# M.Sc. Chemistry

# CBCS Curriculum & Syllabus (2018-19 Onwards)



# **Department of Chemistry**

School of Advanced Sciences
Kalasalingam Academy of Research and Education
(Deemed to be University)
Anand Nagar, Krishnankoil - 626 126.

(January 2018)

#### **UNIVERSITY VISION**

To be a Center of Excellence of International Repute in Education and Research.

#### **UNIVERSITY MISSION**

To Produce Technically Competent, Socially Committed Technocrats and Administrators through Quality Education and Research.

#### VISION OF THE DEPARTMENT

To be a centre of excellence of international repute in education and research in the field of chemistry and other related interdisciplinary sciences.

#### MISSION OF THE DEPARTMENT

To promote the advancement of science and technology in the broadest in chemistry in all of its branches and other related interdisciplinary areas through quality education, research and service missions that produce technically competent, socially committed technocrats and scientists.

# **Programme Educational Objectives (PEOs):**

PEO: 1	The graduates would have attained an expertise in major areas of chemistry such
	as organic, inorganic, physical and analytical chemistry.
PEO: 2	The graduates would have acquired skills so as to exploit the opportunities in
	research and development.
PEO: 3	The graduates would have gained an in-depth knowledge and hands-on training in
	diverse areas of Chemistry to specialize in one of the areas of their interest.
PEO: 4	The graduates would be ready to take up responsible positions in different sectors
	such as industry, teaching and research.

# **Programme Outcomes (POs)**

PO: 1	Have an advanced level of understanding of the theories and fundamental concepts in major as well as allied areas of chemistry.
PO: 2	Have specific skills in planning and conducting advanced chemistry experiments and applying the same for the structure elucidation and characterization of various compounds/materials.
PO: 3	Should possess critical thinking and problem solving abilities.
PO:4	Recognize, analyze and deal-with complex chemistry related problems associated with biology, physics and material science.
PO: 5	Acquire knowledge on basic tools needed to execute independent research in chemistry.
PO: 6	Have ability to converse knowledge of chemistry not only in oral but also in writing, including research reports.
PO: 7	Become proficient in their specialized areas of chemistry and effectively complete advanced research projects.
PO: 8	Work effectively and with a safety-conscious attitude.

## **Programme Specific Outcomes (PSOs)**

DCO. 1	Ability to serve as an efficient scientist / researcher in well reputed						
PSO: 1	institutes/industry.						
DCO. 2	Competent to crack national/state level competitive examinations including CSIR-						
<b>PSO: 2</b>	NET, TN-SET etc.						
PSO: 3	Pursue higher studies in well reputed institution around the globe.						

# COURSE STRUCTURE OF M.Sc. CHEMISTRY (2-YEARS) PROGRAMME SCHEME OF INSTRUCTION

<b>Course Code</b>	Course	Course Category	L	Т	P	C			
CHY18R4001	Inorganic Chemistry-I	Theory with Practical	4	0	2	4			
CHY18R4002	Organic Chemistry-I	Theory	5	0	0	4			
CHY18R4003	Physical Chemistry-I	Theory	5	0	0	4			
CHY18R4004	Analytical Techniques	Theory	5	0	0	4			
CHY18R40XX	Elective Course-I	Theory	5	0	0	4			
CHY18R4081	Physical Chemistry Laboratory	Practical	0	0	6	3			
CHY18R4083	Seminar & Comprehensive Viva-I	Viva	0	1	1	2			
CHY18R4005	Inorganic Chemistry-I	Theory	5	0	0	4			
CHY18R4006	Organic Chemistry-II	Theory with Practical	4	0	2	4			
CHY18R4007	Physical Chemistry-II	Theory	5	0	0	4			
CHY18R40XX	Elective Course-II	Theory	5	0	0	4			
CHY18R40XX	Elective Course-III	Theory	5	0	0	4			
CHY18R4082	Inorganic Chemistry Laboratory	Practical	0	0	6	3			
CHY18R4084	Seminar & Comprehensive Viva-II	Viva	0	1	1	2			
CHY18R4061	Materials Characterization Techniques	Practical	0	0	2	2			
CHY18R5001	Synthetic Strategies in Natural Product Chemistry	Theory	5	0	0	4			
CHY18R5002	Electrochemistry and Photochemistry	Theory with practical	4	0	2	4			
CHY18R5003	Statistical Thermodynamics and Equlibrium Phenomena	Theory	5	0	0	4			
CHY18R5051	Research Methodology	Theory	2	0	0	2			
CHY18R50XX	Elective Course–IV/ Online Course*	Theory	5	0	0	4			
CHY18R5081	Organic Chemistry Laboratory	Practical	0	0	6	3			
CHY18R5082	Seminar & Comprehensive Viva - III	Viva	0	1	1	2			
CHY18R5098	Project Work (Phase-I)	Project	0	0	4	3			
CHY18R50XX	Elective Course–V/Online Course*	Theory	5	0	0	4			
CHY18R5099	Project Work (Phase-II)	Project	0	0	30	8			
	Total Credits 90								

<sup>\*</sup>Elective may be replaced if the students get pass in the discipline specific online courses with exam (other than courses offered by the Dept.) before the commencement of the fourth. The courses should be approved by the department.

## **ELECTIVE COURSES**

Sl. No.	<b>Course Code</b>	Course	L	T	P	C
1.	CHY18R4031	Spectroscopy	5	0	0	4
2.	CHY18R4032	Environmental Chemistry	5	0	0	4
3.	CHY18R4033	Industrial Chemistry	5	0	0	4
4.	CHY18R4034	Medicinal Chemistry	5	0	0	4
5.	CHY18R4035	Supramolecular Chemistry	5	0	0	4
6.	CHY18R4036	Nanomaterials	5	0	0	4
7.	MAT18R4001	Mathematics for Chemistry (Interdepartmental Elective)	5	0	0	4
8.	CHY18R5031	Corrosion Science	5	0	0	4
9.	CHY18R5032	Green Chemistry	5	0	0	4
10.	CHY18R5033	Modern Methodologies in Organic Synthesis	5	0	0	4
11.	CHY18R5034	Polymeric Materials	5	0	0	4
12.	CHY18R5035	Advanced Organometallic Chemistry and Catalysis	5	0	0	4
13.	BIT18R4001	Biology for Chemists (Interdepartmental Elective)	5	0	0	4

## **Non-CGPA Courses**

Category	Courses	Credit	Credit Requirement
I	NET/SET/ GATE etc. coaching classes <i>Note:</i> Minimum attendance is 80%. Exam will be conducted by the department at the end of the third. 30% Weightage for attendance 70 % Weightage for Exam.		Minimum of 2 credits earned from any of the
II	Paper presentation in National/International Conferences/Seminars		five categories.
III	Participation in workshops (2 days) [OR] Participation in Guest Lectures (5 Nos.)		
IV	Internship	2	
V	Foreign Language/National Language	2	

<sup>\*80%</sup> attendance is compulsory in this category even if the student earns Non-CGPA credit under any of the rest of the categories.

CHY18R4001	Inaugania Chamistus I	L	T	P	C
Cn 1 18K4001	Inorganic Chemistry-I	4	0	2	4

CO1	Understand the basic concepts and explain the advanced theories of coordination
	chemistry.
CO2	Describe the VB and MO theory of complexes and electronic and bonding reactivities
	of transition metals.
CO3	Discuss the properties of the non-transition elements like C, B and Si and other p-
	block elements.
CO4	Illustrate the properties of Nitrogen, Phosphorus, sulphur and noble gas compounds.
CO5	Understand the Chemistry of lanthanides and Actinides and explain the magnetic and
	electronic properties of them.

#### **Mapping of Course Outcomes:**

CO/PO	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8
CO1	S	M	M				L	
CO2	S	M	M	M				
CO3	M	M					L	
CO4	S	M	M					
CO5	S	M	L					

#### **Unit – I: Chemistry of Coordination Compounds:**

General Characteristics of transition elements, Basic concepts of coordination chemistry, types of ligands, nomenclature of coordination complexes, chelate effect, geometry and isomerism, Theories of coordination compounds, Werner, Sidgwick's theory. Crystal field theory, crystal field splitting application of d-orbital splittings to explain magnetic properties, low spin (L-S) and high spin (H-S) complexes, crystal field stabilization energy, spectrochemical series, weak and strong field complexes, thermodynamic and related aspects of crystal fields, ionic radii, heats of ligation, lattice energy, site preference energy and spinels.

#### Unit – II: Electronic Structure, Bonding and Reactivity of Transition Metal Complexes:

VB and MO theory of complexes (quantitative principles involved in complexes with pi and without pi bonding) and ligand field theories and molecular symmetry, angular overlap model, Jahn Teller effects, electronic spectra of transition metal complexes, Orbital angular momentum, spin angular momentum, Term symbols, J-J coupling, L-S coupling, Selection rule, Orgel and Tanabe –Sugano diagrams, charge transfer and d-d transitions, nephelauxetic series.

#### **Unit – III: Chemistry of Non-Transition Elements-I:**

Brief discussion on the properties of the non-transition elements like C, B and Si: special feature of individual elements; synthesis, properties and structure of their halides and oxides, polymorphism of carbon, properties and structure of boranes (small boranes and their anions  $B_1$ - $B_4$ ), boron nitride, borazines, metallacarboranes, silicates, silicones, diamond, graphite, Zeolites.

#### **Unit – IV: Chemistry of Non-Transition Elements-II:**

Nitrogen, Phosphorus, sulphur and noble gas compounds, Hydrides, Oxides and oxy acids of nitrogen, phosphorus, sulphur and halogens, phosphazenes, sulphur-nitrogen compounds, inter halogen compounds, pseudohalogens, noble gas compounds.

#### Unit - V: Chemistry of Lanthanides and Actinides:

Magnetism: dia, para, ferro and antiferromagnetism, magnetic susceptibility measurements - Gouy method – quenching of orbital angular moment - spin orbit coupling- orbital contribution to magnetic moments-application of magnetic measurements to structure elucidation - Spin crossover phenomena in coordination complexes. Chemistry of lanthanides and actinides, lanthanide contraction, oxidation states, spectral and magnetic properties, use of lanthanide compounds as shift reagents.

#### **Reference Books:**

- 1. F.A.Cotton and G.Wilkinson, Advanced Inorganic Chemistry, 6<sup>th</sup> Ed., John Wiley & Sons, Inc., New York, 2004.
- 2. J.E.Huheey, Inorganic Chemistry, Principles, Structure and Reactivity, Harper and Row, 3<sup>rd</sup>Edn, 1983.
- 3. Wahid.U.Malik, G.D.Tuli and R.D.Madhan, Selected Topics in Inorganic Chemistry, S.Chand& Company Ltd, New Delhi, 2004.
- 4. Morris Sylvin, Bioinorganic Chemistry, Sarup& Sons, New Delhi, 2003.
- Banerjea, Coordination Chemistry, Tata McGraw-Hill Publishing Co. Ltd., New Delhi, 1997.
- 6. W.L. Jolly, Modern Inorganic Chemistry, 2<sup>ndEd.</sup>, McGraw-Hill, 1991.
- 7. B.Douglas, D.McDaniel, J.Alexander, Concepts and Models of Inorganic Chemistry, 3<sup>rdEd.,</sup> John Wiley, 2001.
- 8. N.N.Greenwood, A. Earnshaw, Chemistry of the Elements, 2<sup>nd</sup>Edn, Pergamon Press, 1989.
- 9. S.F.A.Kettle, Coordination chemistry ECBS (1973).
- 10. R.Gopalan and V.Ramalingam, Concise Coordination Chemistry, Vikas publishing House (P) Ltd, New Delhi, 2003.

#### **List of Experiments for Practical**

- 1. Volumetric Analysis: Potassium iodate titrations Determination of iodide.
- 2. Volumetric Analysis: Potassium bromate titrations Determination of antimony (III).
- 3. EDTA titration: Determination of copper
- 4. Gravimetric and volumetric methods: Analysis of Copper and Nickel from the mixture solution.
- 5. Green method of preparation of Bis(acetylacetonato)copper(II) complex.

CHY18R4002	Organic Chemistry – I	L	T	P	C
CH Y 18K4002	Organic Chemistry – I	5	0	0	4

CO1	Evoke the fundamental concepts in chemistry needed for any individual belongs to
	organic chemistry.
CO2	Recognize three dimensional structures of any organic molecule from simple ones to
	complicated ones with orientation of atoms or groups.
CO3	Envisage/Illustrate reactivity, reaction centre, selectivity, mode of reaction and
	kinetics of aliphatic compounds.
CO4	Predict/exemplify the fundamentals of major types of reactions on aromatics with
	their specific reactivity.
CO5	Well versed in green chemistry approaches in organic synthesis especially through
	free radical mode.

#### **Mapping of Course Outcomes:**

CO/PO	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8
CO1	S	M	M				L	
CO2	S	M		L				
CO3	S	M	M				L	
CO4	S	M	S		L			
CO5	S	M				M	M	

Unit – I: Structure, Bonding, and polar bonds and their consequences:

Atomic structure – Orbitals, electron configuration; Development of chemical bonding theory – Valence bond theory and molecular orbital theory; Hybridization – sp3, sp2 and sp, hybridization of other atoms (nitrogen and oxygen); Polar covalent bonds – Electronegativity and dipole moment; Resonance - Rules for resonance forms and technique for drawing resonance forms; Acids and bases – The Bronsted-Lowry and Lewis definition, acid base strength, predicting acid base reactions from pKa, organic acids and bases.

#### **Unit – II: Stereochemistry and conformational analysis:**

Enantiomers and tetrahedral carbon, Pasteur's discovery of enantiomers, optical activity, specific rotation, sequence rules, diastereomers, meso compounds; Molecules with more than two chiral centres; Racemic mixtures and their resolution; Isomerism – A brief review; Fischer projections – assigning R, S configurations; Chirality – Atoms other than carbon; Chirality in nature; Stereochemistry of alkanes and cycloalkanes – Conformations of ethane, propane, butane; Conformation and stability of cycloalkanes – The Baeyer-Strain theory; Cyclopropane – an orbital view, conformations of cyclobutane, cyclopentane and cyclohexane; conformational mobility of cyclohexane; Conformational analysis of mono and disubstitutedcyclohexanes.

# Unit – III: Nucleophilic Substitution Reactions, Elimination Reactions and Addition to Carbon-Carbon Multiple Bonds

Nucleophilic substitution reactions -  $S_N1$ ,  $S_N2$ , and  $S_Ni$  reactions, mechanisms and stereochemistry. Parameters influencing reaction rates; Neighbouring group participation by  $\pi$  and  $\sigma$  bonds, Synthetic applications of nucleophilic substitution reactions involving alcohols, thiols, amines and hydrides: Elimination reactions – E1 and E2 reactions, Mechanism and stereochemistry; Effects of substrate structure, attacking base, leaving group and medium; Formation of other double bonds (C=N, C=O) and triple bonds by elimination reactions; Mechanism and orientation in pyrolytic elimination. Addition reactions – Mechanism and stereochemistry of addition reactions involving electrophiles, nucleophiles and free radicals.

#### Unit-IV: Aromaticity, Aromatic Electrophilic and Nucleophilic Substitution Reactions:

Aromaticity – Criteria, Huckel's rule, Aromatic hydrocarbons, Aromatic heterocyclic compounds, Chemical consequences of aromaticity; Antiaromaticity; Molecular orbital description of aromaticity and antiaromaticity, Aromaticity of compounds with more than  $10\pi$  electrons –a few representative examples including fullerenes, annulenes, and hetero annulenes. General mechanism for aromatic electrophilic substitution reactions - Orientation-Reactivity-mechanism of nitration, halogenation-Friedel-Crafts reaction, sulfonation and Gattermann-Koch Formylation-Aromatic nucleophilic substitution – Addition-elimination and elimination-addition strategies.

#### **Unit – V: Free Radicals and Application to Green Chemistry:**

Free radicals –Aspects, Types, Reaction styles, Orientation in radical additions, Reactivity in radical additions, Reaction patterns of radicals, Generation of radicals; Familiar and close radicals in our life; Stable free radicals; Physical and chemical characteristics of free radicals – Orbital interactions between radicals and olefins, Baldwin's rule; Functional group conversion – Radical coupling reaction, Radical reduction, Conversion to hydroxy and other functional groups; Free radicals for green chemistry – Design of free radical precursors, Application to environmentally benign synthesis.

- 1. R. T. Morrison and R. N. Boyd, "Organic Chemistry", 6<sup>th</sup> Ed., Prentice-Hall of India (P) Ltd., New Delhi, 1995.
- 2. P. S. Kalsi, Stereochemistry-Conformation and Mechanism, New Age International (P) Ltd, VI <sup>Ed.</sup>, New Delhi, 2005.
- 3. Jerry March, Advanced organic chemistry-reactions mechanisms and structure, McGraw-Hill, 1968.
- 4. P.Y.Bruice, Organic Chemistry, 6<sup>th</sup> Ed.,, 2011.
- 5. F.A.Carey and R.J.Sundberg: Advanced Organic Chemistry, Third Edition, Plenum Press, 1990.
- 6. John McMurry, Fundamentals of Organic Chemistry (Fifth Edition), Brooks/Cole, Thomson-Brooks/Cole, 2003.
- 7. I.L. Finar, Organic Chemistry, Vol I & II, Pearson, Education Singapore, 2004.
- 8. H. Togo, Advanced Free Radical Reactions for Organic Synthesis, Elsevier, 2004.

CHY18R4003	Physical Chemistry – I	L	T	P	C
CH 1 10K4005	Physical Chemistry – I	5	0	0	4

CO1	Understanding the basic concepts of thermodynamics and its applications.
CO2	Acquire the knowledge in statistical thermodynamics and its application.
CO3	Gathering the knowledge about chemical kinetics and its applications.
CO4	Gathering the knowledge about Solid state chemistry and its applications.
CO5	Details the study of the principle and applications of electrochemistry.

#### **Mapping of Course Outcomes:**

CO/PO	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8
CO1	S	M					L	
CO2	S	M	S	M				
CO3	M	M						
CO4	S	M	M	M				
CO5	S	M	M		L			

#### **Unit – I: Equilibrium Thermodynamics:**

Concept of entropy, second and third law of thermodynamics, residual entropy. Free energy, chemical potential, fugacity, liquids and solutions: ideal and non-ideal solutions, chemical equilibrium Non-equilibrium thermodynamics Entropy of irreversible processes – Clausius inequality; entropy production (heat flow, chemical reactions, electrochemical reactions) and entropy flow; Entropy production in open systems; Rate of entropy production – generalized forces and fluxes; Phenomenological equations, Onsager reciprocity relation; Stationary non-equilibrium states - states of minimum entropy production.

#### **Unit – II: Statistical Thermodynamics:**

MB statistics and distribution, ensembles, partition functions and molecular partition function, Vibrational, rotational, electronic partition functions-thermodynamic functions in terms of partition functions. Mean energy BE, FD statistics, Comparison between MB, BE and FD. Residual entropy, heat capacity of mono and diatomic gases, chemical equilibrium, Einstein and Debye theories of heat capacity of solids

#### **Unit – III: Chemical Kinetics**

Molecularity, order and rate of reactions, Arrhenius theory, Collision and activated complex theory comparison of results with Eyring and Arrhenius equation-reactive collisions, molecular beam experiments, introduction to potential energy surface—ionic reactions: salt effect Complex reactions: reversible, pre-equilibrium, consecutive, chain and photochemical, oscillatory reactions, enzyme kinetics-Lindemann's theory of unimolecular reactions Molecular reaction dynamics: Fast reaction kinetics Flow method, Flash photolysis

#### **Unit – IV: Solid State Chemistry:**

Types of solids, covalent, ionic, molecular and metallic solids, lattice energy, cohesive energy and Madelung constants, Van derWaals forces, hydrogen bonding, unit cell, crystal lattice, structure of simple ionic compounds (AX, AX<sub>2</sub>, ABX<sub>3</sub>), z radius ratio and closed packed structures. Imperfection and related phenomena-defects in solids: point defects, line defects and plane defects. Thermal properties-Heat capacities of solids: Dulong –Petit law, thermal conductivity of insulators and thermal expansion coefficient. Electrical conductivity origin of band gap. Fermi energy, density of states, thermal conductivity of metals, semiconductors and superconductivity.

#### **Unit – V: Electrochemistry:**

Activities in electrolytic solutions mean activity coefficient, Debye-Huckel treatment of dilute electrolyte solutions, origin of electrode potential, half cell potential, electrochemical cell, Nernst equation, thermodynamics of electrochemical cell: Electrical double layer-electrode kinetics; rate of charge transfer, current density, Butler–Volmer equation- Different approximations to it. Mechanism determination of electrode reactions-H<sub>2</sub> evolution.

- 1. F.W.Sears, "An Introductions to Thermodynamics, Kinetic Theory of Gases and Statistical Mechanics" Addison Wesley Pub. Cambridge, 1969.
- 2. F.C.Andrews, "Equilibrium to Statistical Mechanics" John Wiley, 2<sup>nd</sup> Ed., 1975.
- 3. Malcolm Dole, "Introduction to Statistical Thermodynamics" Prentice Hall, 1954.
- 4. L.K.Nash, "Statistical Thermodynamics" Addison Wesley, 2<sup>nd</sup> Ed., Addison-Wesley Pub. Co., 1974.
- 5. Joseph Kestin and J.R. Dorfman, "A course in statistical thermodynamics", Academic press, 1971.
- 6. IIya Prigogine, Introduction to thermodynamic irreversible processes, 3<sup>rd</sup> Ed., Interscience Publishers, 1968.
- 7. H. V. Keer, Principles of Solid State, Wiley Eastern Limited, 1993.
- 8. W.R.West, Solid State Chemistry and its Application, John Wiley and Sons, New York, 1984.
- 9. J. O'M. Bockris and A.K.N. Reddy, Modern Electrochemistry, <sup>2nd</sup> Ed., Vols 1, 2A, 2B, Kluwer/Plenum, 1998 (Vol 1), 2001 (Vols 2A, 2B),(<sup>1st</sup>Ed.Vols. 1, 2, Plenum 1973 QD 553 B6).
- 10. P. W. Atkins Physical Chemistry, 6<sup>th</sup> Ed., Oxford, 1998.
- 11. Y. V. C. Rao, An introduction to Thermodynamics, Wiley Eastern, 1993.
- 12. M. Ladd, Introduction to Physical Chemistry, Cambridge, 1998.
- 13. D.A.McQuarrie and J.D.Simon Physical Chemistry, A molecular Approach, Viva 1998.
- 14. F.W.Sears&G.L.Salinger, Thermodynamics, Kinetic theory & Statistical thermodynamics, Narosa, 1986.
- 15. J.Rajaram and J.C. Kuriacose, Thermodynamics, ShobanLal Chand & Nagin Lal (P) Ltd, 1999.
- 16. K. J. Laidler "Chemical Kinetics, 3<sup>rd</sup> Ed., Pearson Education Inc., New Delhi, 2004.

CHY18R4004	Analytical Techniques	L	T	P	C
CH 1 10K4004		5	0	0	4

CO1	Understand the principle of different chromatography techniques and Apply that
	knowledge for the separation and purification of different samples.
CO2	Describe the various types of electroanalytical methods and importance in the
	characterization of compounds.
CO3	Understand the basic principle and applications of cyclic voltammetry and
	hydrodynamic methods.
CO4	Apply the knowledge of SEM, TEM and AFM for the characterization of samples.
CO5	Detail the principle and applications of TGA, DTA and DSC for the characterization
	of polymer and other samples.

#### **Mapping of Course Outcomes:**

CO/PO	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8
CO1	S	M			S		L	
CO2	S	M			S			
CO3	S	M			S			
CO4	S	M			S		L	
CO5	S	M			S			

#### **Unit – I: Chromatographic Methods:**

Introduction to Chromatography and types of techniques: ion exchange chromatography, Column Chromatography, Paper Chromatography, Thin Layer Chromatography (TLC), Gas Chromatography (GC), High Pressure Liquid Chromatography, Ion Chromatography, Gel Permeation Chromatography—Applications.

#### **Unit – II: Electroanalytical Methods:**

Electron transfer-mass transport (diffusion, convection, migration) IIkovic equation-Polarography analysis-sampled current voltammetry: Potentiometry and Amperometric analytical methods -Chronoamperometry, chronocoulometry-Polarography- pulse polarographic methods: Tast pulse, normal pulse, and differential pulse - Applications.

#### **Unit – III: Voltammetry Methods**

Voltammetry- Cyclic voltammetry- reversible, totally irreversible, quasi-reversible processes-applications. Controlled Potential methods: current –time behaviour, Electrogravimetry, Electroseparation- Coulometric measurements: controlled current methods: Stripping voltammetry and Hydrodynamic electrochemical methods of analysis.

#### **Unit – IV: Imaging Methods:**

Basic Studies and Principles of SEM, TEM, AFM, Scanning Tunnelling Microscope (STM) – Applications.

#### **Unit – V: Thermoanalytical Methods:**

Thermal methods of analysis: Principles and instrumentations of TG and DTA. Complementary nature of TG and DTA. Differential scanning calorimeter (DSC). Applications of thermal methods in analytical chemistry and in the study of minerals and polymers.

- 1. C.N.R.Rao, A.Muller, A.K.Cheetham, Chemistry of Nanomaterials (Vol. 1&2), Wiley-VCH Verlag GmbH & Co. KGaA, Germany, 2004.
- 2. Charles P. Poole Jr and Frank J. Owens, Introduction to Nanotechnology Wiley Student Edition, Singapore, 2003.
- A.J.Bard and L.R.Faulkner, Electrochemical Methods, Fundamentals and applications, John Wiley, 1980.
- 4. P. Kissinger and W. R. Heineman, Laboratory Techniques in Electroanalytical Chemistry, Taylor & Francis, Inc., 1996.
- 5. P.H.Rieger, Electrochemistry, Prentice, Hall, 1987.
- James A. Plan Beck, Electroanalytical Chemistry-Basic Principles and Applications, John Wiley & Sons, 1982.
- 7. B. H. Vassos and G. W. Ewing Electroanalytical Chemistry, John Wiley and Sons, Inc., 1983.
- 8. D. A. Skoog, D. M. West, F. J. Holler, S. R. Crouch, Fundamental of Analytical Chemistry, 7<sup>th</sup> Ed., Saunders College Publishing Co., New York, 1999.
- 9. A.I.Vogel, A.R.Tatchell, B.S.Furnis, A.J.Hannaford, P.W.G.Smith, Vogel's Textbook of Practical Organic Chemistry (5<sup>th</sup> Ed.), Longman, 1989.
- 10. F.W. Fifield and D. Kealey, Principles and Practice of Analytical Chemistry, 2<sup>nd</sup> Ed., International Book Company, London, 1983.

CHY18R4081	Physical Chemistry Laboratory	L	T	P	C
CH 1 10K4001	Physical Chemistry Laboratory	0	0	6	3

CO1	Understand the basic principles of chemistry and capable of writing the procedure for
	carrying out physical chemistry experiments.
CO <sub>2</sub>	Observe and note various types of observable parameters, physical properties,
	chemical changes etc that occurred during a chemical reaction.
CO3	Calculate and arrive the result through systematic way by applying the existing rules,
	formulas and concepts in chemistry.
CO4	Interpret and analyze the data obtained from an experiment and also able to
	communicate the same orally in an efficient and correct manner.
CO5	Create a record of practicals by documenting the obtained data and using it for future
	reference.

#### **Mapping of Course Outcomes:**

CO/PO	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8
CO1		S		M	M	S		L
CO2	M		S	L			S	
CO3	M	S		S		M		S
CO4			S		M		L	
CO5	S	M	M		L	L		M

#### **List of Experiments:**

- 1. Molecular weight determination by cryoscopic methods, Formula of complexes.
- 2. Phase diagrams: Two component liquid–liquid and solid-liquid systems. Three component liquid-liquid systems.
- 3. Kinetics Acid hydrolysis of ester determination of activation energy (Ea).
- 4. Kinetics–Acid hydrolysis of ester-Comparison of strength of acids/ Determination of Ea.
- 5. Kinetics- Saponification of ester –Determination of Ea.
- 6. Distribution law-study of iodine-iodide equilibrium.
- 7. Adsorption –Oxalic Acid/Acetic Acid on Charcoal using Freundlich isotherm.
- 8. Conductometry: Cell constant, conductivity of a weak-acid, solubility of sparingly soluble salt, conductometric titrations.
- 9. Potentiometer: Measurement of electrode potentials, activity coefficients and potentiometric titrations.

- 1. Alexander Findlay, Bryan Philip Levitt, Findlay's Practical Physical Chemistry, 9<sup>th</sup> Ed., Wiley, 1972.
- 2. J.B. Yadav, Advanced Practical Physical Chemistry, Goel Publishing House, 2001.

CHY18R4083	Seminar & Comprehensive Viva - I	L	T	P	C
CH110K4003	Seminal & Comprehensive viva - 1	0	1	1	2

Chemistry of Coordination Compounds - Electronic Structure, Bonding and Reactivity of Transition Metal Complexes - Chemistry of Non-Transition Elements - Chemistry of Lanthanides and Actinides - Structure, bonding of carbon compounds - polar bonds and their consequences - Stereochemistry and conformational analysis - Nucleophilic Substitution Reactions - Elimination Reactions and Addition to Carbon-Carbon Multiple Bonds - Aromaticity - Aromatic Electrophilic and Nucleophilic Substitution - Free Radicals and their application to Green Chemistry - Thermodynamics - Statistical Thermodynamics - Chemical Kinetics - Solid State Chemistry - Electrochemistry - Chromatographic Methods - Electroanalytical Methods - Voltammetry Methods - Imaging Methods - Thermoanalytical Methods.


-II

CHY18R4005	Inorgania Chamiatry II	L	T	P	C
CH 1 18K4005	Inorganic Chemistry-II	5	0	0	4

#### **Course Outcomes (COs)**

CO1	Understand the nomenclature, metal-ligand reactions and their mechanism and the							
	concepts of hard and soft acids and bases.							
CO2	Describe the basic concepts of organometallic chemistry and their bonding patterns							
	especially with unsaturated ligands.							
CO3	Detail the mechanism of different organometallic reactions and catalysis.							
CO4	Understand the role of Metal ions in biological systems.							
CO5	Describe the basic photochemical processes in biological systems and Photo synthesis							
	in plants.							

#### **Mapping of Course Outcomes:**

CO/PO	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8
CO1	S	L	M	M				
CO2	S	M		L				
CO3	S	M					L	
CO4	S	M					L	
CO5	S	L					M	

#### **Unit – I: Inorganic Reaction Mechanism:**

Isomerism and nomenclature of coordination compounds, Formation of complexes, stability constants Inert and labile compounds, substitution reactions of octahedral complexes, dissociative, associative, anation, aquation, conjugate base mechanism; substitution reactions of square planar complexes, trans effect, trans effect series, theories of trans effect; electron transfer reactions. Concept of hard and soft acids and bases. Stabilisation of unusual oxidation states-stereochemistry of coordination compounds

#### **Unit – II: Organometallic Chemistry-I:**

Compounds with transition metal to carbon bonds: classification of ligands nomenclature, eighteen electron rule; transition metal carbonyls: range of compounds and structure, bonding vibrational spectra, preparation, reactions; transition metal organometallics: square planar complexes, metal alkyls, metal alkylidenes and metal alkylidenes; structure and bonding: metal-olefin bond and arene metal bond. Compounds with ligands having extended pi systems: bis(cyclopentadienyl) compounds, cyclopentadienyl carbonyl compounds, bis(arene) compounds, arene carbonyl compounds-fluxional molecules.

#### **Unit – III: Organometallic Chemistry-II:**

Organometallic reactions and catalysis: oxidative addition, reductive elimination, insertion, hydride elimination, abstraction; olefin hydrogenation, hydroformylation, Wacker process, Ziegler-Natta polymerization, Olefin metathesis, Monsanto acetic acid synthesis, Fischer-Tropsch process, Hydroxylation.

#### **Unit – IV: Bioinorganic Chemistry:**

Metal ions in biological systems; heme proteins, haemoglobin, myoglobin, hemerythrin, hemocyanin, ferritin, transferring, cytochromes and vitamin B12; Iron-Sulphur Proteins: rubredoxin, ferredoxin and model systems. Metalloenzymes: active sites, carboxypeptidase, carbonic anhydrase, superoxide dismutase, xanthine oxidase, peroxidase and catalase; photosynthesis, water oxidation, nitrogen fixation, nitrogenase; ion pump, metallodrugs.

#### **Unit – V: Inorganic Photochemistry:**

Basic Principles, Basic photochemical processes, Kasha's rule, Thexi state, Photo substitution reactions, Adamson's rules, Photo substitution reactions of Cr(III)-Polypyridyl, Rh(III) Ammine Complexes, Ru-Polypyridyl complexes, Ligand photo reactions, photoredox reactions, comparison of Fe(II) and Ru(II) complexes, Photo reactions and Solar energy conversions, Photosynthesis in plants and Bacteriochlorophyll photosynthesis, photolysis of water using Inorganic precursors.

- 1. J. D. Lee, A New Concise Inorganic Chemistry, 3<sup>rdEd.</sup>, ELBS, 1987.
- 2. P. Powell, Principles of Organometallic Chemistry, 2<sup>ndEd.</sup>, ELBS, 1991.
- 3. M. F. Purcell, J.C.Kotz, Inorganic Chemistry, Saunder, 1977.
- 4. R. W. Hay, Bioinorganic Chemistry, Ellis, Horwood, 1987.
- 5. R. M. Roat-Malone, BioInorganic Chemistry, John Wiley, 2002.
- 6. T. M. Loehr, Iron carriers and Iron proteins, VCH, 1989.
- 7. S. L. Lippord, Progress in In organic Chemistry, John, Wiley, Vol.30, 1983.
- 8. J. E. Huheey, Inorganic Chemistry, Principles, Structure and Reactivity, Harper and Row, 3<sup>rd</sup>Edn, 1983.
- 9. Inorganic Photochemistry, J. Chem. Educ., vol. 60, no. 10, 1983.
- 10. Elements of Inorganic Photochemistry, G. J. Ferraudi, John Wiley & Sons, 1988.
- 11. K. K. Rohatgi-Mukherjee, *Fundamentals of Photochemistry*, Wiley, New York, <sup>3rd</sup> Ed.,, 2002.
- 12. Turro, N. J., "Modern Molecular Photochemistry", Benjamin-Cummings, NY, 1978.

CHY18R4006	Organic Chemistry-II	L	T	P	C

	4	Λ	2	4
	-	U	4	

CO1	Capable of preferring suitable reagent for important reactions/building appropriate							
	bonds.							
CO <sub>2</sub>	Skilled in constructing homo/heterocyclic rings of significant molecules and							
	rearranging functionalities within the important chemical entities.							
CO3	Well versed in applying unique methodologies to furnish major classes of oxidized							
	and reduced organic compounds.							
CO4	Skilled in fundamental concepts of photochemistry and its applications to various							
	synthetic organic reactions							
CO5	Proficient in fundamental / reactivity of most significant biopertimentheterocycles and							
	nucleic acids.							

#### **Mapping of Course Outcomes:**

CO/PO	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8
CO1	S	M	S	M			M	
CO2	S	S	S	M			M	
CO3	S	M	M	M			M	
CO4	S	M	M	L			M	
CO5	S		M	M			L	

#### **Unit – I: Reagents in Organic Synthesis:**

Palladium on Carbon, Lithium tri-tert-butoxyaluminum hydride, Diazomethane, Sodium Periodate, Grignard Reagents, Dicyclohexylcarbodiimide (DCC), Pyridiniumchlorochromate, *Di*-isobutyl aluminum hydride (DIBAL), Lithium *diisopropylAmide* (LDA), Sodium amide, Aluminum chloride, Osmium tetroxide, N-Bromo succinimide, Wilkinson's catalyst, Phase-transfer catalysts, Introductory treatment to the application of palladium, ruthenium and indium reagents in organic synthesis.

#### **Unit – II: Ring Constructions and Rearrangements:**

Construction of ring systems - Darzens condensation, Simmons–Smith reactions, Staudinger reaction ( $\beta$  - lactams synthesis), Reaction of isocyanates with alkenes, Borsche–Drechsel cyclization, Paal-Knorr pyrrole syntheses, Pechmanncoumarin synthesis, Bischler–Napieralski synthesis, Corey–Nicolaoumacrolactonization. Rearrangements – Baker–Venkataraman, Evans-Mislow, Wagner–Meerwein rearrangements, Beckmann, Overman, Schmidt, Curtius, Wolff rearrangements, Boulton–Katritzky.

#### **Unit – III: Oxidation and Reduction:**

Oxidation - Alcohols to carbonyls/acids - Corey-Kim, and Swern oxidations; Aldehyde to phenol - Dakin oxidation; Alkenes to epoxides - Sharpless asymmetric and Jacobsen epoxidation; Alkenes to diols - Prevost reaction; Ketones to esters/lactones -

Baeyer-Villiger oxidation; Alkenes to alcohols - Hydroboration, Wacker oxidations, Silanes to alcohols/ketones - Fleming-Kumada and Saegusa oxidations; Halides to aldehydes - Sommelet reaction; Reduction - Imine to amine - Borch reductive amination; Ketones/Esters/thiolesters/alkenes to alcohols/aldehydes/alkanes - Corey-Bakshi-Shibata, Bouveault-Blanc, Fukuyama, Midland, and Wolff-Kishner reductions, Noyori hydrogenation; Acetylenic alcohol to allyl alcohol - Chan alkyne reduction; Alcohols to alkenes - Corey-Winter reductive olefination.

#### **Unit – IV: Organic Photochemistry and Pericyclic Reactions:**

Photochemistry – Definitions- Grotthuss-Draper law, Stark-Einstein law, quantum yield; Mechanistic background – Franck-Condon principle, Jablonski diagram, singlet and triplet states, photosensitization, quenching; Photochemical reactions – Alkene isomerisation, carbonyl compounds (background, reactions – Norrish type-I and Type-II reactions, Paterno-Buchi reaction, photo enolization reaction), Enone reactions ([2+2] cycloaddition and the de Mayo reactions), di-π-methane rearrangements, Barton reaction. Molecular orbitals and Pericyclic reactions; Electrocyclic reactions; Stereochemistry of thermal and electrocyclic reactions; photochemical electrocyclic reactions; Cycloaddition reactions, stereochemistry of cycloaddition reactions; Sigmatropic rearrangements with examples; Rules for pericyclic reactions.

#### **Unit – V: Heterocycles and nucleic acids:**

Five-membered unsaturated heterocycles; Structure of pyrrole, furan and thiophene; Electrophilic substitution reactions of pyrrole, furan and thiophene; Six membered heterocycle – Pyridine and its electrophilic and nucleophilic substitutions; Fused ring heterocycles; Nucleic acids and nucleotides; Structure of nucleic acids; Base pairing in DNA – The Watson-Crick model; Nucleic acid and heredity; Replication of DNA; Structure and synthesis of RNA – Transcription; RNA and protein biosynthesis – translation; DNA sequencing; DNA synthesis; polymerase chain reaction.

- B.P.Mundy, M.G.Ellerd, F.G.Favaloro, Name Reactions and Reagents in Organic Synthesis, 2<sup>nd</sup> Ed., 2005.
- 2. Adam Jacobs; Understanding Organic Reaction Mechanism, Cambridge University Press 1997.
- 3. Jie Jack Li, Name Reactions, 5<sup>th</sup> Ed., (Springer), 2014
- 4. M.A.Fox and J.K.Whitesell., Organic Chemistry, Jones and Bartlett Publishers 1994.
- 5. F.A.Carey and R.J.Sundberg (Part A and B) Kluwer Academic/ Plenum Publishers 2000.
- 6. Clayden et al Advanced organic chemistry 2004.
- 7. R.J.Simmonds: Chemistry of Biomolecules: An Introduction, RSC

8. John McMurry, Fundamentals of Organic Chemistry (Fifth Edition), Brooks/Cole, Thomson-Brooks/Cole, 2003.

#### **List of Experiments for Practical**

- 1. Synthesis of one molecule each by using any two of the following reagents:
  - 1. Dicyclohexylcarbodiimide
  - 2. Pyridinium chlorochromate
  - 3. Aluminum chloride
  - 4. N-Bromosuccinimide
  - 5. Phase-transfer catalysts
- 2. Synthesis of one molecule each by adopting any three of the following reactions:
  - 1. Pechmann condensation
  - 2. Swern Oxidation
  - 3. Baeyer–Villiger oxidation
  - 4. Beckmann Rearrangement
  - 5. Wolff–Kishner reduction
  - 6. Biginelli reaction
  - 7. Knoevenagel reaction
  - 8. Sommelet reaction

CHY18R4007	Physical Chemistry-II	L	T	P	C
	Physical Chemistry-11	5	0	0	4

CO1	Gathering the knowledge in the Quantum Chemistry and its applications.
CO2	Understand the basic knowledge in group theory and its applications.
CO3	Describe the importance of surface phenomena.
CO4	Details the study of the principle and applications of photochemistry.
CO5	Acquire the knowledge of nucleus, nuclear reaction, radioactive techniques and application of radioisotopes.

#### **Mapping of Course Outcomes:**

CO/PO	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8
CO1	S	L	S	M				
CO2	S	M	S	S			M	
CO3	S	L			M			
CO4	S	L			S		M	
CO5	S	L	M		S		L	

#### **Unit – I: Quantum Chemistry:**

Inadequacy of classical mechanics-Wave particle dualism-Heisenberg's uncertainty principle-Eigen functions-Postulates of quantum mechanics —Application of wave mechanics to simple systems-Particle in one and three dimensional boxes- degeneracy. Application of wave mechanics to one dimensional simple harmonic oscillator-Rigid rotor-Hydrogen atom-Pauli's exclusion principle-Slater determinant-Approximation methods to helium atom.

#### **Unit – II: Group Theory-Concept and Applications:**

Symmetry elements and symmetry operations Group-Definition-Group multiplication table-Reducible and irreducible representation–Point groups-Systematic methodology for fixing point groups for simple compounds-Great orthogonality theorem (Non-Mathematical) and its consequences-Construction of character table ( $C_2V$  and  $C_3V$  groups)-Direct product representation. Application of group theory to vibrational and Raman spectra-ammonia and water molecules-Application of group theory to electronic spectroscopy –formaldehyde and ethylene.

#### **Unit – III: Surface Phenomena:**

Adsorption of gases on solids-Physical and chemical adsorption-Solid-gas interface-Langmuir and BET isotherms, Surface area determination –mechanism of uni and bimolecular surface reactions –Langmuir and Hinshelwood and Langmuir-Riedel mechanisms –Gibbs adsorption isotherm.

#### **Unit – IV: Photochemistry:**

Photochemical principles – Absorption of light by atoms and molecules-Reaction paths of excited molecules- Jablonski diagram – Fluorescence and Phosphorescence – Photochemical chain reaction – Chemiluminescence, fluorescence quenching: concentration quenching, quenching by excimer and exciplex emission, fluorescence resonance energy transfer between photoexcited donor and acceptor systems. Stern-Volmer equation, critical energy transfer distances, energy transfer efficiency, examples and analytical significance, bimolecular collisional V quenching and Stern-Volmer equation.

#### **Unit – V: Nuclear Chemistry:**

Properties of nucleus – different types of nuclear forces –liquid drop model, shell model nucleus. Nuclear reactions induced by charged particles. Q value- nuclear reactions cross sections, significance and determination. Types of reactions-radioactive decay and equilibrium-chemical effects of nuclear transformation-fission and fusion, fission products and fission yields. Production of feed materials for nuclear reactors, radioactive techniques-tracer techniques, neutron activation analysis, counting techniques such as G.M. ionisation and proportional counter. Application of radioisotopes.

- 1. S.N.Datta: Lectures on Chemical bonding and quantum chemistry, 1998.
- 2. P.W.Atkins: Molecular Quantum Mechanics, Clarendon Press, Oxford, 1983.
- 3. F.A.Cotton; Chemical Applications of Group Theory, Wiley Eastern, 1985.
- 4. Karplus and Porter Atoms and Molecule 1973.
- 5. R.K.Prasad:Quantum Chemistry, New Age International Publishers, Revised Edition, 2006.
- 6. A.K.Chandra, Introductory Quantum Chemistry, 4<sup>th</sup>Ed.,,Tata McGraw-Hill Education, 1994.
- 7. K.V.Raman, Group theory and its application to Chemistry, Tata McGraw Hill Publishing Co.,1990.
- 8. K.K.Rohatgi Mukherjee "Fundamental of Photochemistry", New Age International (P) Ltd, Publisher, New Delhi, 2003.
- 9. H.J.Arnikar, Essential of nuclear Chemistry, 4<sup>th</sup> Ed., New Age International (P) Ltd., New Delhi, 1997.
- 10. A.K.Chandra, "Introductory Quantum Chemistry", 4<sup>th</sup> Ed., Tata McGraw Hill, New Delhi, 1994.

CHY18R4082	Inorganic Chemistry Laboratory	L	T	P	C	
	Thorganic Chemistry Laboratory	0	0	6	3	

CO1	Understand the basic preparation of coordination complexes.
CO2	Interpret the electronic spectrum of first row transition metal ions.
CO3	Analyze the common and rare cations in a mixture by semimicro qualitative analysis.
CO4	Estimate the metal ions by complexometric and cerimetric titrations.
CO5	Apply the softwares: Excel, Origin, Mercury and Powerpoint.

#### **Mapping of Course Outcomes:**

CO/PO	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8
CO1	L	S					M	
CO2	L	S					S	
CO3	M	S					S	
CO4	M	S					S	
CO5	L	S					S	

#### **List of Experiments Experiments:**

- 1. Preparation of any five coordination complexes.
- 2. Interpretation of the electronic spectrum and calculation of Dq values in respect of Ni(II) complex.
- 3. Semimicro qualitative analysis: Analysis of common and rare cations in a mixture
- 4. Estimation of metal ions by complexometric and Cerimetric titrations.
- 5. Spectro Colorimetric analysis.
- 6. Training to use software: Excel, Origin, Mercury, Powerpoint.

- 1. Vogel's Text Book of Inorganic Qualitative Analysis, 4<sup>th</sup> Ed., ELBS, London, 1974.
- 2. V.V.Ramanujam, Inorganic Semi Micro Qualitative Analysis, 3<sup>rd</sup> Ed., The National Publishing Company, Chennai, 1974.

CHY18R4084	Seminar & Comprehensive Viva -II	L	T	P	C
CH 1 10K4004	Seminal & Comprehensive viva -11	0	1	1	2

Inorganic Reaction Mechanism - Organometallic Chemistry - Bioinorganic Chemistry - Inorganic Photochemistry - Reagents in Organic Synthesis - Ring Constructions and Rearrangements - Oxidation and Reduction - Organic Photochemistry and Pericyclic Reactions - Heterocycles and nucleic acids - Quantum Chemistry - Group Theory: Concept and Applications - Surface Phenomena – Photochemistry - Nuclear Chemistry.

CHY18R4061	Materials Characterization Techniques	L	T	P	C
CH 1 10K4001	Materials Characterization Techniques	0	0	2	2

(Skill Enhancement Course)

#### **Unit I: UV-Visible and Fourier Transform Infrared Spectrometer**

Basic concepts - Working Principles Instrumentation and Applications including Hands-on training.

#### **Unit II: X-Ray Diffractometer**

Basic concepts - Working Principles - Instrumentation and Applications including Hands-on training.

#### **Unit III: Atomic Absorption Spectrometer and Scanning Electron Microscopy**

Basic concepts - Working Principles - Instrumentation and Applications including Hands-on training.

#### **Unit IV: Cyclic voltammetry**

Basic concepts - Working Principles - Instrumentation and Applications including Hands-on training.

#### **Unit V: Chromatography techniques**

Basic concepts and Applications including Hands-on training on thin layer (TLC) and column chromatography.

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#### -III

CHV10D5001	Synthetic Strategies in Natural Products Chemistry	L	T	P	C
CHITOKSUUI	Synthetic Strategies in Natural Products Chemistry	5	0	0	4

#### **Course Outcomes (COs)**

CO1	Gathering of knowledge about the classification, isolation techniques, structural elucidation of natural products and to study the biosynthetic pathway of forming metabolites.
CO2	Describe the various retrosynthetic approaches in Natural Products synthesis.
CO3	Understand the various synthetic approaches in Natural Products synthesis.
CO4	Details the synthesis and stereochemistry of Carbohydrates and amino acids.
CO5	Explain the structure determination, synthesis and classification of biomolecules like peptide, proteins and lipids.

#### **Mapping of Course Outcomes:**

CO/PO	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8
CO1	S	M			L			
CO2	S	L	M		L			
CO3	S	M	L					
CO4	S	L	M		L			
CO5	S		L		M		L	

#### **Unit – I: Classification of natural products:**

Introduction to natural product chemistry; classification of natural products, isolation techniques and physiochemical data, Structural elucidation of Natural Products based on joint application of UV,IR, PMR, CMR and mass spectroscopy. alkaloids, peptides and amino acid derivatives, and carbohydrates Present examples of natural products and some simple biosynthetic pathways showing how metabolites are formed in nature.

#### **Unit – II: Retrosynthetic approaches in Natural Products Synthesis**

Origin for retrosynthetic analysis –Types of approaches for retrosynthesis; Transform-based approaches - goal guidance, Structure-based and topological approaches - Structure-goal (S-goal) approaches Retrosynthesis of fumagillol: Stereochemical approaches - Stereochemical simplification - Transform stereoselectivity, Stereochemical convolution - Clearable stereocenters, Stereochemical approaches for polycyclic and acyclic systems; retrosynthetic analyses of Longifolene

#### **Unit – III: Total synthesis of Important Natural Products:**

Total synthesis of Recifeiolide, Biotin, Humulene, Farnesol, Kahweol, Cafestol, Fumagillin, Longifolene Prostaglandins  $E_1$ ,  $F_{1\alpha}$  and their 11-epimers, (±)-Prostaglandins  $E_1$ ,  $F_{1\alpha}$ ,  $F_{1\beta}$ ,  $A_1$  and  $B_1$ , General synthesis of prostaglandins Lipoxins, Bongkrekic acid

#### **Unit – IV: Biomolecules – Carbohydrates and amino acids:**

Classification of carbohydrates, configuration of monosaccharides, D, L sugars, configuration of aldoses, cyclic structure of monosaccharides, monosaccharide anomers, reactions of monosaccharides, stereochemistry of glucose; Disaccharides; polysaccharides and their synthesis; Other important carbohydrates; cell-surface carbohydrates and carbohydrate vaccines; Structure of amino acids, isoelectric points, synthesis of  $\alpha$ -amino acids, resolution of R, S amino acids.

#### **Unit – V: Biomolecules – Peptides, proteins and lipids:**

Peptides and proteins, covalent bonding in peptides; Structure determination of peptides – amino acid analysis; Sequencing of peptides – The Edman degradation and C-terminal residue determination; Synthesis of peptides; Automated peptide synthesis – The Merrifield solid-phase technique; Classification of proteins; Protein structure; Enzymes – working of enzyme, citrate synthase; Protein denaturation; Lipids – Waxes, fats, oils and soap; Phospholipids; Prostaglandins; Terpenes, biosynthesis of terpenes; Steroids, stereochemistry of steroids; steroid biosynthesis.

- S. Warren & P. Wyatt. Organic Synthesis: The Disconnection Approach, John Wiley & Sons (2008).
- 2. R. Xu, Y. Ye&W. Zhao. Introduction to Natural Products Chemistry, CRC Press (2011).
- 3. E. J. Corey &Xue-Min Cheng. The Logic of Chemical Synthesis, John Wiley & Sons (1995).
- 4. D. Goldsmith, M. C. Pirrung& A. T. Morehead. Total Synthesis of Natural Products, John Wiley & Sons (2007).
- 5. W. H. Pearson. Advances in Heterocyclic Natural Product Synthesis, Jai Press (1996).
- 6. D. Barton, K. Nakanishi&O. Meth-Cohn. Comprehensive Natural Products Chemistry, Elsevier (1999).
- 7. I. L. Finar, Organic Chemistry Vol. I & Vol. II- Pearson Education,
- 8. F. A. Carey and R. J. Sundberg, (Eds) <sup>3rd</sup> Ed., Part B. Plenum/Rosetta, 1990.
- 9. Atta-ur-Rahman, Studies in Natural Products Chemistry, Vol.1 and 2, Elsevier, 1988.
- 10. John McMurry, Fundamentals of Organic Chemistry (Fifth Edition), Brooks/Cole, Thomson-Brooks/Cole, 2003.
- 11. R. Krishnaswamy, Chemistry of Natural Products; A Unified Approach, Universities Press.

CHY18R5002	Electrochemistry and Photochemistry	L	T	P	C
CH 1 10K5002	Electrochemistry and Photochemistry	4	0	2	4

CO1	Understand the Debye-Huckel theory of strong electrolytes and related concepts.							
CO2	Details the structure of electrode-electrolyte interface with various models such as							
	Helmholtz - Perrin, Gouy - Chapman and Stern model of electrical double layers.							
CO3	Illustrate the mechanism of electrode reactions and Butler-Volmer equations.							
CO4	Discuss the principle of absorption and emission of radiation and explain the							
	mechanism of Jablonski diagram.							
CO5	Describe the methods of measurements and kinetics of photochemical reactions.							

#### **Mapping of Course Outcomes:**

CO/PO	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8
CO1	S		M		M			
CO2	S		M		S			
CO3	S		M	L	M			
CO4	S		L		M			
CO5	S	S	L		L			

#### **Unit-I: Electrochemistry I:**

Mean ionic activity and mean ionic activity coefficient - concept of ionic strength, Debye - Huckel theory of strong electrolytes - activity coefficient of strong electrolytes - determination of activity coefficient by electrochemical method. Debye Huckel limiting law - qualitative and quantitative verification - limitation of Debye Huckel limiting law at appreciable concentrations of electrolytes - Huckel equation - Debye - Huckel - Bronstedequation .

#### **Unit-II: Electrochemistry II:**

Electrode - electrolyte interface - adsorption at electrified interface - electrical double layer - electro capillary phenomenon - Lippmann equation - Structure of double layers - Helmholtz - Perrin, Gouy - Chapman and Stern model of electrical double layers. Diffusion - Fick's law of diffusion - Effect of ionic association on conductance-electrokinetic phenomenamembrane potential.

#### **Unit-III: Electrochemistry III:**

Mechanism of electrode reactions - polarization and overpotential - the Butler-Volmer equation for one step and multistep electron transfer reactions - significance of electron exchange current density and symmetry factor - transfer coefficient and its significance - mechanism of the hydrogen and oxygen evolution reactions. Corrosion and passivation of

metals - Pourbaix diagram - Evan's diagram - fuel cells - electrodeposition - principle and applications.

#### **Unit-IV: Photochemistry I:**

Absorption and emission of radiation - Franck - Condon Principle - decay of electronically excited states - Jablonski diagram - radiative and nonradiative processes - fluorescence and phosphorescence - spin forbidden radiative transition - internal conversion and intersection crossing - energy transfer process - kinetics of unimolecular and bimolecular photophysical processes-excimers and exciplexes - static and dynamic quenching - Stern-Volmer analysis.

#### **Unit-V: Photochemistry II:**

Experimental methods - quantum yield and lifetime measurements - steady state principle - quantum yield and chemical actinometry. kinetics of photochemical reactions: hydrogen and halogen reactions, photoredox, photosubstitution, photoisomerization and photosensitized reactions - photovoltaic and photogalvanic cells, photoelectrochemical cells, photoassisted electrolysis of water, aspects of solar energy conversion. Radiation chemistry - Interaction of high energy radiation with matter - primary and secondary processes - G value - radiolysis of water - hydrated electron.

- S.Glasstone, Introduction To Electrochemistry, Affiliated East West Press , New Delhi, 1960.
- 2. D.R.Crow, Principles And Applications To Electrochemistry, Chapman And Hall, 1991.
- 3. R.Crow, Principles and Applications to Electrochemistry, Chapman and Hall, 1991.
- 4. P.H.Rieger, Electrochemistry, Chapman and Hall, New York, 1994.
- 5. M.C.Gupta, Statistical thermodynamics, Wiley Easter, New Delhi, 1990.
- 6. R.Hasee, Thermodynamics Of Irreversible Process, Addison Wesley, Reading, Mass, 1969.
- 7. N.J.Turro, Modern Molecular Photochemistry, Benjamin, Cumming, Menlo Park, California, 1978.
- 8. K.K.Rohatgi Mukherjee, Fundamentals Of Photochemistry, Wiley Eastern Ltd., 1978.
- 9. S.Glasstone, Textbook Of Physical Chemistry

#### **List of Experiments for Practical**

- Corrosion rate measurement: Determination of corrosion rate of mild steel and zinc in 1M HCl medium by weight loss method(by individual and by combining both metals).
- 2. Electrode potential measurement: Determination of electrode potential of copper and zinc electrodes.
- 3. Corrosion testing for metals and alloys: Salt spray tests for corrosion of mild steel in 3.5% NaCl solution.
- 4. Photodimerisation of maleic anhydride.
- 5. Determination of dye concentration by colorimetric method.
- 6. Estimation of Nickel/Manganese by photocolorimetric method.

CHY18R5003	Statistical Thermodynamics and Equilibrium	L	T	P	C
CH 1 10K5005	Phenomena		4		

CO1	Understand the basic knowledge about partition functions and their significance.									
CO2										
	thermodynamic parameters.									
CO3	Gathering knowledge about phase equilibria and its applications.									
CO4	To understanding the chemical equilibria and its application.									
CO5	Understand about the entropy changes involved in irreversible processes.									

#### **Mapping of Course Outcomes:**

CO/PO	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8
CO1		S		M	M	S	M	
CO2	M		S	L				M
CO3	M	S		S		M	S	S
CO4			S		M			
CO5	S	M	M		L	S		S

#### **Unit - I: Introduction:**

Objectives of statistical thermodynamics – concept of thermodynamics and mathematical probabilities- distribution of distinguishable and indistinguishable particles. Partition function – evaluation of translational, vibrational and rotational partition functions for mono, diatomic ideal gases- thermodynamic functions in terms of partition functions – application of partition function to heat capacity of ideal gases – nuclear partition function – contribution to heat capacity of ortho and para hydrogen. Heat capacity of solids – Einstein and Debye models.

#### **UNIT – II: Statistical Mechanical Ensembles:**

Need for statistical approach- Permutations and combinations – Distribution – probability – Relation between entropy and probability – stirling approximation- Types of particles-Boson, Fermion, Boltzmannons – Microstate – most probable distribution –derivation of Maxwell –Boltzmann distribution law- statistical weight factor (gi), Different types of ensembles, ensemble averaging, Applications of statistical thermodynamics, equipartition theorem, heat capacity behavior of crystals.

#### **UNIT – III: Phase Equilibria and Phase Rule:**

Phase-components-Degree of freedom-Derivation of the phase rule- one component system: water system – two component systems- simple eutectic systems – Thermal analysis – cooling curves – Lead-silver system – Bismuth-Cadmium system – Three component systems-solid-liquid systems – Acetic acid-chloroform-water system – three component system consisting of two salts and water.

#### **UNIT – IV: Free energy and Chemical equilibria:**

Spontaneous reactions- Standard free energy change – the law of mass action – van't Hoff reaction isotherm – De Donder's treatment of chemical equilibria – reaction potential – Homogenous Equilibria – Temperature-dependent of the equilibrium constants van't Hoff equation – Heterogeneous equilibria – Equilibrium constants for reaction involving real gases – Le Chatelier principle.

#### **Unit – V: Non-equilibrium Thermodynamics:**

Entropy of irreversible processes- Clausius inequality, entropy production ( heat flow, chemical reactions, electrochemical reactions) and entropy flow, entropy production in open systems, Rte of entropy production – generalized forces fluxes, phenomenological equations, Onsager reciprocity relation, electrokinetic phenomena, stationary non-equilibrium statesstates of minimum entropy production.

- 1. G.S.Rush Brooke, Statistical Mechanics, Oxford University Press.
- 2. T.L.Hill, Introduction to statistical Thermodynamics Addison Wesley.
- 3. M.C.Gupta, Statistical thermodynamics, Wiley Easter, New Delhi, 1990.
- 4. R.Hasee, Thermodynamics of irreversible process, Addison Wesley, Reading mass, 1969
- 5. Elements of statistical Thermodynamics- L.K.Nash, Addison Wesley.
- 6. Thermodynamics of Irreversible Processes by Ilya Prigogine.
- 7. Advanced physical chemistry by S.N.Blinder, The Macmillan Company 1967
- 8. Thermodynamics by R.C.Srivastava, S.Saha and A.K.Jain, Prentice hall, India.
- 9. Elements of statistical thermodynamics L. K. Nash, Addison Wesley
- 10. Theoretical Chemistry by S. Glasstone.
- 11. J. Rajaram, J.C. Kuriakose, Thermodynamics, S Chand and Co., 1999.
- 12. M.C. Gupta, Statistical Thermodynamics, New age international, 2007
- 13. B. R. Puri, L. R. Sharma, M. S Pathania, Principles of Physical Chemistry, Vishal Publishing Co.,2017.
- C. Kalidas, M.V. Sangaranarayanan, Non-equilibrium Thermodynamics, Macmillan India, 2002.

CHY18R5051	Doggovah Mothodology	L	T	P	C
CH 1 10K5051	Research Methodology	2	0	0	2

CO1	Details the selection of research problem.
CO2	Understand the various sources of information for literature survey.
CO3	Exemplify the information technology and library resources for research.
CO4	Understand the writing of research papers and presentations.
CO5	Analyse the writing of research proposal.

#### **Mapping of Course Outcomes:**

CO/PO	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8
CO1	S		M		S	M	S	
CO2	S		M		S	M	S	
CO3	S		M		S	M	S	
CO4	S		M		S	M	S	
CO5	S		M		S	M	S	

#### **UNIT-I: Introduction to Scientific research**

Selection of research problem, meaning of research problems, sources of research problems, criteria / characteristics of a good research problem, errors in selecting a research problem.

#### **UNIT-II: Literature Survey**

Sources of information, Primary, Secondary, Tertiary sources, Journals, Journal abbreviations, Abstracts, Current titles, Reviews, Monographs, Textbooks, Current contents, Introduction to Chemical Abstracts. Online searching, Database, *Scifinder*, *Scopus*, Citation Index, Impact Factor.

#### **UNIT-III:** Use of Information technology resources

The Internet and World Wide Web, internet resources for chemistry, internet search engines, using spreadsheets, word processors, databases and other packages, finding and citing information.

#### **UNIT-IV: Communicating information**

General aspects of scientific writing, reporting practical and project work, writing literature surveys and reviews, Paper writing for International Journals, submitting to editors, organizing a poster display, giving an oral presentation in seminars/conferences.

**UNIT-V: Writing of Research Report:** Format of the research report, style of writing the report, references and bibliography. Research Proposal: Format of research proposal, individual research proposal and institutional proposal.

- 1. Dr.C.R. Kothari, Research Methodology: Methods and Techniques, New Age International Publishers, 2<sup>ndEd.,</sup> New Delhi (2014.)
- 2. Ranjitkumar, Research Methodology: A Step by Step Guide for Beginners, Pearson Education; 2<sup>nd</sup> Ed., (2005).
- 3. M.D. Barbara Gastel and Robert A. Day, How to Write and Publish a Scientific Paper, Greenwood Publishing Group Inc, 8<sup>th</sup> Ed., 2016.
- 4. Tanmoy Chakraborty and LalitaLedwani, Research Methodology in Chemical Sciences: Experimental and Theoretical Approach, Apple Academic Press; 1<sup>st</sup> Ed.,, 2016.

CHY18R5081	Organic Chemistry Laboratory	L	T	P	C
CHITOKSUOI	Organic Chemistry Laboratory	0	0	6	3

CO1	Understand the basic preparation of organic reactions.
CO2	Gathering the knowledge about various spectroscopic techniques such as IR, NMR and Mass spectroscopy analysis.
CO3	Details the various organic reactions and their synthetic procedures.
CO4	Analyze the separation processes of various organic compound mixtures and their quality checking processes.
CO5	Explain the use of the software: Excel, Origin, Mercury and Powerpoint.

## **Mapping of Course Outcomes:**

CO/PO	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8
CO1	M	S			S		M	
CO2		S			S		M	
CO3	S	S			S		M	
CO4	M	S			S		M	
CO5			S		L			

## **List of Experiments Experiments:**

- 1. Introductory experiments on Chromatographic technique –TLC, CC and PC.
- 2. Separation and identification of organic compounds in a mixture.
- 3. Preparation of organic compounds illustrating important synthetic reactions.
- 4. Training to use software: ChemDraw, ISI Draw.

- 1. A.I.Vogel, A.R.Tatchell , B.S.Furnis, A.J.Hannaford, P.W.G.Smith, Vogel's Textbook of Practical Organic Chemistry (5<sup>th</sup> Ed.,), Longman, 1989.
- 2. Bansal Raj K, Laboratory Manual of Organic Chemistry, New Age International, 2009.

CHY18R5082 Seminar & Comprenensive viva - III L I P C	CHY18R5082	Seminar & Comprehensive Viva - III	L	T	P	C
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	 <b>N</b>	1	1 1	1 7
	U	1	1 1	4

Classification of natural products - Retrosynthetic approaches in Natural Products Synthesis - Total synthesis of Important Natural Products - Carbohydrates and amino acids – Peptides, proteins and lipids – Electrochemistry – Photochemistry - Statistical Mechanical Ensembles - Quantum Statistics - Classical Statistics of Independent Particles - Non-equilibrium Thermodynamics.

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#### **ELECTIVE COURSES**

CHY18R4031	Chaetmagaany	L	T	P	C
CH 1 10K4031	Spectroscopy	5	0	0	4

## **Course Outcomes (COs)**

CO1	Understand the basic principles, instrumentation and applications of UV-Visible spectroscopy for the structural elucidation of organic compounds.
CO2	Discuss the principles, characteristic frequencies of common functional groups, instrumentation and applications of IR Spectroscopy for the structural elucidation of
	organic compounds.
CO3	Describe the basic theory of Nuclear Magnetic Resonance (NMR) Spectroscopy and obtain structural information from <sup>1</sup> H NMR and <sup>13</sup> C NMR spectroscopy and interpret the data's.
CO4	Identify the components of Mass spectrometer and explain the fragmentation pattern and use them in structural elucidation.
CO5	Details the basic principles and application of Electron spin resonance (ESR) spectroscopy for the structural elucidation of compounds.

## **Mapping of Course Outcomes:**

CO/PO	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8
CO1	S	S	M		S		M	
CO2	S	S	M		S		M	
CO3	S	S	M		S		M	
CO4	S	S	M		S		M	
CO5	S	S	M		S		M	

## **Unit – I: UV-Visible Spectroscopy:**

Electromagnetic radiation, energy and electromagnetic spectrum, units, absorption of energy by organic compounds. UV-Visible spectroscopy: Basic principles, theory, instrumentation and applications of UV-Visible spectroscopy. Application of UV-Visible spectroscopy to structure elucidation of organic compounds. Woodward- Fieser rules for calculating absorption maximum in Dienes,  $\alpha$ ,  $\beta$ -unsaturated carbonyl compounds. Octant rules, Application of ORD-CD to stereochemical assignments.

## **Unit – II: IR and Raman Spectroscopy:**

IR-Spectroscopy-Basic Principles, theory, Molecular vibrations, vibrational frequency, factors influencing vibrational frequency, instrumentation, infrared spectrum, fingerprint region and characteristic frequencies of common functional groups. Application of IR spectroscopy to structure elucidation of organic compounds. Basic Principles of Raman Spectroscopy and its application.

## **Unit – III: NMR Spectroscopy:**

Basic principles-introduction to NPR technique-CW and FT NMR techniques, 1H NMR spectral parameters-Intensity, chemical shift, multiplicity, coupling constant factors affecting. Analysis of first order and second–order spectra, structure determination of organic compounds by <sup>1</sup>H NMR spectra. <sup>13</sup>C NMR Proton coupled, off-resonance decoupled, proton noise decoupled <sup>13</sup>C NMR spectra, Assignment of chemical shifts of common organic compounds and functional groups: Introduction to multinuclear NMR of common heteroatoms present in organic compounds (N, F, O, P, S & D).

<sup>2</sup>D NMR techniques <sup>1</sup>H-<sup>1</sup>H COSY, <sup>1</sup>H-<sup>13</sup>C COSY-NOESY spectra.

## **Unit – IV: Mass Spectroscopy:**

Basic principles, techniques of ion production and ion and daughter ions, molecular ion and isotope abundance, nitrogen rule-energetics of fragmentation. Metastable ions, common fragmentation pathways-fragmentation of common chemical classes. Mclafferty rearrangement. Structural elucidation.

Applications of UV-Visible, IR, NMR and Mass spectroscopy for structure elucidation of organic compounds-problems.

## **Unit – V: ESR, NQR and Mossbauer Spectroscopy:**

**Electron Spin Resonance**: g value, hyperfine structure, esr of hydrogen atom, free radicals, esr of simple free radicals in solutions, Spin densities, spin polarisation, anisotropy of Zeeman and Hyperfine interactions. ESR of spin transition Metal ions: s = 1/2 systems, g and A anisotropy. Effect of spin orbit interaction.  $d^1$  system in a tetragonal field. Covalency effects. EPR spectra of transition ion (s = 1/2), S > 1/2 systems, Zero field splittings, EPR of Metalloenzymes.

**NQR and Mossbauer Spectroscopy**: Principles, isomer shift, quadrupole effect of magnetic field, applications to iron and tin compounds.

- 1. William Kemp, Organic Spectroscopy, Third Edition, MacMillan (1994).
- 2. D.H.William and Ian Fleming, Spectroscopic methods in organic chemistry, Tata McGraw Hill (1998).
- 3. R.M.Silverstein and F.X.Webster, Spectrometric identification of organic compounds; John Wiley and Sons, Inc., Sixth Edition (1997).
- 4. A.B.P. Lever, Inorganic Electronic Spectroscopy, 1986.
- 5. J. Pilbrow; Transition ion EPR (Oxford) 1968.
- 6. C.N.Banwell: Fundamentals of Molecular Spectroscopy, 4<sup>th</sup> Ed., Tata McGraw Hill, 1996
- 7. A.E.Derome: Modern NMR Techniques for Chemical Research, Pergamon Press, 1987.
- 8. R.S.Drago: Physical Methods for Chemists, Second Edition, Saunders College Publication, 1992.
- 9. D.H.Williams and I.Fleming: Spectroscopic Methods in Organic Chemistry, Fourth Edition, McGraw-Hill, 1966.
- 10. Norman B.Colthup, Lawrence H. Daly, Stephen E. Wiberley, Introduction to Infrared and Raman Spectroscopy, 3<sup>rd</sup> Ed., Academic Press, 1990.
- 11. V.R.Dani, Organic Spectroscopy, Tata McGraw Hill Publishing Co. Ltd, New Delhi, 1998.

CHY18R4032	Environmental Chemistry	L	T	P	C
C11110K4032	Environmental Chemistry	5	0	0	4

CO1	Understand the chemistry and effects of Atmospheric pollution.
CO2	Describe the Lithosphere and the chemical composition of the Earth and Hydrosphere.
CO3	Understand the significance of biosphere and explain the effects of thermal pollution.
CO4	Detail the chemistry of water pollution and sewage treatment.
CO5	Illustrate the various industrial Pollution control methods and analysis of different pollutants.

## **Mapping of Course Outcomes:**

CO/PO	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8
CO1	S		L		L		M	
CO2	S			L	L		M	
CO3	S		L					
CO4	S			L				
CO5	S		L		M		M	

## **Unit – I: Atmospheric Chemistry:**

The structure of the earth's atmosphere- chemistry of the lower and upper atmosphere. The chemistry of air pollution- oxides of nitrogen- hydrogen sulphide and oxides of sulphur-Aerosols – ozone depletion and consequences- dioxins burning plastics- other atmospheric chemicals- smog- radioactivity and fall out- air pollution abatement. Greenhouse effect-Global warming, oxides of carbon.

#### **Unit – II: The Earth:**

The lithosphere- the chemical composition of earth- the structure and composition of inner earth - the mantle, and the crust. The exploitation of mineral resources and the abuse of earth - earth resources - changing the face of the land- the earth as a dump- recycle earth resource conservation steps. The hydrosphere: The fresh water chemistry - the structure and properties of liquid water -lakes, rivers, ponds and stream - river chemistry, pollution and aeration - water additives-isotopes- mercury pollution. The chemical constituents of sea water- organic matter and suspended material- ocean dumping- oil pollution. The role of water in our total environment-the hydrologic cycle- snow and ice - nucleation and precipitation - the chemical composition of rain water- phase changes and isotopic fractionation.

## **Unit – III: The Biosphere:**

The structure of the biosphere, Man's perturbation of the biosphere – Man as a chemical factory – material use and waste – energy use and thermal pollution – ecological disruption –chemical sensation, hormonal imbalance and mutagens- internal pollution. Hydrosphere –lithosphere interaction: The structure of water at an interface – chemical composition of mineral water- weathering and the changing face of the land- the origin of the oceans-sedimentation and the deposition of materials from the hydrosphere – chemical exchange between sediments and the water column.

#### **Unit – IV: Interactions:**

Lithosphere- biosphere interaction: soil chemistry — the prospects of agriculture-agricultural pollution — pesticides and other persistent pollutants — the deposition of coal and petroleum —theories of origin of petroleum. Atmosphere — biosphere interaction and atmosphere —hydrosphere interaction: history of earth's atmosphere — the nitrogen cycle — the carbon cycle —air — sea interactions. Biosphere — hydrosphere interaction: The chemistry of water pollution — sewage treatment, primary, secondary— and tertiary — activated sludge — trickling filters— denitrification —biology and energy chain — reactor design theory — anaerobic digestion —eutrophication.

#### **Unit – V: Pollution Control:**

Pollution control in the following: Fertiliser, petroleum, pulp and paper, tanning, sugar, alcohol, electroplating and nuclear reactors. Environmental act and rules: Air and Water. Central and state pollution control boards and their functions. Analysis of pollutants: Sum, specific and group parameters BOD, COD, specific oxygen demand, DOC, DOC, DOS, Fe, Cr, Cu, Pb, and Ni-SOx, NOx, H<sub>2</sub>S, O<sub>3</sub> and CO.

- 1. R. A. Horne., The Chemistry of Our Environment. John Wiley & Sons Ltd., New York 1978.
- 2. A.K.De, Environmental chemistry, Fifth Ed., 2003, New age International (P) limited, new Delhi,
- 3. S.P.Mahajan, Pollution control in process industries, Tata McGraw-Hill Enn. 1985
- 4. Iain L, Marr and Malcolm S. Cresser, Environmental chemical analysis, International Text Book. Co., 1983 science.

CHY18R4033	Industrial Chemistry	L	T	P	C
CH 1 10K4033	muusti iai Chemisti y	4	0	0	4

CO1	Understand the different manufacturing process uses oxidation, hydrogenation and
	halogenations reactions.
CO2	Outline the manufacturing process of esterification and amination reactions.
CO3	Illustrate the manufacture of pulp and paper, common salt and caustic soda.
CO4	Understand the constituents, classification, properties and applications of paints.
CO5	Exemplify the manufacture of cement and ceramics.

## **Mapping of Course Outcomes:**

CO/PO	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8
CO1	S	M			S	M	S	
CO2	S	M			S	M	S	
CO3	S	M			S	M	S	
CO4	S	M			S	M	S	
CO5	S	M			S	M	S	

## **UNIT-I Unit Processes (Oxidation, Hydrogenation and Halogenation)**

**Oxidation:** Introduction, Types of oxidation reactions, various oxidizing agents, manufacturing process of acetic acid, manufacturing process of acetaldehyde, manufacturing process of benzoic acid.

**Hydrogenation:** Introduction, Various methods of reduction, various hydrogenating catalyst, Hydrogenation process of vegetable oils, Synthesis process of methanol.

**Halogenation:** Definition, Types of halogenation reactions, Various halogenating agents, Manufacturing process of monochloroacetic acid, Manufacturing process of chlorol, Manufacturing process of chloro benzene, Manufacturing process of freon-12, Chlorination of methane.

## **UNIT-II Unit Processes (Esterification & Amination)**

**Esterification:** Definition, Types of Esterification reaction, Types of Esterification agents, Manufacturing process of cellulose acetate, Manufacturing process of vinyl acetate, Manufacturing process of ethyl acetate.

**Amination:** Amination by reduction: Definition, Types of amination reaction, Aminating agents, Manufacturing process of aniline, Manufacturing process of m-nitroaniline, Amination by ammonolysis: Definition, Types of amination reaction, Aminating agents, Chemical factors and Physical factors, Outline of chemical kinetics, mechanism and thermodynamics.

#### **UNIT-III Process Industries:**

**Pulp and Paper Industry:** Introduction, manufacture of pulp, sulphite pulp, soda pulp, sulphite pulp, rag pulp, beating, refining filling, sizing and colouring, manufacture of paper, calendering.

Alkali and Chlorine Industry:Introduction, common salt, method of manufacture of salt, caustic soda, cells used diaphragm cell, Hooker diaphragm cell, CastnerKellner cell, physicochemical principle.

## **UNIT-IV Paint Technology**

**Paints and Varnishes:** Introduction and Definitions of paints, pigments, varnishes, lacquers, Anatomy of paints, functions & requirements of constituents of paints, classification of paints on the basis of order of application/ methods of curing / nature of solvent/ uses etc. General characteristics of paint varnishes, lacquers and their functions.

**Paint Properties**: Color, tinting strength, reducing power, pigments-classification of pigments, pigments properties-oil absorption, refractive index, particle size shape, bleeding, resistance to light and heat.

#### **UNIT-V** Cement and Ceramics

**Cement:** Introduction, Composition of cement, Functions of ingredient of ordinary cement, Manufacturing of ordinary cement-Dry process, Wet process, Advantages and disadvantages of both the processes, Uses of cement, various types of cement, Additives of cement, Accelerators.

**Ceramics:**Introduction, Raw materials of ceramic, Types of ceramic, Whitewares, Manufacturing of whitewares, Refractory materials, Uses of refractory materials, Manufacturing of refractories, Properties of refractories, Classification of refractories, Various uses of refractory materials.

- 1. P.H. Groggins, Unit Processes in Organic Synthesis, McGraw Hill Book Co, (1984).
- 2. Philip Groggins, Unit Processes in Organic Synthesis, McGraw Hill Education; 5<sup>th</sup> Ed., (2001).
- 3. Michael B Smith, Organic Synthesis, Academic Press; 3<sup>rd</sup> Ed., (2011).
- 4. Clayden, Organic chemistry, Oxford; Second Edition (2012).
- 5. John E. McMurry, Organic Chemistry, Brooks Cole; 8<sup>th</sup> Ed., (2011).
- 6. George T.Austin, Shreve's Chemical Process Industries, McGraw Hill Education, Fifth Edition (1984).
- 7. B.K.Sharma, Industrial chemistry, KrishnaPrakashan; 17/e Ed., (2014).

CHY18R4034	Medicinal Chemistry	L	T	P	C
	ivicatemai onemistry	5	0	0	4

## **COURSE OUTCOMES (CO'S)**

CO1	Understand the basic principles of drug metabolism, pharmacokinetics and								
CO1	pharmacodynamics.								
CO2	Discuss various cardiovascular diseases, mode of action of cardiovascular drugs and								
COZ	their side effects.								
CO3	Describe the classification of various antibiotics and their mechanism in inhibiting								
	protein synthesis, cell wall biosynthesis.								
CO4	Build knowledge on synthesis of various local antiinfective drugs and their mode of								
	action along with side effects.								
CO5	Details the importance of various antineoplastic agents and their recent developments								
	in cancer therapy.								

## **Mapping of Course Outcomes:**

CO/PO	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8
CO1	S	S		M	S		S	
CO2	S	S		M	S		S	
CO3	S	S		M	S		S	
CO4	S	S		M	S		S	
CO5	S	S		M	S		S	

#### UNIT-1

**Drug Metabolism**: Introduction, oxidation, reduction, hydrolysis, conjugation, Pharmacokinetics: Drug Absorption, drug distribution, drug elimination, drug disposition, pharmacokinetic parameters, uses of pharmacokinetics in drug development process, Pharmacodynamics: Enzyme stimulation, inhibition, sulphonamides, membrane active drug, biotransformation, xenobiotics.

#### **UNIT-2**

**Cardiovascular drugs**: Cardiovascular diseases, arteriolar dilators, diuretics, adrenergic receptor blockers, synthesis mode of action, uses and side effects of cardiovascular drugs, esters of nitrous and nitric acid-amyl nitrate, calcium channel blockers, anti-adrenergic drugs methyldopa, sodium channel blockers - quinidine, -adrenergic blockers - atenolol, oxprenolol.

#### **UNIT-3**

**Antibiotics**: Introduction and classification, synthesis uses and side effects of antibiotics (a) penicillin-V (b) penicilline-G (c) tetracycline (d) ampicillin, (e) cephalosporin, antibiotics inhibiting protein synthesis, cell-wall biosynthesis, inhibitors of cell-wall biosynthesis, mode of action of penicillin and cephalosporin, microorganisms.

## **UNIT-4**

**Local anti-infective agents**: Introduction, mode of action, sulfonamides, synthesis mode of action and side effects of sulfa drugs: sulphanilamide, sulphapyridine,antileprotic drugs: synthesis, mode of action and side effect of dapsone, tuberculosis, antitubercular drugs: Synthesis, mode of actions, and side effects of ethionamide, isoniazid, antifungal drugs: synthesis, mode of action and side effects of (a) fluconazole (b) griseofulvin.

## **UNIT-5**

Antineoplastic agents: Introduction, cancer, classification of antineoplastic agents, role of alkylating agents and antimetabolites in treatment of cancer, carcinolytic antibiotics, synthesis use and side effects antineoplastic agents: Mechlorethamine, cyclophosphamide, melphalan, mustards (mode of action) fluorouracil, 6-mercaptopurine, recent development in cancer chemotherapy, mitotic inhibitors: natural products, hormones.

- 1. D.J.Abraham. Burgers medicinal chemistry and drug discovery, Wiley, 6<sup>th</sup> edition, 2003.
- 2. R. B. Silverman. The organic chemistry drug design and drug action, Academic Press, 3<sup>rd</sup> edition, 2014.
- A.Gringuage. Introduction to medicinal chemistry-how drugs act and why, Wiley-VCH, 1934.
- 4. William O. Foye. Thomas L. Lemice and David A.Williams, Principles of Medicinal Chemistry, Wiley-VCH, 7<sup>th</sup> edition, 2002.
- 5. Goodman and Gilman's Pharmacological Basis of Therapeutics, McGraw-Hill, 12<sup>th</sup> edition, 2011.
- 6. Graham L. Patrick.An Introduction to Medicinal Chemistry, Oxford, 6<sup>th</sup> edition, 2017.
- 7. Wilson, Charles Owens. Textbook of Organic Medicinal and Pharmaceutical Chemistry, Philadelphia, Pa.: Lippincott,6<sup>th</sup> edition, 1971.
- 8. AshutoshKar. Medicinal Chemistry, New Age International, 3<sup>rd</sup> edition, 2005.

CHY18R4035	Supramolecular Chemistry	L	T	P	C
	Supramolecular Chemistry	5	0	0	4

## **COURSE OUTCOMES (CO'S)**

CO1	To learn about the basic concepts of supramolecular chemistry, which relies on the
COI	non-covalent interactions
CO2	To study about various molecular recognition where the molecules that fit into the
COZ	cavity of the host molecules.
CO3	To understand various supramolecular devices such as rotaxanes and catenanes and
	their applications
CO4	To obtain knowledge on the reactivity of supramolecular systems which has been
	extensively used in catalysis
CO5	To study the basic principles and application of organometallic systems in the
	construction of metal organic frameworks

## **Mapping of Course Outcomes:**

CO/PO	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8
CO1	S	S		M	S	M	S	
CO2	S	S		M	S	M	S	
CO3	S	S		M	S	M	S	
CO4	S	S		M	S	M	S	
CO5	S	S		M	S	M	S	

## **UNIT I: Concepts of Supramolecular Chemistry**

Concepts and languages of supramolecular chemistry – various types of non covalent interactions – hydrogen bonds, C-H...X interactions, halogen bonds –  $\pi$ - $\pi$  interactions, non-bonded interactions – various types of molecular recognition.

Chemistry of non-covalent interactions – hydrogen bonded supramolecular patterns involving water / carboxyl /amine motifs – concepts of different types of synthons based on non-covalent interactions

## **UNIT II: Molecular Recognition and host-guest chemistry**

Molecular recognition: Molecular receptors for different types of molecules including anionic and cationic substrates, design and synthesis of synthetic receptor molecules and multiple recognition. H-bonds in supramolecular structures. Use of H-bond in crystal engineering and molecular recognition. Chelate and macrocyclic effects. Cation binding hosts, binding of anions, binding of neutral molecules, binding of organic molecules.

## **UNIT III: Supramolecular Devices**

Synthesis and structure of crown ethers, podands, cryptands, spherands, calixarenes, cyclodextrins and other host molecules. Host-Guest interactions, pre-organization and complementarity, lock and key analogy. Molecular electronic devices, molecular wires, molecular rectifiers, molecular switches, molecular logic and other molecular level devices.

#### **UNIT IV: Supramolecular Reactivity and Catalysis**

Supramolecular reactivity – Organocatalysis mediated through hydrogen bonding, preconcentration, self-assembly of catalysts and preorganisation of catalyst-substrate systems. Influence of organisation (effective molarity) on catalysis and supramolecular photochemical reactions. Cyclodextrins as enzyme mimics reactions.

## **UNIT V: Metal Organic Frameworks**

M.O.F (Metal Organic Frameworks) – organometallic systems – combinations of metal ions with various ligands and their interactions to design molecular rods, triangles, ladders, networks, etc. – design of nanoporous solids – inter ligand hydrogen bonds in metal complexes – implications for drug design and related applications

- 1. J. M. Lehn, Supramolecular Chemistry; VCH, Weinheim, Germany, 1995.
- 2. G. R. Desiraju, Crystal Engineering: The Design of Organic Solids; Elsevier, United States, 1989.
- 3. G. R. Desiraju, and T. Steiner, The Weak Hydrogen Bond in Structural Chemistry and Biology; Oxford University Press, Oxford, 1999.
- 4. G. A Jeffrey, Introduction to Hydrogen Bonding; Oxford University Press: UK, 1997.
- J. M. Lehn, Transition Metals in Supramolecular Chemistry; John Wiley and Sons: New York, 1999.
- 6. G. R. Desiraju, Current Science; 2001, 81, 1038.
- 7. Web source: Crystal Growth and Design,
- 8. http://www.pubs.acs.org/journals/cgdefu/index.html
- Crystal Engineering Communication http://www.rsc.org/Publishing/Journals/ce/index.asp

CHY18R4036	Nanomaterials	L	T	P	C
C11110N4030	Nationiaterials	5	0	0	4

CO1	Describe the various unique characteristics of nanomaterials
CO2	Understand the synthesis of nanomaterials by chemical methods
CO3	Understand the fabrication of nanomaterials by physical methods
CO4	Capable to characterize the nanomaterials by various instrumental methods
CO5	Apply nanomaterials towards multidisciplinary problems.

## **Mapping of Course Outcomes:**

CO/PO	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8
CO1	S	M	L		M		M	
CO2	S	S	L		M		M	
CO3	S	M			M		M	
CO4	S	S	M	L	S	M	S	L
CO5	S	L	L		M	M	M	

#### **Unit – I: Basics of Nanomaterials:**

Basics of nanomaterials: Properties of materials & nanomaterials, quantum confinement effect, surface to volume ratio, surface properties of nanoparticles. Classification of the nanomaterials – zero dimensional, one dimensional, two dimensional and three dimensional nanostructures. Mechanical, optical, electronic, magnetic, thermal and chemical properties of nanomaterials. Size dependent properties-size dependent absorption spectra.

## **Unit – II: Synthesis of Nanomaterials by Chemical Routes:**

Chemical precipitation and coprecipitation, metal nanocrystals by reduction, sol-gel synthesis, microemulsions or reverse micelles, solvothermal synthesis, thermolysis routes, microwave heating synthesis, sonochemical synthesis, electrochemical synthesis, photochemical synthesis, synthesis in supercritical fluids, self-assembly strategies.

## **Unit – III: Fabrication of Nanomaterials by Physical Methods:**

Inert gas condensation, arc discharge, plasma arc technique, RF plasma, MW plasma, ion sputtering, laser ablation, laser pyrolysis, molecular beam epitaxy, chemical vapour deposition method and electro deposition.

## **Unit – IV: Characterization of Nanomaterials:**

X-ray diffraction, Scanning Electron Microscopy (SEM), Scanning Probe Microscopy (SPM), TEM and EDX analysis, Atomic force Microscopy (AFM); Spectroscopic characterizations: UV-Visible and NMR spectroscopy; Surface Characterization: X-ray Photoelectron Spectroscopy (XPS), Secondary Ion Mass Spectroscopy (SIMS); Thermal Characterization: DTA, TGA, DSC.

## **Unit – V: Applications of Nanomaterials:**

Catalysis on nanoparticles, oxide reactions, semiconductors, sensors, and electronic devices, photochemistry and nanophotonics, applications of CNTs, nanomaterials in biology and medicine.

- 1. Charles P. Poole, Frank J. Owens, "Introduction to Nanotechnology", Wiley Interscience, 2003.
- C. N. R. Rao, A. Mu"ller, A. K. Cheetham, "The Chemistry of Nanomaterials: Synthesis, Properties and Applications" WILEY-VCH Verlag GmbH & Co. KGaA, Weinheim, 2004
- 3. G. Schmidt, "Nanoparticles: From theory to applications", Wiley, Weinheim 2004.
- 4. G. B. Sergeev, "Nanochemistry" Kidlington, Oxford OX5 1GB, UK, 2006.
- C. N. R. Rao, A. Mu'ller, A. K. Cheetham, "Nanomaterials Chemistry: Recent developments and new directions" WILEY-VCH Verlag GmbH & Co. KGaA, Weinheim, 2007
- C.N.R. Rao, G.U. Kulkarni, P.J. Thomas, Nanocrystals: Synthesis, Properties and Applications" Springer Series in materials science-95, Springer-Verlag Berlin Heidelberg 2007
- 7. Zhong Lin Wang, "Characterization of nanophase materials" WILEY-VCH Verlag GmbH & Co. KGaA, Weinheim, 2000.

## M.Sc. Chemistry

MAT18R4001	<b>Mathematics for Chemists</b>	L	T	P	C
WIA 1 10K4001		5	0	0	4

(Interdepartmental Elective)

## **Course Outcomes (COs)**

CO1	Understand the basic concepts of Cartesian coordinates, differential calculus and								
	vector calculus.								
CO2	Know the methods of integration and methods of solving differential equations.								
CO3	Inderstand the concepts in matrix theory and its application to chemistry problems.								
CO4	Know about the C-Programming.								
CO5	Apply the C-Programme to solve the problems in chemistry.								

## **Mapping of Course Outcomes:**

CO/PO	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8
CO1	S		S	M				M
CO2	S		S	M				M
CO3	S		S	M				M
CO4	S		S	M				M
CO5	S		S	M				M

## UNIT -I: Differential Calculus and Vectors

Cartesian coordinates: plane polar coordinates, spherical representation of functions, the complex plane, polar coordinates in trigonometric functions.

Differential calculus: functions of single and several variables, partial derivatives, the total derivative, maxima and minima theorem, and simple examples related to chemistry.

Vectors: representation and simple properties of vectors (addition and subtraction) vector addition by method of triangles, resolution of vectors. Scalar product of vector. Concept of normalization, orthogonality and complete set of unit vectors.

## **UNIT -II : Integral Calculus and Differential equations**

Integral calculus: general and special methods of integration, geometric interpretation of integral, evaluation of definite and some standard integrals related to chemistry. The significance of exponential equations.

Differential equations: simple differential equations, separable variables, homogeneous equations, exact equations, linear equations, and equations of first and second order. Application to simple chemistry problems.

#### UNIT -III: Matrix Algebra

Matrices and Determinants: Definition of matrix, types of matrices (row, column, null, square, diagonal).

Matrix algebra: addition, subtraction, and multiplication by a number, matrix multiplication. Transpose and adjoint of matrix, elementary transformation, representation and applications to solutions of linear equations. Definition of determinant, its properties and evaluation of determinants. Application to simple chemistry problems.

## **UNIT -IV: Programming in C**

Programming in C: Character set, constants and variables, reserved words, data types, expressions, scanf and print statements, operators and their hierarchy, conditional, unconditional and loop control structures. One-dimensional and two-dimensional arrays. Functions.

## **UNIT-V: Computer Application in Chemistry**

Computer Application in Chemistry: Developing programs in C involving simple formulae in chemistry such as van der Waals equation, pH titration, kinetics, radioactive decay, evaluation of lattice energy and ionic radii from experimental data. Linear simultaneous equation to solve secular equations within the Huckel theory. Elementary structural features such as bond lengths, bond angles, dihedral angles etc. of molecules extracted from a database such as Cambridge database.

- 1. Mathematical Methods for Scientists and Engineers, D.A. McQuarrie
- 2. Advanced Engineering Mathematics, E. Kreyszig.
- 3. Mathematical Methods for Science Students, G. Stephenson, ELBS.
- 4. The Chemistry Mathematics Book, E. Stener, Oxford University Press.
- 5. Mathematics for Chemistry, Doggett and Sutcliffe, Longman.
- 6. Let Us C, YashwantKanetkar.
- 7. Computational Chemistry, A.C. Norris.

CHY18R5031	Corrosion Science	L	Т	P	C
CHTTOKSUST	Corrosion Science	5	0	0	4

CO1	Describe the corrosion process and its different types.
CO2	Understand the basic principles of corrosion science.
CO3	Detail the different forms of corrosion.
CO4	Evaluate the various methods of corrosion testing.
CO5	Describe the methods of corrosion protection and explain the principles of corrosion
	protection.

## **Mapping of Course Outcomes:**

CO/PO	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8
CO1	S	M	L	L	M		M	
CO2	M	M	L	L			M	
CO3	S	M	L				M	
CO4	S	M	L		M		M	
CO5	S	M	L	L	M		M	

#### **Unit – I: Introduction:**

Corrosion-Definition, Classification, Expressions for corrosion rate, EMF series and Galvanic series-Merits and Demerits, Pourbaix diagram for iron, magnesium and aluminium, High temperature corrosion, Pilling-Bedworth ratio.

## **Unit – II: Corrosion Principles:**

Introduction, Electrochemical reactions, Application of thermodynamics to corrosion, Polarization-Activation polarization and Concentration polarization, Mixed potential theory, Exchange current density, Tafel equation, Passivity-Mechanism of the growth and breakdown of passive film.

## **Unit – III: Forms of Corrosion:**

Uniform corrosion-Atmospheric corrosion, Galvanic corrosion, Crevice corrosion, Pitting corrosion, Intergranular corrosion, Stress corrosion cracking, Dezincification, Erosion corrosion, Corrosion fatigue, Hydrogen damage.

## **Unit – IV: Corrosion Testing:**

Introduction, Classification, Purpose of corrosion testing, Huey test for stainless steel, Streicher test for stainless steel, Stress corrosion test, salt spray test, humidity and porosity tests, Accelerated weathering tests. Electrochemical methods of corrosion rate measurements

by Tafel polarization, linear polarization, and impedance spectroscopy-ASTM Standards for corrosion testing.

## **Unit - V: Corrosion Protection:**

Introduction, Material selection, Alteration of environment, Design, Cathodic protection and Anodic protection, Coatings-metallic and other inorganic coatings, Organic coatings, Electroless plating and Anodizing, Corrosion inhibitors, Failure analysis.

- 1. Fontana and Greene, Corrosion Engineering, McGraw Hill Book Co, New York, 1983.
- Raj Narayan, An introduction to metallic corrosion and its prevention, Oxford and IBH, New Delhi, 1983.
- S.N.Banerjee, "An Introduction to Corrosion Science and Corrosion Inhibition", Oxonian Press P.Ltd, New Delhi, 1985.
- 4. Denny A. Jones, Principles and Prevention of corrosion, Macmillan Publishing Company, 1991.
- 5. Zahi Ahmed, Principles of corrosion engineering & corrosion control, Butterworth Heinemann, 2006.
- Budinski, K.G., Surface Engineering for wear resistance, Prentice Hall Inc, Englewood Cliff, New Jersey, USA, 1988.
- Uhlig, H.H., Corrosion and Corrosion control, John Wiley and sons, New York, USA, 1985.

CHV10D 5022	Conserve Charminton	$\mathbf{L}$	T	P	C
CHY18R5032	Green Chemistry	5	0	0	4

CO1	Understand the principle and importance of green chemistry.
CO2	Describe the typical chemical reactions essential for designing green chemical synthesis.
CO3	Detail the chemical transformations induced by physical factors such as microwave, sunlight and ultrasound.
CO4	Familiarizing with the various concepts in heterogeneous catalysis.
CO5	Illustrate the synthesis of complex organic compounds through green chemistry approaches.

## **Mapping of Course Outcomes:**

CO/PO	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8
CO1	S	M	L		M		M	
CO2	S	M		L	L		M	
CO3	S	M	L				M	
CO4	M	M		L			M	
CO5	S	M	L				M	

## **Unit – I: Basic Concepts of Green Chemistry:**

Definition of green chemistry, need of green chemistry and eco-efficiency, Environmental protection laws, challenges and green chemistry education, pollution control and pollution prevention-Principle of green chemistry.

#### **Unit – II: Green Solvents:**

Aqueous phase reactions: Mechanism and application of Baeyer-Villiger Oxidation, Claisen rearrangement, Claisen-Schmidt reaction, Diels-Alder reaction, Heck reaction, Knoevenagel condensation, Michael addition, Mukaiyama Reaction and Wurtz reaction. Ionic liquids: Properties of ionic liquids and applications in organic synthesis (illustrate with three examples such like Diels-Alder reaction, Heck reaction, Knoevenagel condensation, Michael addition, Wittig reaction.

## **Unit – III: Non-conventional energy sources:**

Microwave Solvent free reaction: Solid state reactions-Deacetylation, deprotection, Saponification of esters, alkylation of reactive methylene compounds, synthesis of nitriles from aldehydes, reductions. Microwave assisted reactions in water-Hofmann elimination,

hydrolysis, oxidation, saponification reactions. Microwave assisted reactions in organic solvents-Esterification reactions, Fries rearrangement, Orthoester rearrangement, Diels-Alder reaction, decarboxylation. Microwave assisted reactions under PTC conditions: Ultrasound assisted reaction: Introduction, substitution reactions, addition, oxidation and reduction reactions. Photochemical reactions using sunlight: Benzopinacol, conversion of trans azobenzene to cis azobenzene and conversion of trans stilbene to cis stilbene.

## **Unit – IV: Green catalysis:**

Heterogeneous catalysis: use of zeolites, silica, alumina, clay, polymers, cyclodextrin and supported catalysts. Biocatalysis: enzymes, microbes etc Phase-transfer catalysis: micellar/surfactant etc.

## **Unit – V: Designing Green Synthesis:**

Designing Green Synthesis- choice of starting materials, choice of reagents, choice of catalysts-biocatalysts, polymer supported catalysts, choice of solvents. Synthesis involving basic principles of green chemistry - Examples-Synthesis of ibuprofen, adipic acid, methyl methacrylate and paracetamol.

- 1. Green Chemistry, Theory and Practical, Paul T.Anastas and John C.Warner, Oxford University Press.
- 2. New Trends in Green Chemistry by Ahluwalia and M. Kidwai.
- 3. Green Chemistry, Introductory Text, M.Lancaster, Royal Society of Chemistry, London.
- 4. Introduction to green chemistry, M. A. Ryan and M. Tinnesand, American Chemical Society, Washington.
- 5. Real World Cases in Green Chemistry, M.C. Cann and M.E. Connelly, American Chemical Society, Washington.
- 6. Alternative Solvents for Green Chemistry, F.M. Kerton, Royal Society of Chemistry, London.
- 7. Recoverable and Recyclable Catalysis, M. Benaglia, Wiley.
- 8. Handbook of Green Chemistry and Technology, J.Clark and D. Macquarrie, Blackwell Publication.
- 9. Solid-Phase Organic Synthesis, k. Burgess, Wiley-Interscience.
- 10. Eco-Friendly synthesis of Fine Chemicals, R. Ballini, Royal Society of Chemistry, London.

CHY18R5033	Modern Methodologies in Organic Synthesis	L	T	P	C	
		5	0	0	4	

#### **COURSE OUTCOMES (COs)**

CO1	Understand the basic concepts and construction of carbon – carbon and carbon –							
	heteroatom bond formations through carbene and nitrene chemistry.							
CO2	Well versed in applying carbanion and ylid chemistry for the construction of carbon							
	– carbon and carbon – heteroatom bond formations.							
CO3	Capable of applying various mechanisms for the Catalytic C-C, C-N and C-X bond							
	formations.							
CO4	Proficient in selecting Multi-component reactions (MCR's) for the construction of							
	significant molecules.							
CO5	Skilled in applying protecting and deprotecting strategy for molecules with multi							
	reactive centres.							

## **Mapping of Course Outcomes:**

CO/PO	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8
CO1	S	S	M		M		M	
CO2	S	S		L	M		M	
CO3	S	S	M		M		M	
CO4	S	S		L	M		M	
CO5	S	S	M		M		M	

# Unit – I: C-X bond (X = C, O, N) formations through the intermediacy of Carbenes and Nitrenes:

Structure of carbenes, generation of carbenes, addition and insertion reactions of carbenes. Structure of nitrene, generation and reactions of nitrene and related electron deficient nitrogen intermediates.

## Unit – II: C-X bond (X = C, O, N) formations through the intermediacy of Carbanions and Ylids:

Organolithium, Organomagnesium, Organozinc, Organocopper reagents (restricted to 1,4-addition) in synthesis; Chemistry of Phosphorous and Sulfurylids - Wittig and related reactions, Peterson olefination.

## **Unit – III: Catalytic C-C and C-X bond formations:**

C-C Bond formation - Baylis-Hillman, Henry, Wittig, Horner-Wadsworth-Emmons, Mukaiyamaaldol, and Hosomi-Sakurai reactions, Mukaiyama Michael addition, Cadiot-Chodkiewicz, Glaser, Kumada, Ullmann, Eglinton, Sonogashira, Heck, Stille, Hiyama, McMurry, Suzuki-Miyaura, and Negishi coupling reactions; C-X bond formation - Buchwald-Hartwig amination, Chan-Lam C-X

coupling, Miyauraborylation, Tsuji-Trost, Pinner, Diels-Alder, and Ritter reactions.

## **Unit – IV: Multi-component reactions (MCR's):**

Mannich, Passerini, Biginelli, Petasis, Ugi, Pauson–Khand, and Asinger reactions, Strecker, Hantzschdihydropyridine, Radziszewski imidazole, Robinson's tropinone, and Kobayashi's pyrroloquinoxline syntheses, Palladium catalyzed synthesis of tetrahydrofuran, pyrroles, imidazolines, oxazolines, Iodine catalyzed synthesis of pyrroles, Base catalyzed synthesis of substituted benzenes, Catalyst free synthesis of azepines, Solvent free synthesis of thioamides.

## **Unit – V: Protecting groups:**

Protection and deprotection of hydroxy, carboxyl, carbonyl, carboxy amino groups and carbon-carbon multiple bonds; chemo- and regioselective protection and deprotection; illustration of protection and deprotection in synthesis.

- 1. F. A. Cary & R. I. Sundberg, Advanced Organic Chemistry, Part A & B, 5<sup>th</sup>Edn. Springer (2009).
- 2. B. P. Mundy, M. G. Ellerd, & F. G. Favaloro. Name Reactions and Reagents in Organic Synthesis, Wiley-Interscience (2005).
- 3. W. Carruthers and I. Coldham, Modern methods of Organic Synthesis, First South Asian Edition, Cambridge University Press (2005).
- 4. <u>A. Hassner & I. Namboothiri</u>. Organic Syntheses Based on Name Reactions, Elsevier (2012).
- 5. W. Carruthers, Modern Methods of Organic Synthesis, Cambridge University Press (1996).
- 6. L. Kurti& B. Czako. Strategic Applications of Named Reactions in Organic Synthesis, Elsevier (2005).
- 7. M. Beller& C. Bolm, Transition metals for organic synthesis, Wiley-VCH (2004).
- 8. J. Tsuji, Palladium Reagents and Catalysts, New Perspectives for the 21<sup>st</sup> Century, John Wiley & Sons (2003).
- 9. R. Noyori, Asymmetric Catalysis in Organic Synthesis, John Wiley & Sons (1994).
- 10. J. Zhu & H. Bienaymé, Multicomponent Reactions, Wiley-VCH (2005).

CHY18R5034	Dalymania Mataniala	L	T	P	C
CH 1 10K5U34	Polymeric Materials	5	0	0	4

CO1	Understand the chain-growth and step-growth polymerization and preparation,					
	property uses of some industrially important polymers.					
CO2	Describe the morphology, structure and physical properties of polymers.					
CO3	Determine the number, weight and viscosity average molecular weight of polymers.					
CO4	Details the chemistry and physical aspects of vulcanization.					
CO5	Illustrate the different polymer processing techniques.					

## **Mapping of Course Outcomes:**

CO/PO	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8
CO1	S	M	L				M	
CO2	S	L		M	S		M	
CO3	M	L	M	M	L		M	
CO4	S	M	L	L	M		L	
CO5	S	M	L	L	M		M	

## **Unit – I: Basic Concept and Polymeric Materials:**

Introduction - classification - polymerization: chain growth - step growth - coordination - copolymerization - ring opening metathesis polymerization (ROMP) - polymerization techniques: bulk - solution - suspension - emulsion. Thermoplastic polymers: Polyvinyl chloride - PTFE - polyacrylonitrile. Thermosetting resins: phenolic resins - epoxy resins - silicones - polyurethane, UF resin, ABS polymer.

## **Unit – II: Structure and Properties:**

Morphology and order in crystalline polymers: configurations of polymer chains - crystal structures of polymers - morphology of crystalline polymers - crystallization and melting. Polymer structure and physical properties: crystalline melting point Tm - melting point of homologous series, effect of chain flexibility and other steric factors - glass transition temperature (Tg) - Factors affecting the Tg - Relationship between Tm and Tg.

## **Unit – III: Characterization and Testing:**

Determination of molecular weight: Number, weight and viscosity average molecular weights - characterization of polymers by IR and NMR - thermal properties by TGA and DSC. Mechanical test: tensile strength - impact strength - Rockwell hardness - abrasion resistance. Test for electrical resistance: dielectric constant - arc resistance - dielectric strength.

## **Unit – IV: Elastomers Technology:**

Compounding and elastomers properties, vulcanization - chemistry of vulcanization, sulfur vulcanization, physical aspects of vulcanization. Reinforcement, types of fillers, carbon black.

## **Unit - V: Polymer Processing Techniques:**

Plastics - elastomers - fibres - calendaring - diecasting - rotational casting - film casting-compression moulding - injection moulding - blow moulding - extrusion moulding - thermoforming - fibre spinning.

- 1. Textbook of Polymer Science: F. W. Billmeyer JR. John Wiley & Sons, 3<sup>rd</sup> Ed., 1984.
- Polymer Science: V. R.Gowariker, N. V. Viswanathan and J. Sreedhar, New age International Publishers, Reprint 2013.
- 3. Encyclopedia of Polymer Science and Engineering: H.F.Mark (Ed.), Wiley-Interscience, New York, 1991.
- 4. Plastic Materials: A. Brydson, 4<sup>th</sup> Ed.,, Butterworth Heinemann Ltd., London, 2002.
- 5. Polymer Chemistry An Introduction: R.B.Seymour and C.E. Carraher, JR., Marcel Dekker Inc., 2005.
- 6. Rubber Technology: Maurice Morton, Van Nostrand Reinhold, New York, 2002.
- 7. Principles of Polymerization: G. Odian, 3<sup>rd</sup> Ed., Wiley-Interscience, 2009.
- 8. Polymer Science and Technology, Joel R. Fried, 2<sup>nd</sup> Ed., PHI Learning Private Limited, 2010.
- 9. Journal articles from current literature.

CHY18R5035	Advanced Organometallic Chemistry and Catalysis	L	T	P	C	
CH 1 10K5055	Auvanceu Organometame Chemistry and Catalysis	5	0	0	4	1

## **COURSE OUTCOMES (CO'S)**

CO1	To learn about the basic concepts of Organometallic chemistry that include the bonding pattern of transition metals.
CO2	To study the basic concepts of homogeneous and heterogeneous catalysis.
CO3	To understand various catalysts that have been used currently in the important
	industrial process such as petrochemical industries.
CO4	To obtain knowledge on the reactivity of various organometallic catalysts in the field of
	organic chemistry.
CO5	To study the basic principles and application of organometallic systems in biology
	especially to study the role of biocatalysts.

## **Mapping of Course Outcomes:**

CO/PO	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8
CO1	S	S		M	S		S	
CO2	S	S		M	S		S	
CO3	S	S		M	S		S	
CO4	S	S		M	S		S	
CO5	S	S		M	S		S	

## **UNIT I: Basic Organometallic chemistry**

Transition Metal  $\pi$ -Complexes: Transition metal  $\pi$ -complexes with unsaturated moleculesalkenes, alkynes, allyl, & dienyl(metallocene) complexes, preparation, properties and nature of bonding and structural features

## **UNIT II: Homogeneous and Heterogeneous catalysis**

Types of catalysis: homogeneous catalysis and heterogeneous catalysis: introduction, phase transfer and tri-phase catalysis, liquid – liquid and solid – liquid catalysis,

## **UNIT III: Industrial Catalysis**

Introduction to catalysis, application to industrial processes – one example each from inorganic, fine organic chemical, petroleum refining, petrochemical and biochemical industries.

## **UNIT IV: Organometallic catalysts in Organic chemistry**

Applications of Organometallic catalysts in various organic coupling reactions: Kumada coupling, Suzuki-Miyaura coupling, Hiyama coupling, Sonogashira coupling, Negeshi coupling, Stille coupling, Buchwald-Hartwig Coupling, Heck reaction, Click Reactions.

## **UNIT V: Biocatalysts (Metalloenzymes)**

General features - proximity and orientation, strain and distortion, acid base and covalent catalysis (chymotrypsin, lysozyme). Metal activated enzymes and metalloenzymes: carboxypeptidase, carbonic anhydrase, superoxide dimutase, xanthine oxidase, peroxidase, catalase.

- Basic Organometallic Chemistry: Concepts, Syntheses and Applications, B.D. Gupta, Anil J. Elias, Universities Press (2013)
- 2. Organometallics, ChristophElschenbroich, Wiley-VCH (2006)
- 3. March's Advanced Organic Chemistry: Reactions, Mechanisms and structures J., March, and M. B. Smith, John Wiley (2007) 6th ed.
- 4. Heterogeneous Catalysis in Industrial Practices, N. Satterfield Charles, McGraw-Hill International Editions, 2nd Edition 1993.
- 5. Organotransition Metal Chemistry: From Bonding to Catalysis, John Hartwig, University Science Books (2010)
- Concepts and Models of Inorganic Chemistry, B. Douglas, D. McDaniel and J. Alexander, 3rd Ed., Wiley (1994).
- 7. Bioinorganic chemistry: Inorganic Elements in the Chemistry of Life, W. Kaim and B. Schwederski, Wiley (2006).
- 8. Priniciples of Bioinorganic Chemistry. S. J. Lippard and J.M. Berg.

DIT1QD/001	Biology for Chemists	L	T	P	C
BIT18R4001	protogy for enemists	5	0	0	4

## **COURSE OUTCOMES (CO'S)**

CO <sub>1</sub>	To learn about the basic concepts of various cell types and their structural aspects.						
CO2	To study about structural variations of carbohydrates and their function in cells.						
CO3	To understand various lipid types located in cell membrane and their role in						
	safeguarding the cells from external environment.						
CO4	To obtain knowledge on the various types of proteins and enzymes and their specific						
	role in running the cell mechanism						
CO5	To study the basic principles and application nucleic acid parts and preservation of their						
	genetic code during the cell cycle.						

## **Mapping of Course Outcomes:**

CO/PO	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8
CO1	S		M	S	M		M	
CO2	S		M	S	M		M	
CO3	S		M	S	M		M	
CO4	S		M	S	M		M	
CO5	S		M	S	M		M	

#### **UNIT I: Cell Structure and Functions**

Structure of prokaryotic and eukaryotic cells, intracellular organelles and their functions,

comparison of plant and animal cells. Overview of metabolic processes - catabolism and anabolism. ATP - the biological energy currency.

## **UNIT II: Structure and functions of Carbohydrates**

Conformation of monosaccharides, structure and functions of important derivatives of monosaccharides like glycosides, deoxy sugars, myoinositol, amino sugars. N acetylmuramic acid, sialic acid, disaccharides and polysaccharides. Structural polysaccharides - cellulose and chitin. Storage polysaccharides - starch and glycogen. Structure and biological functions of glycosaminoglycans. Carbohydrates of glycoproteins and glycolipids. Role of sugars in biological recognition. Blood group substances. Ascorbic acid. Carbohydrate metabolism - glycogenesis and glycogenolysis and pentose phosphate pathway.

## **UNIT III: Cell membrane Lipids**

Fatty acids, essential fatty acids, structure and function of triacylglycerols, glycerophospholipids, sphingolipids, cholesterol, bile acids, prostaglandins. Lipoproteins-

composition and function. Properties of lipid aggregates-micelles, bilayers, liposomes and their possible biological functions. Biological membranes. Fluid mosaic model of membrane structure. Lipid metabolism - -oxidation of fatty acids.

#### **UNIT IV: Proteins and Enzymes**

Chemical and enzymatic hydrolysis of proteins to peptides, Secondary structure of proteins, forces responsible for holding of secondary structures. -helix, -sheets, super secondary structure, triple helix structure of collagen. Tertiary structure of protein-folding and domain structure. Quaternary structure.

## **UNIT V: Nucleic Acids and Genetic Code**

Structure of nucleotides, nucleosides, DNA (Watson-Crick model) DNA structure and conformation, Replication of DNA, transcription, translation of genetic material, genetic code, universality of the code, codon, anticodon pairing, RNA, protein biosynthesis

- 1. A. L. Lehninger, Principles of Biochemistry, Worth Publishers Inc., U.S.; 3rd edition edition (2000).
- 2. Berg JM, Tymoczko JL, Stryer L., Biochemistry, W H Freeman 5<sup>th</sup> edition New York (2002).
- 3. J. David Rawn, Biochemistry, Neil Patterson publishers (1989)
- 4. Donald Voet, Judith G. Voet, Biochemistry, Wiley (2004).
- 5. E. E.Conn and P. K. Stump, Outlines of Biochemistry, John Wiley and sons, 5<sup>th</sup> edition (2009).

## LIST OF ONLINE COURSES RECOMMENDED (not limited in the given list)

Sl. No.	Name of the Course	Offered by
1.	Organometallic Chemistry	IIT Bombay
2.	Thermodyanamics and Kinetics	IISER, Mohali
3.	Biochemistry	IIT Kharagpur
4.	Organic Chemistry III (Reaction Mechanisms 2)	MHRD and AICTE
		(SWAYAM)
5.	Application of Spectroscopic Methods in Molecular	MHRD and AICTE
	Structure Determination	(SWAYAM)
6.	Forensic Chemistry and Explosives	MHRD and AICTE
		(SWAYAM)