	P
Type: Program Elective	3	0	0

Course Description:

- To enable the students to understand the structure, bonding, and reaction mechanism involved in the biological, bioinorganic complexes.
- To facilitate the student to apply the practical aspects of bio-inorganic chemistry in basic and advanced research and development.
- To understand the basic need of bio-inorganic chemistry in industrial applications.

Course Content

Module 1 (8L)	**Transition metal ions in biology** Metallo-biomolecules, electron carriers, oxygen carriers and enzymes, Biogeoinorganic chemistry - environment, their occurrence and function, active-site structure and function of metallo-proteins and metallo-enzymes with various transition metal ions and ligand systems.
Module 2 (14L)	Transport and storage of Dioxygen: Heme proteins and oxygen uptake, and their coordination geometry, electronic structure and functions of hemoglobin, myoglobin and characterization of O_2 bound species by Raman and infrared spectroscopic methods, representative synthetic models of heme- and non-heme systems, hemocyanins and hemerythrin, model synthetic complexes of iron, copper and cobalt etc. Zinc enzymes-carboxypeptidase and carbonic anhydrase, Iron enzymes-catalase, peroxidase and cytochrome P-450, Metallo enzyme-II Copper enzymes-superoxide dismutase, Molybdenum oxotransferase enzymes-xanthine oxidase, Coenzyme vitamin B12
Module 3 (8L)	Calcium in Biology - Ion channels in biomembrane, calcium in living cells, transport and regulation, molecular, aspects of intramolecular processes, extracellular binding proteins
Module 4 (10 L)	Metals in medicine, metal deficiency and disease, toxic effects of metals (Cd, Hg and Cr toxic effects with specific examples), metals used for diagnosis and chemotherapy with particular reference the anticancer drugs and MRI (Mn and Fe) agents
Reference Books	1. Principles of Bioinorganic Chemistry, S. J. Lippard and J. M. Berg, University Science Books, Mill Valley, 1994. 2. Bioinorganic Chemistry: Inorganic Elements in the Chemistry of Life, W. Kaim and B. Schwederski, John Wiley & Sons Inc., 1994.
Course Outcomes	CO1. Understand the importance of minerals for living organisms. CO2. Understand role of iron, copper, zinc etc. containing biological molecules

	CO3. Understand the applications of Bioinorganic chemistry such as in chemotherapy, imaging and other similar applications CO4. Explain the reaction mechanism of different metal complex reactions. CO5. Become familiar with the various transition metal-based inorganic materials.

Symmetry and Group Theory (21CYT813)			
Prerequisite: Basic knowledge of structure and bonding of inorganic compounds and coordination compounds	**L**	**T**	**P**
Type: Program Elective	**3**	**0**	**0**

Course Description: To impart the knowledge of symmetry and group theory in inorganic/organic compounds and its applications in various molecular spectroscopy

Course Content	
Module 1 (6L)	**Introduction** Concept of symmetry, symmetry in nature, polygons, pyramids, prism, concept of symmetry in molecules - Symmetry operation, rotational axis of symmetry, plane of symmetry, improper axis of rotation, centre of symmetry and inversion centre, identity and determinations of various symmetry elements.
Module 2(4L)	**Molecular Point Group** Schonfilies symbols, identification of molecular point group, cyclic point group, dihedral point group, improper point groups, molecules with special point group, molecules of high symmetry.
Module 3(8L)	**Properties of Group** Properties of group, sub-group, abelian and non-abelian group, class and order of the group, matrices representations of groups.
Module 4(15L)	**Representations, Character Table and its applications** Representations, reducible and irreducible representations, derivation of reducible representation by 3N system and bond vector method **Character Table and its applications** Structure of character table, the great orthogonality theorem (without proof) and its importance, derivation of character tables for water and ammonia molecule, Mullikan symbols determination for translations and rotations, applications of group theory in FTIR and Raman and spectroscopy, molecular hybridization and NMR spectroscopy
Module 6 (2L)	**Direct product** Concept of direct product and its application in spectroscopy
Reference Books	1. Physical methods in Chemistry, R. S Drago, Saunders college 2. K. Veera Reddy, Symmetry and spectroscopy of molecules, New Age Science. 2009 3. Chemical application of group theory, F. A Cotton 4. Group Theory in Chemistry, M. S. Gopinathan and V. Ramakrishnan, Vishal Publishing Co., 2nd edition.
Course Outcome	CO1. Basic knowledge of structure and geometry as per symmetry point of view

	CO2. Derivation of point group in various structures and general molecules, shapes, polygons CO3. Understanding of character table and its its fundamental in various spectroscopy

<table>
<tr><th colspan="4">Organic Synthesis (21CYT814)</th></tr>
<tr><td>Prerequisite: Basics of organic reaction mechanism</td><td>L</td><td>T</td><td>P</td></tr>
<tr><td>Type: Program Elective</td><td>3</td><td>0</td><td>0</td></tr>
<tr><td colspan="4">Course Description: To impart knowledge of advanced concepts in organic chemistry such as asymmetric synthesis, retrosynthetic analysis, disconnections approach and organometallic reagents with their applications. Common organic reactions and rearrangements will also be discussed.</td></tr>
<tr><td colspan="4">Course Content</td></tr>
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<table>
<tr><td>Module 1 (12L)</td><td>General concepts in Organic synthesis
Asymmetric Synthesis, Retrosynthesis analysis, disconnection approach, Synthons, linear and convergent synthesis, Umpolung of reactivity and protecting groups in organic synthesis. Organic transformations and functional group interconversion.</td></tr>
<tr><td>Module 2 (14L)</td><td>Organometallic Reagents and their applications
Principle, preparations, properties and applications and role of catalysts and reagents including organic, inorganic, organometallics and enzymatic in organic synthesis with mechanistic details. Group I and II metal organic compounds Li, Mg, Hg, Cd, Zn and Ce Compounds.</td></tr>
<tr><td>Module 3 (14L)</td><td>Common Organic Reactions and Rearrangements
General mechanistic considerations-nature of migration, migratory aptitude, memotry effects. A detailed study of the following rearrangements. Pinacol-pinacolone, Wagner-Meerwein, Demjanov, Benzil-Benzillic acid. Favorskii, Arndt-Eister synthesis, Neber, Beckmann, Hofmann, Curtius, Schmidt, Baeyer-Villiger, Shapiro reaction.</td></tr>
<tr><td>Reference Books</td><td>1. Modern Synthetic Reactions. H.O. House, W.A. Benjamin
2. Some Modern Methods of Organic Synthesis, W. Carruthers, Cambridge Univ. Press
3. Advanced Organic Chemistry, Reactions Mechanisms and Structure, J. March. John Wiley
4. Principles of Organic synthesis, R.O.C. Norman and J.M. Coxon, Blackie Academic & Professional
5. Advanced Organic Chemistry Part B.F.A. Carey and R.J. Sundberg Plenum Press
6. Rodd's Chemistry of Carbon Compounds. Ed. S. Coffey, Elsevier
7. Name Reactions, Jie jack Li, Springer
8. Organic Syntheses Based on Name Reactions, A. Hassner and I. Namboothiri, Elsevier</td></tr>
<tr><td>Course Outcomes</td><td>CO1. Explain advanced organic chemistry concepts such as asymmetric Synthesis, retrosynthesis, disconnection approach etc.
CO2. Demonstrate the role of catalysts and reagents including organic, inorganic,</td></tr>
</table>

	organometallics and enzymatic in organic synthesis with mechanistic details CO3. Understand various rearrangement reactions with mechanistic approach.

Applied Biocatalysis (Enzymes) (21CYT815)				
Prerequisite: Basics of enzyme catalysis		**L**	**T**	**P**
Type: Program Elective		**3**	**0**	**0**
Course Description: To impart knowledge of biological catalysis including enzyme catalysis in different reactions.				
Course Content				
Module 1 (4L)	**Introduction** Basic considerations, Proximity effects and molecular adaption.			
Module 2 (14L)	**Enzymes** Introduction and historical perspective, chemical and biological catalysis, remarkable properties of enzymes like catalytic power, specificity and regulation. Nomenclature and classification, extraction and purification. Fischer's lock and key and Koshland's induced fit hypothesis, concept and identification of active site by the use of inhibitors, affinity labeling and enzyme modification by site-directed mutagenesis. Enzyme kinetics, Michael's-Menten and Lineweaver Burk plots, reversible and irreversible inhibition.			
Module 3 (8L)	**Mechanism of Enzyme Action** Transition-state theory, orientation and Steric effect, acid-base catalysis, covalent catalysis, strain or distortion. Examples of some typical enzyme mechanisms for chymotrypsin, ribonuclease, lysozyme and carboxypeptidase.			
Module 4 (8L)	**Enzyme Catalyzed Reactions** Nucleophilic displacement on a phosphorus atom, multiple displacement reactions and the coupling of ATP cleavage to endergonic processes. Transfer of sulphate, addition and elimination reactions, enolic intermediates in Isomerization's reactions, α-Cleavage and condensation, some isomerization and rearrangement reactions. Enzyme catalyzed carboxylation and decarboxylation.			
Module 5 (8L)	**Biotechnological Applications of Enzymes** Large-scale production and purification of enzymes, techniques and methods of immobilization of enzymes, effect of immobilization on enzyme activity, application of immobilized enzymes, use of enzymes in food and drink industry-brewing and cheese-making, syrups from corn starch, enzymes as targets for drug design. Clinical uses of enzymes, enzyme therapy, enzymes and recombinant DNA Technology.			
Reference Books	1. Bioorganic Chemistry: A Chemical Approach to Enzyme Action, Hermann Dugas and C. Penny, Springer Verlag. 2. Understanding Enzymes, Trevor Palmer, Prentice Hall. 3. Enzyme Chemistry: Impact and applications, Ed. Collin J suckling, chemistry.			

	4. Enzyme Mechanisms Ed. M.I. Page and A Williams, Royal Society of Chemistry. 5. Fundamentals of Enzymology, N.C. Price and L. Stevens. Oxford University Press. 6. Immobilized Enzymes: An Introduction and Applications in Biotechnology, Michael ID. Trevan, John Wiley. 7. Enzymatic Reaction Mechanisms. C. Walsh. W.H. Freeman. 8. Enzyme Structure and Mechanism, A Fersht, W.H. Freeman. 9. Biochemistry: The Chemical Reactions of Living Cells, D.E. Metzler, Academic Press.
Course Outcome	CO1. Understand the theories of enzyme kinetics in the cell CO2. Mechanisms of enzyme catalysis, and the mechanisms of enzyme regulation in the cell CO3. Describe and use the equations of enzyme kinetics.

Heterocyclic Chemistry (21CYT816)			
Prerequisite: Basics of Heterocyclic Chemistry	**L**	**T**	**P**
Type: Program Elective	**3**	**0**	**0**

Course Description: Heterocyclic compounds are very interesting due to their distinct structure and their availability in Nature and in Medicinal Drugs. So, the technique of synthesis of heterocyclic compounds is important in the synthesis of different drugs. This course gives quantitative ideas about the synthesis, properties and uses of such heterocyclic compounds like pyrole, pyridine quinoline, thiophene, furan and their benzo-fused derivatives.

Course Content	
Module 1 (8L)	**Nomenclature of Heterocycles** Replacement and systematic nomenclature (Hantzsch-Widman system) for monocyclic fused and bridged heterocycles.
Module 2 (12L)	**Benzo-Fused Five-Membered Heterocycles** Synthesis and reactions including medicinal applications of benzopyrroles, bezofurans and benzothiophenes.
Module 3 (10L)	**Six-Membered Heterocycles with one Heteroatoms** Synthesis and reactions of pyrylium salts and pyrones and their comparison with pyridinium & thiopyrylium salts and pyridones. Synthesis and reactions of quinolizinium and benzopyrylium salts, coumarins and chromones.
Module 4 (10L)	**Six Membered Heterocycles with Two or More Heteroatoms** Synthesis and reactions of diazines, triazines, tetrazines and thiazines. Seven-and Large-Membered Heterocycles Synthesis and reactions of azepines, oxepines, thiepines, diazepines thiazepines, azocines.
Reference Books	1. Heterocyclic Chemistry Vol. 1-3, R.R. Gupta, M. Kumar and V. Gupta, Springer Verlag 2. The Chemistry of Heterocycles, T. Eicher and S. Hauptmann, Thieme 3. Heterocyclic chemistry J.A. Joule, K. Mills and g. F. Smith, Chapman and Hall 4. Heterocyclic Chemistry, T.L. Gilchrist, Longman Scientific Technical 5. Contemporary Heterocyclic Chemistry, G. R. Newkome and W.W. Paudler, Wiley-Inter Science 6. An Introduction to the Heterocyclic Compounds, R.M. Acheson, John Wiley 7. Comprehensive Heterocyclic Chemistry, A.R. Katritzky and C.W. Rees, eds. Pergamon Press
Course Outcome	CO1. Explain nomenclature, synthesis and reactivity of smaller, five and six membered heterocyclic compounds CO2. Explain various methods of ring synthesis, reactivity and applications of heterocyclic compounds and their derivatives.

	CO3. Acquire knowledge on various biosynthetic pathways.

Chemistry of Natural Products (21CYT817)

	L	T	P
Prerequisite: Basic knowledge of natural products	**L**	**T**	**P**
Type: Program Elective	**3**	**0**	**0**

Course Description: Alkaloids and terpenes are two very important class of organic chemicals available in different kind of drugs and perfumery chemicals like ephedrine, conium, citral, jasmone etc. The contents of this course deals with synthesis and structural determination of these class of chemicals. Few reactions of them are also discussed here.

Course Content

Module 1 (14L)	**Terpenoids and Carotenoids** Classification, nomenclature, occurrence, isolation, general methods of structure determination, isoprene rule. Structure determination, stereochemistry, biosynthesis and synthesis of the following representative molecules: Citral, Geraniol α-Terpeneol, Menthol, Farnesol, Zingiberence, Santonin, Phytol, Abietic acid and b-Carotene.
Module 2 (14L)	**Alkaloids** Definition, nomenclature and physiological action, occurrence, isolation, general methods of structure elucidation, degradation, and classification based on nitrogen heterocyclic ring, role of alkaloids in plants. Structure, stereochemistry, synthesis and biosynthesis of the following: Ephedrine, (+) - Coniine, Nicotine, Atropine, Quinine and Morphine.
Module 3 (10L)	**Steroids** Occurrence, nomenclature, basic skeleton, Diel's hydrocarbon and stereochemistry, Isolation, Structure determination and synthesis of Cholesterol, Bile acids, Androsterone, Testosterone, Estrone, Progesterone, Aldosterone, Biosynthesis of Steroids.
Module 4 (4L)	**Porphyrins** Structure and synthesis of Haemoglobin and Chlorophyll.
Reference Books	1. Natural Products: Chemistry and Biological Significance, J. Mann, R.S. Davidson, J.B. Hobbs, D.V. Banthrope and J.B. Harbome, Longman, Esses. 2. Organic Chemistry: Vol. 2 1L. Finar, ELBS 3. Stereoselective Synthesis: A Practical Approach, M. Norgradi, VCH. 4. Rodd's Chemistry of Carbon Compounds, Ed. S. Coffey, Elsevier. 5. Chemistry, Biological and Pharmacological Properties of Medicinal Plants from the Americas, Ed. Kurt Hostettmann, M.P. Gupta and A. Marston. Harwood Academic Publishers. 6. Introduction to Flavonoids, B.A. Bohm. Harwood Academic Publishers. 7. New Trends in Natural Product chemistry, Ata-Ur-Rahman and M.L. Choudhary, Harwood Academic Publishers. 8. Insecticides of Natural Origin, Sukh Dev, Harwood Academic Publishers.

Course Outcome	CO1. Acquire knowledge about basic structure and occurrence of the natural products CO2. Able to understand the chemistry of natural products like alkaloids, steroids, terpenoides, carotenoids and porphyrins

Pharmaceutical Chemistry (21CYT818)

	L	T	P
Prerequisite: Basic knowledge of pharmaceutical Chemistry	**L**	**T**	**P**
Type: Program Elective	**3**	**0**	**0**

Course Description: Nowadays synthesis of medicine is a very important issue for pharmaceutical industry. The medicines can be antipyretic drugs like paracetamol or antibiotic like penicillin. This course mainly deals with the structural determination, synthesis and uses of some drugs such as antipyretics, analgesic, sulpha-drugs penicillin etc.

Course Content

Module 1 (14L)	**Disinfectants and Antiseptics** Phenol and homologs (chlorocresol, chloroxylenol, hexachlorophene, thymol), hydroxyquinolines, quaternary ammonium compounds, halogen derivatives, chloramine, chlorohexidine HCL, Dyes (crystal violet, brilliant green), thiomersol, alcohol.
Module 2 (14L)	**General and local anesthetics** Ethers, halogenated hydrocarbons (halothane), Cyclopropane, nitrous oxide, intravenous anaesthetics, local anaesthetics: esters, benzoic acid derivatives, amides, miscellaneous anaesthetics, local anaesthetics, and their mechanism of action.
Module 3 (12L)	**Antibiotics and other antibacterial drugs** Synthesis and therapeutic used of penicillin G, penicillin V, Ampicillin, Amoxycillin, Chloramphenicol, Sulphonamides, Sulphanilamide, silver sulphadiazine, Aminglycosides and their Mechanism of Action including Enzymatic Drug modification.
Reference Books	1. Alex Grigauz, Introduction to Medicinal Chemistry, Wiley-VCH 2. Wilson and Gisvolds Text Book of Organic Medicinal and Pharmaceutical Chemistry, Ed., Robert F. Dorge. 3. Burgers Medicinal Chemistry and Drug Discovery, Vol I-V Ed. Monfred E. Wolff John Wiley. 4. Goodman and Gilman Pharmacological Basis of Therapeutics, McGraw- Hill 5. Umezawa**,** Hamao, Hooper and Irving R, Aminoglycoside Antibiotics, Springer
Course Outcome	CO1. Explain the chemistry and mechanism of action of medicines used as disinfectants, antiseptics, local anesthetics and antibiotics CO2. Explain the chemistry of antibacterial drugs

<table>
<tr><th colspan="4">Cell Structure & Biomolecules (21CYT819)</th></tr>
<tr><td colspan="1">Prerequisite: Basic knowledge of biology and cell structure.</td><td>L</td><td>T</td><td>P</td></tr>
<tr><td>Type: Program Elective</td><td>3</td><td>0</td><td>0</td></tr>
<tr><td colspan="4">Course Description: This course includes basic knowledge of biology including cell structure, its functions, lipids and proteins.</td></tr>
<tr><td colspan="4">Course Content</td></tr>
<tr><td>Module 1 (12L)</td><td colspan="3">Cell Structure and Functions
Structure of prokaryotic and eukaryotics cell. Intracellular organelles and their function, comparison of plant and animals cells. Overview of metabolic processes – catabolism and anabolism. ATP the biological energy currency. Origin of life -unique properties of carbon, chemical evolution and rise of living systems. Introduction to Biomolecules, building blocks of bio macromolecules.</td></tr>
<tr><td>Module 2 (12L)</td><td colspan="3">Lipids
Fatty acids, essential fatty acids. Structure and function of triacycerols, glycerophospholipilds. Sphingolipids, cholesterol, bile acids, prostaglandins. Lipoproteins composition and function. Properties of lipid aggregate-micelles, bilayers, liposomes and their possible biological functions, Biological membranes. Fluid mosaic model of membrane structure. Lipid metabolism, β-oxidation of fatty acids.</td></tr>
<tr><td>Module 3 (12L)</td><td colspan="3">Amino acids, peptides and protein
Chemical and enzymatic hydrolysis of properties to peptides, amino acid sequencing. Secondary structure of proteins, forces responsible for holding of secondary structure α-helix, β-sheets, super secondary structure, triple helix structure of collagen. Tertiary structure of protein-folding and domain structure. Quaternary structure. Amino acid metabolism-degradation and biosynthesis of amino acids, sequence determination: chemical/enzymatic/mass spectral, racemization/detection. Chemistry of oxytocin and tryptophan releasing hormone (TRH)</td></tr>
<tr><td>Reference Books</td><td colspan="3">1. Principles of biochemistry, A.L. Lehninger, Worth Publishers.
2. Biochemistry, L. Stryer, W.H. Freeman.
3. Biochemistry, J. David Rawn, Neil Patterson</td></tr>
<tr><td>Course Outcome</td><td colspan="3">CO1. Understand the basics of cell and its components
CO2. Understand the foundation on the basic module of life
CO3. Understand the structure, properties and biosynthesis of important biomolecules like lipids and proteins.</td></tr>
</table>

Biochemistry (21CYT820)			
Prerequisite: Basic knowledge of physical, organic and inorganic chemistry	**L**	**T**	**P**
Type: Program Elective	**3**	**0**	**0**

Course description: This course examines the chemical and physical properties of the building blocks of cell, with special emphasis on the structures of proteins and nucleic acids, their roles in propagation of genetic codes, roles of enzymes in catalyzing biochemical processes and basic principles of metabolism.

Course Content

Module 1 (12L)	**Proteins** Primary structure: Amino acids, peptide bonds, polypeptide chains Secondary structure: α-, 310-, π-helices, parallel and antiparallel β-sheets, β-turns, γ-turns, Ramachandran plot Tertiary structure: Protein folding, Levinthal's paradox, Motifs and domains: Rossmann fold, helix turn helix, 4 helix bundle, beta barrel Protein sequencing and structure determination: Mass & NMR spectroscopy, X-ray crystallography
Module 2 (14L)	**Nucleic acids** Nucleobases, nucleosides and nucleotides, Single stranded RNA, Double helix DNA, A, B and Z-DNA structures, DNA replication: polymerases, Transcription: mRNA, reverse transcription, Translation: codon, role of tRNA and ribosome Genomes, genes, Polymerase chain reaction (PCR), Use of modified bases in PCR, mutagenesis (random and site directed), recombinant DNA technology
Module 3 (4L)	**Enzymes and their kinetics** Enzymes as Catalysts: role of cofactors, active sites and enzyme-substrate complex Michaelis-Menten kinetics and its extension, competitive, Inhibition of enzymes: reversible (competitive, uncompetitive and noncompetitive) and irreversible. Effect of pH and temperature on enzyme activity
Module 4 (12L)	**Metabolism** ATP: Universal currency of free energy, ATP hydrolysis, Glycolysis and gluconeogenesis, Krebs cycle, Oxidative phosphorylation, Photosynthesis, Calvin cycle, Pentose phosphate pathway
References	Text Books: 1. J. M. Berg, J. Timoczko, L. Stryer, Biochemistry, WH Freeman, 2019 2. D. L. Nelson, M. Cox, Lehninger Principles of Biochemistry, WH Freeman, 2017 3. D. Voet, J. Voet, C. Pratt, Fundamentals of Biochemistry, Wiley, 2012 Reference Books:

	1. C. I. Branden, J. Tooze, Introduction to protein structure, Garland Science, 1998 2. R. A. Copeland, Enzymes: A Practical Introduction to Structure, Mechanism, and Data Analysis, Wiley, 2000
Course Outcomes	CO1. Introduction to the chemical processes of life: Their structures, chemistry and functions CO2. Gain basic ideas about the flow of genetic codes via chemical transformation occurring inside cells CO3. Understand the role of enzymes in realizing complex chemical reactions under mild conditions CO4. Introduction to the central pathways of metabolism and understanding the associated chemical transformations involved therein

Physical Organic Chemistry (21CYT821)			
Prerequisite: Basic understanding of Physical and Organic Chemistry	**L**	**T**	**P**
Type: Program Elective	**3**	**0**	**0**
Course Description: This course will connect the knowledge of physical chemistry to traditional organic synthesis and mechanism.			
Course Content			

Module 1 (6L)	**Description of molecules:** (includes reactive intermediates as radicals, carbenes, carbocations and carbanions) based on the Quantum mechacanical valence bond theory and molecular orbital theory.
Module 2 (6L)	**Conformational analysis of organic molecules:** NMR analysis of hindered rotation (determination of the rate constant at the coalescence temperature), energy-reaction coordinate diagram for simultaneously rotation of two C-C bonds and a short introduction to molecular mechanic calculations.
Module 3 (15L)	**Energy surfaces (2D and 3D) and kinetic analyses in the study of reaction mechanisms:** Ke More O'Ferral-Jencks plot (variable transition-state diagram), reaction order and rate laws, the steady-state approximation in the study of complex reactions, kinetic versus thermodynamic control, the principle of microscopic reversibility, the Curtin-Hammett principle, the Hammonds postulate. Energy functions from rate constants and reaction temperatures: The Arrhenius (activation energy) and the Eyring (enthalpy and entropy of activation) equations. Kinetic isotope effects (primary and secondary). Polanyi' rule of mode selectivity.
Module 4 (15L)	**Linear free energy relationships (LFERs):** (a) The Hammett equation for aromatic compounds, substituent and reaction constants, significance of the Hammett reaction constant values, deviations from linearity mechanistic information in multi-step reactions. (b) The Swain-Scott equation (nuclophilicity versus basicity). (c) The Grunwald-Winstein and the Schleyer equations(quantifying solvent effects and nucleophilicity).
Module 5 (6L)	**Classification of solvents based on physical properties:** dielectric constant, refractive index, dipole moment, donor number, acceptor number, hydrogen bond acceptor capacity alpha, hydrogen bond donor capacity beta and the Reichardt's Et scales.
References	Text Books: 1. E. V. Anslyn; D. A. Dougherty: Modern Physical Organic Chemistry, University Science Books Reference Books:

	1. F. A. Carey; R. J. Sundberg: Advanced Organic Chemistry, Part A: Structure and Mechanisms, Springer 2. T. H. Lowry and K. S. Richardson: Mechanism and Theory in Organic Chemistry, Pearson
Course Outcomes	CO1. To connect the physical chemistry knowledge to the organic synthesis and mechanism. CO2. Invoke known mechanisms and intermediates to explain observed chemical phenomena

<table>
<tr><th colspan="4">Electrochemistry: Ionics and Electrodics (21CYT822)</th></tr>
<tr><td>Prerequisite: Basic understanding of Physical Chemistry and Electrochemistry</td><td>L</td><td>T</td><td>P</td></tr>
<tr><td>Type: Program Elective</td><td>3</td><td>0</td><td>0</td></tr>
<tr><td colspan="4">Course Objectives: To apply theories in electrochemistry to analyse electrochemical processes in liquid as well as solid phases.</td></tr>
<tr><td colspan="4">Course Content</td></tr>
<tr><td>Module 1 (6L)</td><td colspan="3">Introduction to Electrode Processes: Electrochemical cells and reactions,Faradaic and nonfaradaic electrode processes, Nature of electrode-solution interface in nonfaradaic processes, Factors effecting rates of faradaic electrode reactions, Mass transfer controlled reactions.</td></tr>
<tr><td>Module 2 (8L)</td><td colspan="3">Ionics: Introduction to electrochemistry of solutions, Ion-solvent interactions, ion-ion interactions, ionic transport and diffusion in solutions, Equilibrium electrode potentials, Liquid junction potential, Selective electrodes.</td></tr>
<tr><td>Module 3 (6L)</td><td colspan="3">Electric Double layer: Models for double-layer structure - The Helmholtz model, Stern’s modification, Gouy and Chapman model, Specific adsorption of ions and neutral compounds, Influence of electric double layer on charge transfer processes.</td></tr>
<tr><td>Module 4 (8L)</td><td colspan="3">Electrodics and Electrode kinetics: The electrode/electrolyte interface, Current-potential relationship (Butler-Volmer and Tafel equations), Overpotential, Hydrogen evolution and oxygen reduction reactions, Underpotential deposition of metals</td></tr>
<tr><td>Module 5 (6L)</td><td colspan="3">Electrochemical Methods: Potential step methods, Potential sweep methods, Pulse techniques, Controlled current techniques, Basic concepts of impedance, Bulk electrolysis.</td></tr>
<tr><td>Module 6 (2L)</td><td colspan="3">Reference electrodes: Polarizable and non-polarizable electrodes, Types of reference and working electrodes.</td></tr>
<tr><td>Module 7 (6L)</td><td colspan="3">Solid State Electrochemistry: Interface electrical phenomena in ionic solids, Defect chemistry in solid state electrochemistry, Solid electrolytes, Mixed ionic–electronic conductors, Experimental methods, Electrochemical membranes, Important applications.</td></tr>
<tr><td>Reference Books</td><td colspan="3">1. Modern Electrochemistry, J. O′M. Bockris and A.K.N Reddy, Springer 2000.
2. Gileadi, Physical Electrochemistry, Fundamental, Techniques and Applications, Wiley-VCH, 2011
3. J. Bard and L. R Faulkner Electrochemical Methods: Fundamentals and Applications, 2nd Edition, Wiley, 2001</td></tr>
</table>

	4. H. Rieger, Electrochemistry, 2nd Edition, Springer 1994 5. Newman and K. E. Thomas-Alyea, Electrochemical Systems, 3rd Edition, Wiley Interscience, 2004 6. P. J. Gellings, H. J. M. Bouwmeester, CRC Press, 1997
Course Outcome	CO1. Representation of an electrochemical cell and write relevant electrochemical equations CO2. Explanation of potential, overpotential and thermodynamics involved during the operation of the cell. CO3. Calculation of electrochemical cell parameters, understand the mass transfer process during electrochemical reactions involving migration and diffusion. CO4. Calculation of electroactive active surface area, plotting current vs. overpotential, potential vs. current, and understand basic electrochemical methods.

Solid State Chemistry: Fundamentals and Applications (21CYT823)			
Prerequisite: Basic understanding of Physical Chemistry	**L**	**T**	**P**
Type: Program Elective	**3**	**0**	**0**
Course Objectives: To identify and apply the concepts involved in the structure, physical properties, syntheses and characterization of crystalline inorganic solids.			

Course Content	
Module 1 (6L)	**Crystal Structure:** Crystalline and amorphous solids, The crystal lattice and unit cells, crystal systems and Bravais lattices, Close packing in solids, Interstitial sites, Structures based on close packing, Layered structures based on close packing, Crystal defects and their classification, Grain boundaries and crystallographic shear
Module 2 (8L)	**Solid Solutions and Preparative Methods of Solids:** Substitutional solid solutions, Interstitial/vacancy solid solutions, Monitoring of solid solution formation, Fundamentals and mechanistic aspects of solid state reactions, Film deposition, Chemical precursor method, Co-precipitation, Sol-gel, Metathesis, Solution combustion synthesis, Ion exchange reactions, Intercalation/de-intercalation reactions, Hydrothermal, Solvothermal and template synthesis, Microwave and sonochemistry approach for the synthesis of solids.
Module 3 (6L)	**Preparative Methods for Single Crystals of Solids:** Solution growth, Hydrothermal method, Chemical vapor transport, Melt growth - Bridgeman, Czochralski, Kyropoulus, Verneuil, Epitaxial growth of thin films, Flux growth.
Module 4 (4L)	**Characterization of Solids by Physical Techniques**: Powder X-ray diffraction (PXRD) – Indexing the PXRD patterns, Determination of lattice type, Unit cell parameter and density from the PXRD patterns, Electron and neutron diffraction, Microscopic and Spectroscopic techniques
Module 5 (5L)	**Electronic and Electrical Properties of Solids:** Band structures of metals, semiconductors and insulators, Controlled vacancy semiconductors, Thermoelectric effects - Thomson, Peltier and Seebeck, Hall effect, Dielectric materials, Ferroelectricity, Pyroelectricity, Piezoelectricity and Multiferroics
Module 6 (6L)	**Ionic Conductivity and Magnetic Properties of Solids:** Common ionic crystals, Stoichiometry and ionic conductivity, Fast ion conducting solids, Halide and oxide ion conductors, Selected magnetic materials - spinels, garnets, perovskites, hexaferrites and lanthanide-transition metal compounds.

Module 7 (4L)	**Thermal Analysis of Solids:** TGA, DTA and DSC, Applications – Glasses, Polymorphic phase transition, Decomposition pathway determination, Enthalpy and heat capacity measurements
Reference Books	1. A. R. West, Solid State Chemistry and its Applications, John Wiley & Sons, 2007. 2. L. E. Smart and E. A. Moore, Solid State Chemistry - An Introduction, 4th Edition, CRC Press, 2012. 3. H. V. Keer, Principles of the Solid State, 2nd Edition, New Age International, 2017. 4. David Segal, Chemical Synthesis of Advanced Ceramic Materials, Cambridge University Press, 1989. 5. Richard Tilley, Crystals and Crystal Structures, John Wiley & Sons, 2006.
Course Outcome	CO1. Learning unit cell contents and fractional coordinates, index cubic powder XRD patterns, determine unit cell parameter and lattice types CO2. Indexing non-cubic powder XRD patterns based on unit cell parameters provided, and calculating densities from powder XRD data. CO3. Identifying and applying suitable strategies for synthesizing inorganic crystalline solids in polycrystalline and single crystal forms CO4. Correlation and prediction of structure-composition-properties (magnetic, electrical and optical) in inorganic crystalline solids

Laser Spectroscopy: Theory and Applications (21CYT824)				
Prerequisite: Basic Mathematics, Quantum Mechanics and Spectroscopy		**L**	**T**	**P**
Type: Program Elective		**3**	**0**	**0**
Course description: The course would impart fundamental and application based knowledge to understanding the construction and function of laser and its various uses in spectroscopic methods used in physics, chemistry and biology				
Course Content				
Module 1 (6L)	**Light Matter Interaction** Absorption, emission and scattering, Einstein A & B coefficient, polarizability model, light-matter interaction: semiclassical treatment, Rabi oscillation, linewidth, homogeneous and inhomogeneous line broadening			
Module 2 (10L)	**Laser Operation** Population inversion: 3 & 4 level system, gain and threshold, resonator cavity, optical pumping, CW lasers, Q-switching and mode locking: pulsed lasers. Different types of lasers: atomic lasers (He-Ne), gas lasers (CO_2 and N_2), excimer lasers, solid state lasers (Nd:YAG, Ti:Saphire), semiconductor diode lasers and dye lasers.			
Module 3 (9L)	**Spectroscopy in Molecular Beam** Cavity ring-down spectroscopy, laser induced fluorescence, double resonance spectroscopy (UV-UV and IR-UV), resonance enhanced two-photon and multi-photon ionisation spectroscopy (R2PI and REMPI) and their applications.			
Module 4 (7L)	**Laser Raman Spectroscopy** Resonance Raman spectroscopy, hyper Raman Spectroscopy, stimulated Raman spectroscopy, surface enhanced Raman spectroscopy (SERS), coherent anti-Stokes Raman spectroscopy (CARS) and their applications			
Module 5 (7L)	**Ultrafast Spectroscopy** Pump-probe spectroscopy, transient absorption spectroscopy, fluorescence up-conversion spectroscopy, 2D IR spectroscopy and their applications			
References	Text Books: 1. W. Demtröder, Laser Spectroscopy Vol. 1: Basic Concepts and Instrumentation, Springer, 2002 2. W. T. Silfvast, Laser Fundamentals, Cambridge University Press, 2016 3. J. M. Hollas, High Resolution Spectroscopy, Wiley, 1998 4. H. H. Telle, A. G. Urena, R. J. Donovan, Laser Chemistry: Spectroscopy, Dynamics and Applications, Wiley, 2007 Reference Books: 1. W. Demtröder, M. Inguscio, Applied Laser Spectroscopy, Plenum Press, 1990 2. J. C. Diels, W. Rudolph, Ultrashort Laser Pulse Phenomena, Elsevier, 2006			

Course Outcomes	CO1. The course provides an overview of the fundamental concepts of laser operation. CO2. It enables the students to compare the function, properties and application of various types of common lasers. CO3. It gives a detailed idea of a number of fundamental as well as advanced laser based spectroscopic methods and their applications in studying photochemical and photophysical processes important from chemical and biological perspectives.

<table>
<tr><th colspan="4">Advanced Analytical Chemistry (21CYT825)</th></tr>
<tr><td>Prerequisite: Knowledge of advanced topics in analytical techniques</td><td>L</td><td>T</td><td>P</td></tr>
<tr><td>Type: Program Elective</td><td>3</td><td>0</td><td>0</td></tr>
<tr><td colspan="4">Course Description:
To enable the students to acquire advance knowledge of analytical techniques for various applications
To bring adaptability to recent developments in analytical chemistry and a knowledge of contemporary issues
To make them apply the knowledge of advanced analytical chemistry for identification of structures of organic molecules as well as their estimation</td></tr>
<tr><td colspan="4">Course Content</td></tr>
<tr><td>Module 1(8L)</td><td colspan="3">Atomic spectrometric methods: Principle, instrumentation and applications of atomic absorption, atomic emission and atomic fluorescence, beam modulation in AAS, spectral and chemical interferences in atomic spectroscopy, qualitative and quantitative analysis, Internal standard and standard addition calibration, Inductively Coupled plasma technique (ICP)</td></tr>
<tr><td>Module 2(8L)</td><td colspan="3">Nuclear and radiometric methods: Concept of radiotracers and radiolabelling, radioisotope production and their properties, radioactivity and radiation measurement, activation analysis, isotope dilution method. Isotope dilution and substoichiometric analysis - advantages, limitations, and applications, radioimmunoassay and radio reagent methods, Positron emission spectroscopy</td></tr>
<tr><td>Module 3(4L)</td><td colspan="3">X-ray methods: X-ray spectra, x-ray absorption, emission, fluorescence and diffraction methods, Particle Induced X-ray Emission, Optical and electron microscopy</td></tr>
<tr><td>Module 4(6L)</td><td colspan="3">Liquid-liquid extraction: Principle, significance of various terms, batch and counter current extraction, classification of extractants systems, Examples of various extractants, synergism, stripping, backwashing, salting out agents, masking agents, emulsion formation, identification of extracting species.</td></tr>
<tr><td>Module 5(12L)</td><td colspan="3">Chromatographic techniques: Gas chromatography, high pressure liquid chromatography, instrumentation, detector characteristics, ion chromatography, size exclusion chromatography, affinity chromatography. Ion exchange: Introduction, kinetic and thermodynamic considerations, synthetic inorganic ion-exchangers – classification and applications, chelating resins.
Hyphenated systems with mass spectrometry, Ion sources (ESI, APCI, CI), source and compound parameters, LC-MS, GC-MS, ICP-MS, MS-MS;</td></tr>
<tr><td>Reference Books</td><td colspan="3">Mendham J., Denney R.C., Barnes J.D. and Thomas M.J.K., “Vogel’s Text Book of Quantitative Chemical Analysis”, 6th Ed., Pearson Education. 2004
Skoog D.A., West D.M., Holler F.J. and Crouch S.R., “Fundamentals of Analytical Chemistry”, 8th Ed., Thomson Brooks/Cole. 2004
Christian G.D., “Analytical Chemistry”, 6th Ed., John Wiley & Sons Inc. 2004
Fifield F.W. and Kealey D., “Principles and Practice of Analytical Chemistry”, 5th Ed., Blackwell Science. 2000</td></tr>
</table>

	5. Mendham J., Denney R.C., Barnes J.D. and Thomas M.J.K., "Vogel's Text Book of Quantitative Chemical Analysis", 6th Ed., Pearson Education. 2004 6. Ewing G.W., "Instrumental Methods of Chemical Analysis", 5th Ed., McGraw Hill Book Company, Inc. 2004 7. Rochow T.G. and Tuckor P.A. "Introduction to microscopy by means of light, electron, X- rays or Acoustics", Springer, 2nd Ed. 2005 8. Jenkins R., "X-ray fluorescence spectrometry (Chemical Analysis; A series of Monographs on Analytical Chemistry and its application", Wiley-Interscience, 2nd Ed.) 1999
Course Outcome	CO1. Students will be able to understand various aspects and importance of advanced analytical tools to understand their importance and applications CO2. Students will be able to interpret structures of compounds by the advanced working on the principles of analytical chemistry. CO3. Students will be able to conduct investigations of complex problems by the use research-based knowledge and research methods including design of experiments, analysis and interpretation of data, and synthesis of the information to provide valid conclusions. CO4. Students will learn about various methods used for separation of complex mixtures

Dyes and Pigments (21CYT826)			
Prerequisite: Basic knowledge of dyes and pigments	**L**	**T**	**P**
Type: Programme Elective	**3**	**0**	**0**

Course Description: This course is to acquire knowledge of dyes and pigments and their application	
Course Content	
Module 1 (10L)	**Introduction** Introduction of pigments, colour index, generic names of pigments, colour constitution number, polymorphism, properties required in a pigment and extender, dyes, pigment dyestuffs, and hue of the pigment (Bathochromic and hyper chromic shift),practices and requirement of pigments
Module 2 (14L)	**Classification of dyes** Various Module operations in the manufacture of intermediates and dyes, Introduction of various functional groups, synthesis of dyes, basics of azo dyes, diazotisation and coupling reactions, azoic colours; vat dyes, reactive dyes, acid dyes, mono azo dye; disazo, nitro, diphenylamine and anthraquinone dyes; acid mordant dyes, azo metal complex dyes
Module 3 (8L)	**General methods of processing and synthesis of inorganic pigments** Crushing and grinding, vaporization, co-precipitation, filtration, drying, flushing, calcinations/roasting, vapour phase oxidation etc.
Module 4 (8L)	**Raw materials for organic pigments** A brief study of coal tar distillation and the role of distillation products in the manufacture of synthetic dyes: bases and precipitants used in the colour striking
Reference Books	1. Zollinger, H. (2003). Color Chemistry: Syntheses, Properties, and Applications of Organic Dyes and Pigments. John Wiley and Sons 2. Venkataraman, K. (Ed.). (2012). The Chemistry of Synthetic Dyes (Vol. 4). Elsevier 3. Buxbaum, G. (Ed.). (2008). Industrial Inorganic Pigments. John Wiley and Sons 4. Herbst, W., and Hunger, K. (2006). Industrial Organic Pigments: Production, Properties, Applications. John Wiley and Sons
Course Outcome	CO1. Understand the chemistry of dyes and pigments CO2. Understand the applications of dyes and pigments in various fields CO3. Understand the synthetic methods and physical properties of pigments and dyes

Molecular Spectroscopy (21CYT827)			
Prerequisite: None	**L**	**T**	**P**
Type: Program Elective	**3**	**0**	**0**

Course description: The course provides an introduction to the knowledge of underlying theory and methods of various spectroscopy methods encompassing a large window of the electromagnetic spectrum starting from radio wave to X-ray

Course Content	
Module 1 (6L)	**Matter and radiation** Classical and quantum theory of light, absorption and emission of radiation by molecular species, Einstein A and B coefficient, matter-wave interaction: semiclassical treatment, Rabi oscillation, types of molecular motion and associated spectroscopy, spectral broadening: homogeneous and inhomogeneous
Module 2 (5 L)	**Symmetry** Complete nuclear permutation inversion group, Molecular symmetry group, Non-Rigid Molecules
Module 2 (4L)	**Rotational spectroscopy** Rigid rotor, classification of molecular rotors, rotational spectroscopy of diatomic molecules, non-rigid rotor, centrifugal distortion, selection rules, rotational spectra of polyatomic molecules
Module 3 (6L)	**Vibrational spectroscopy** Review of harmonic oscillator, vibrational selection rules, anharmonic vibrations and Morse oscillator, bond dissociation energies and Birge-Sponer plot, overtones and hot bands, isotopic shift, vibration of polyatomic molecules, normal modes
Module 4 (5L)	**Raman Spectroscopy** Description of Raman scattering, Rayleigh scattering, Stokes and anti-Stokes shift, polarizability of the molecules, Placzek theory, selection rules for rotational Raman spectra of diatomic molecules, rotational, vibrational and ro-vibrational Raman spectra, Raman spectra of polyatomic molecules
Module 5 (9L)	**Electronic Spectroscopy** Born-Oppenheimer approximation, electronic transition, selection rules, Franck-Condon principle, term symbols for atomic and molecular states, Fermi-Golden Rule, selection rules, Jablonski diagram, deactivation processes, internal conversion and inter-system crossing, non-radiative and radiative transitions, vibrational predissociation
Module 6 (7L)	**Advanced spectroscopy topics** Wilson-Howard-Watson rovibrational Hamiltonian, Vibronic effect, spectroscopy at high energies, resonances, polyads

References	Text Books: 1. C. N. Banwell & E. M. McCash, Fundamentals of Molecular Spectroscopy, McGraw Hill, 2017. 2. P. Bernath, Spectra of Atoms and Molecules, OUP, 1995 3. J. M. Hollas, Modern Spectroscopy, Wiley, 2004. 4. P. R. Bunker & P. Jensen, Molecular Symmetry and Spectroscopy, NRC, 2006 5. Molecular Vibrations, Wilson Decius Cross, Dover Reference Books: 1. J. M. Hollas, High Resolution Spectroscopy, Wiley, 2004. 2. Gerhard Herzberg, Spectra of Diatomic Molecules, Krieger Publishing Company 1950 3. Gerhard Herzberg , Molecular Spectra and Molecular Structure. Volume II: Infrared and Raman Spectra of Polyatomic Molecules , D. Van Nostrand Company 1945
Course Outcomes	CO1. Understand the nature and underlying physical laws of interaction between molecules and electromagnetic radiation CO2. Know the various factors responsible for the observed spectral shapes CO3. Gain fundamental information on how different molecular motions result in different spectroscopic methods CO4. Select molecular spectroscopy methods suitable for solving given scientific problem CO5. Analyse measured spectra to shed light on the structure, activity of the molecule as well as the environment and physical conditions

<table>
<tr><th colspan="4">Concepts in Chemical Kinetics and Dynamics (21CYT828)</th></tr>
<tr><td>Prerequisite: Basic understanding of Chemical kinetics</td><td>L</td><td>T</td><td>P</td></tr>
<tr><td>Type: Program Elective</td><td>3</td><td>0</td><td>0</td></tr>
<tr><td colspan="4">Course Description: There are some basic concepts which all physical chemists use to describe chemical reactions. This course five a detailed mathematical introduction of all key concepts with various applications in chemistry.</td></tr>
<tr><td colspan="4">Course Content</td></tr>
<tr><td>Module 1 (6L)</td><td colspan="3">Chemical Equilibrium: Legendre Transformation, Gibbs Free Energy and other thermodynamic potentials</td></tr>
<tr><td>Module 2 (8L)</td><td colspan="3">Activation Energy: Temperature dependence of rate constants, Arrhenius equation, Tolman Interpretation, Negative activation energy, Modern Interpretation of Activation energy</td></tr>
<tr><td>Module 3 (6L)</td><td colspan="3">Potential Energy Surface: Born-Oppenheimer Approximation, Adiabatic and Diabatic representation, Non-Adiabatic coupling</td></tr>
<tr><td>Module 4 (6L)</td><td colspan="3">Reaction Coordinate: Generalized coordinate, Lagrangian and Hamiltonian mechanics, Minimum Energy Path, Reaction path Hamiltonian, Path Curvature</td></tr>
<tr><td>Module 5 (8L)</td><td colspan="3">Reaction Rate Theory: Concept of Flux, Statistical rate theories, Rate from correlation functions</td></tr>
<tr><td>Module 6 (6L)</td><td colspan="3">Tunneling in Chemistry: Simple 1-D models (Echart, Wigner, Bell, WKB approximation) , Small curvature tunneling, Large Curvature Tunneling</td></tr>
<tr><td>Module 7 (6L)</td><td colspan="3">Reaction in Solution Phase: Kramers Theory, Marcus Theory</td></tr>
<tr><td>References</td><td colspan="3">Text Books:
1. Keith J. Laidler ; Chemical Kinetics (Pearson)
2. Paul L. Houston ; Chemical Kinetics and Reaction Dynamics (Dover Publications)
3. J. I. Steinfeld, J. S. Francisco, W. L. Hase; Chemical kinetics and dynamics (Pearson(
4. George C. Schatz, Mark A. Ratner; Quantum Mechanics in Chemistry (Dover Publications)
Reference Books:
1. Herbert Goldstein ; Classical Mechanics (Pearson Education)
2. R. D. Levine ; Molecular Reaction Dynamics (Cambridge University Press)</td></tr>
<tr><td>Course outcome</td><td colspan="3">CO1. To learn all key concepts required in the description of chemical dynamics.
CO2. To learn mathematical descriptions for all the chemical dynamic concepts.</td></tr>
</table>

Green and Industrial Organic Chemistry (21CYT829)			
Prerequisite: Basic knowledge of organic chemistry and green chemistry	**L**	**T**	**P**
Type: Program Elective	**3**	**0**	**0**
Course Description: To acquire knowledge of Green aspects of a chemical reaction and various industrial processes			
Course Content			

Module 1 (10L)	**Green Chemistry** Principles of green chemistry, atom economy, tools of green chemistry: green solvents (ionic liquids, supercritical fluids), abundant natural feedstocks/starting precursor, multicomponent reactions (MCRs), tandem/domino reactions, microwave assisted organic synthesis (MAOS), solid phase synthesis, aqueous media reactions, General introduction to Combinatorial Chemistry.
Module 2 (10L)	**Applications of Green Chemistry** Green synthesis of ibuprofen, design and use of CO_2-surfactants for precision cleaning in industries, environmentally preferable marine antifoulant, use of molting accelerators in place of toxic and harmful insecticides, oxidant activators to replace chlorine-based delignification process in paper and pulp industry, green chemistry process for polyester regeneration, Biocatalytic promiscuity of enzymes for C-C bond formation. Recent applications of ionic liquids as solvent and catalysts in chemical industry.
Module 3 (10L)	**Industrial Organic Syntheses:** The raw material and basic processes, chemical processes used in industrial organic synthesis: production of methanol, ethanol, ethyl acetate, ammonia, sulfuric acid, acetaldehyde, acetic acid, ethylene glycol, glycerine, acetone, phenol, formaldehyde, 1,3-butadinene and styrene.
Module 4 (10L)	**Chemistry of Soaps and Detergents** Introduction, methods of preparation of Soap, types of soaps, structure and properties of Soaps cleansing mechanism, limitation of soap as cleansing agent. Introduction, Principal groups of synthetic detergents, Classification of surfactants; anionic, cationic, amphoteric and non-ionic detergents, alkyl/aryl/ amide sulphonates, binders and builders; eco-friendly detergents: detergents containing enzymes and zeolites.
Reference Books	1. Anastas, P. T., and Warner, J. C. (2000). Green chemistry: theory and practice. Oxford university press. 2. Sauer, N. N. (2000). Green Chemistry: Frontiers in Benign Chemical Syntheses and Processes Ed. Anastas P. T., and Williamson T. C., (US Environmental Protection Agency). Oxford University Press: New York, NY. 2. Malhotra, S. V. (2007). Ionic Liquids in Organic Synthesis, Oxford University Press, US.

	3. Howard, W.L., (1986). Introduction to Industrial Chemistry. Wiley Inter-science. 4. Weissermel, K., and Arpe, H.J., (1997) Industrial Organic Chemistry. Wiley-VCH. 5. Sheldon, R.A., Arends, I., and Hannefed, U., (2007). Green Chemistry and Catalysis. Wiley-VCH Verlag GmbH and Co. 6. Ahluwalia, V. K. and Kidwai, M., (2004). New Trends in Green Chemistry. Anamaya Publishers. 7. Scragg, A.H. (2009) Biofuels: Production, Application and Development, CAB International, UK.
Course Outcome	CO1. Understand the green chemistry principles and their applications CO2. Understand organic chemistry of industrial chemical manufacturing