M.Sc. Chemistry

(Revised Framework- 2024-25 Batch onwards)

Syllabus

Learning Outcomes-Based Curriculum Framework

CENTRAL UNIVERSITY OF KARNATAKA

Department of Chemistry

School of Chemical Sciences

Central University of Karnataka

Department of Chemistry
School of Chemical Sciences
Central University of Karnataka, Kalaburagi

VISION

To be one of the well-recognized Departments of Chemistry for higher learning in India and the world in terms of producing skilled and employable chemists, researchers, teachers and entrepreneurs who are go-getters in meeting the challenges in chemistry and society.

MISSION

MS1: To impart quality education at postgraduate and doctoral levels through the well-designed curriculum to meet the demands of academia, research laboratories and industry.

MS2: To provide the state-of-art research facilities to carry out pioneering research in the cutting-edge areas of Chemistry.

MS3: To become a hub for human resource development and sponsored research projects with funding from national and global agencies.

MS4: To associate with national and international reputed institutions for academic excellence and collaborative research.

M.Sc. Chemistry

Department of Chemistry
School of Chemical Sciences
Central University of Karnataka, Kalaburagi

Name of the Academic Program: M.Sc in Chemistry

Qualification Descriptors (QDs)

After completion of this academic program, the students will be able to

QD-1: Demonstrate comprehensive knowledge and skills in Organic, Inorganic, Physical, analytical and Materials Chemistry and other modern areas of Chemistry.

QD-2: Employ advanced tools, techniques, and methodologies to achieve the evidence-based solutions for local and global problems related to Chemistry

QD-3: Apply disciplinary knowledge and transferable skills in the interdisciplinary areas of chemistry to solve problems with well-defined solutions.

QD-4: Develop benchmark standards in writing, communications, team-work, and ethics to disseminate results of studies undertaken in Chemistry.

QD-5: Prepare for self-learning and lifelong-learning to meet one's learning needs using research and development work and professional materials.

QD-6: Demonstrate knowledge and transferable skills in cutting-edge-areas of chemistry that empower them for employment opportunities in academia, research laboratories, chemical and allied industries.

Mapping Qualification Descriptors (QDs) with Mission Statements (MS)

	MS-1	MS-2	MS-3	MS-4
QD-1	3	3	1	1
QD-2	1	3	3	3
QD-3	2	3	1	2
QD-4	2	3	3	1
QD-5	3	3	3	2
QD-6	2	3	3	1

(Note: 3- indicates High-level; 2- Medium-level; and 1 for 'Low-level' mapping)

Name of the Academic Program: M.Sc in Chemistry

Program Learning Outcomes (PLOs)

After the completion of the M.Sc. Chemistry program, the student will be able to:

PLO-1: Demonstrate comprehensive knowledge and skills in different areas of Chemistry, viz; Organic, Inorganic, Physical, Analytical and Materials Chemistry

PLO-2: Apply knowledge and experimental skills to synthesize and analyze chemicals/ materials of immediate need for the society and relevance to chemical and allied industries

PLO-3: Develop eco-friendly protocols/procedures for chemical processes in the industry.

PLO-4: Critically evaluate practices, rules, and theories based on empirical evidence, by following the scientific approach to knowledge development in Chemistry.

PLO-5: Demonstrate effective communication skills both orally and in writing using appropriate media in all the aspects related to Chemistry and one's profession

PLO-6: Demonstrate a sense of inquiry and ability to define problems; use research methods, analyze, interpret and draw conclusions from data; plan, execute and report the results of an experiment or investigation in intra/interdisciplinary areas of chemistry.

PLO-7: Apply the knowledge of chemistry associated with critical thinking to achieve sustainable solutions for energy and environment and other problems in day-today life.

PLO-8: Demonstrate ability to work effectively with diverse teams, facilitate cooperative effort as a member or leader of a team to achieve the deliverables of any project

PLO-9: Demonstrate the capability to use computational tools, software, and databases relevant to different fields of Chemistry

PLO-10: Demonstrate the ability to identify ethical issues related to one's work, avoid unethical behaviour such as committing plagiarism, not adhering to intellectual property rights and adopt objective and truthful actions in all aspects of work.

PLO-11: Demonstrate knowledge of the values of multiple cultures and a global perspective effectively engage in a multicultural society for employment or further studies

PLO-12: Demonstrate the ability of self-learning and lifelong-learning using ICT and Open Education Resources

Mapping of Program Learning Outcomes (PLOs) with Qualification Descriptors (QDs)

	QD-1	QD-2	QD-3	QD-4	QD-5	QD-6
PLO-1	3	3	2	2	2	3
PLO-2	3	2	3	1	3	3
PLO-3	3	2	3	3	1	3
PLO-4	3	3	2	1	3	1
PLO-5	1	2	1	3	2	3
PLO-6	3	3	2	2	2	3
PLO-7	3	3	3	1	3	3
PLO-8	2	1	3	2	1	3
PLO-9	3	3	3	3	3	2
PLO-10	1	3	3	3	2	3
PLO-11	1	2	2	1	3	3
PLO-12	2	3	2	3	2	1

M.Sc. Chemistry_ Course Structure
Department of Chemistry
Central University of Karnataka, Kalaburagi

Semester-I — No. of credits = 20

Code	Type	Title	Credits	Hours	L	T	P
PCHTC11400	Core -1	Inorganic Chemistry – I	4	4	3	1	0
PCHTC11401	Core-2	Organic Chemistry – I	4	4	3	1	0
PCHTC11402	Core-3	Physical Chemistry – I	4	4	3	1	0
PCHTC11403	Core-4	Introduction to Analytical Chemistry	2	2	2	0	0
PCHTC11404	Core-5	Mathematics for Chemistry	2	2	1	1	0
PCHPC11400	Core-6	Organic Chemistry Laboratory	2	4	0	0	4
PCHPC11401	Core-7	Analytical & Computational Chemistry Laboratory	2	4	0	0	4
Total			**20**	24	12	4	8

(L=Lecture; T=Tutorial; P=Practical)

Semester-II — No. of credits = 20

Code	Type	Title	Credits	Hours	L	T	P
PCHTC21500	Core-8	Inorganic Chemistry – II	4	4	3	1	0
PCHTC21501	Core-9	Organic Chemistry – II	4	4	3	1	0
PCHTC21502	Core-10	Physical Chemistry – II	4	4	3	1	0
PCHTC21503	Core-11	Chemistry of Life	2	2	2	0	0
PCHTC21504	Core-12	Chemical applications of Group Theory	2	2	1	1	0
PCHPC21500	Core-13	Inorganic Chemistry Laboratory	2	4	0	0	4
PCHPC21501	Core-14	Physical Chemistry Laboratory	2	4	0	0	4
Total			**20**	24	13	5	8

(L=Lecture; T=Tutorial; P=Practical)

Semester-III — No. of credits = 20

Code	Type	Title	Credits	Hours	L	T	P
PCHTC31505	Core-15	Molecular Spectroscopy	4	4	3	1	0
PCHTC31506	Core-16	Organic Spectroscopy	3	3	2	1	0
PCHTC31507	Core-17	Organometallic Chemistry	4	4	3	1	0
PCHTC31508	Core-18	Organic Chemistry-III	4	4	3	1	0
PCHTD31500	Generic Elective Course-01	MOOC Course (NPTEL; SWAYAM) / Other Department Elective	3	3	2	1	0
PCHWS31500	Skill Enhancement Course-01	Literature Survey and Seminar	2	4	0	0	4
Total			**20**	**22**	**13**	**5**	**4**

(L=Lecture; T=Tutorial; P=Practical)

Semester-IV — No. of credits = 20

Code	Type	Title	Credits	Hours	L	T	P
PCHRC41500	Research Project/ Dissertation - 01	Research training & Project report	20	40	0	2	38
Total			**20**	**40**	**0**	**2**	**38**

(L=Lecture; T=Tutorial; P=Practical)

Semester-wise distribution of courses

Semester	I	II	III	IV	Total
Core Course	20	20	15	00	**55**
Skill Enhancement Course			02		**02**
Research (Project / Dissertation)				20	**20**
Generic Elective Course			03		**03**
Total	**20**	**20**	**20**	**20**	**80**

Total No. of Credits = 80

M.Sc. Chemistry
Course Content/Syllabus
Central University of Karnataka, Kalaburagi

Semester-I

PCHTC11400: Inorganic Chemistry-I **Credit 4**

Code	Type	Title	Credits	Hours	L	T	P
PCHTC11400	Core -1	Inorganic Chemistry – I	4	4	3	1	0

Prerequisite Course/Knowledge (If any): **Fundamentals of Inorganic Chemistry**

Course Learning Outcomes (CLOs)

After completion of this course successfully, the students will be able to……

CLO-1: Categorize inorganic solids into different classes based on its structure, chemical property, and applications.
CLO-2: Understand the structure, bonding, and properties of electron-deficient clusters and cages of boron, silicon, and phosphorus and Sulphur compounds.
CLO-3: Apply the knowledge of radioactivity and nuclear reactions into various applications such as radio-dating, reaction mechanisms, and nuclear energy.
CLO-4: Apply basic concepts into other branches of chemistry and other allied subjects.
CLO-5: Understand the fundamentals and applications of supramolecular chemistry.

Mapping of Course learning outcomes (CLOs) with Program learning outcomes (PLOs)

	PLO 1	PLO 2	PLO 3	PLO 4	PLO 5	PLO 6	PLO 7	PLO 8	PLO 9	PLO 10	PLO 11	PLO 12
CLO-1	3	1	1	3	1	2	2	1	2	--	--	3
CLO-2	2	2	1	3	1	1	3	1	3	1	--	2
CLO-3	3	2	1	3	1	1	3	1	3	2	--	2
CLO-4	3	2	3	3	3	3	2	2	3	--	1	3
CLO-5	3	1	3	3	1	1	3	3	1	3	1	1

Detailed Syllabus:

UNIT I-Inorganic Solids: Types of forces-cohesive energy, van der Waals forces, hydrogen bonding. Types of solids, covalent, ionic, molecular and metallic solids. Unit cell, density and crystal lattice structures of ionic crystals AX, AX_2, ABX_3, AB_2X_4 and layered structures. Defects in ionic solids and associated theories. Band theory, semiconductors and its type & superconductors. **(16 Hrs)**

UNIT II-Main group chemistry:

Structure, bonding and reactivity of polyhedral boranes and carboranes, styx notation; Wade's rules; electron count in polyhedral boranes; synthesis of polyhedral boranes; Carboranes, Metallaboranes, Metalla Carboranes, m+n+o+p rules, isolobal analogy; Synthesis, structural features and reactivity of reactivity of B-N, P-N and S-N heterocycles; Synthesis and properties- Intercalation compounds of graphite, C 60 and its compounds (Fullerenes) - carbon nanotubes, Silicate Minerals, Layered and Framework Silicates, Zeolites, Di, tri, tetra and hexa nuclear Metal clusters, Polyatomic Zintl anions and cations. **(20 Hrs)**

Unit-III: Nuclear chemistry

Nucleus and its classification, stability of nucleus, magic numbers, binding energy, units of radioactivity, types of radioactive decay, kinetics of decay, carbon dating. Nuclear fission: the process, fragments, mass distribution, and fission energy. Liquid drop and shell model of nucleus. Generation of radioisotopes and measurement of radioactivity using Geiger-Muller and Scintillation detectors, Classification of nuclear reactors and nuclear power generation in India. Application of radioisotopes in chemical reactions and medicine. Nuclear disaster and its management, disposal of nuclear waste. **(16 Hrs)**

UNIT IV- Supramolecular chemistry: Supramolecular chemistry, definition, host-guest interaction, cation, anion & neutral molecule binding hosts, crown ethers, calixarenes, application of supramolecular chemistry; supramolecular chemistry in biology **(12 Hrs)**

Reference books:

1. C. E. Housecroft, A. G. Sharpe, *Inorganic Chemistry*, 4th Edn, Pearson, 2012.
2. J. E. Huheey, *Inorganic Chemistry, Principles, Structure and Reactivity*, Harper and Row, 3rd Edn, 1983.
3. N. N. Greenwood, A. Earnshaw, *Chemistry of the Elements*, 2nd Edn., Pergamon Press, 1989.
4. G. Wulfsberg, *Inorganic chemistry*, 1st Edn, Viva books Pvt Ltd. 2002.
5. M. Weller, T. Overton, J. Rourke, F. Armstrong, Inorganic Chemistry, 7th Edn, Oxford University Press India, 2018.
6. F. A. Cotton and G. Wilkinson, *Advanced Inorganic Chemistry- A comprehensive Text*, John Wiley, 5th Edn, 1987.
7. A. R. West, *Solid state Chemistry and its Applications*, 2nd Edn, Wiley, 2007.
8. C. Kettel, *Introduction to Solid state Physics*, 8th Edn, Wiley, 2012.
9. H. J. Arnikar, *Essentials of nuclear chemistry*, New Age International Publisher, 4th Edn, 2018.
10. G. Friedlander, J. W. Kennedy, E. S. Macias, J. M. Miller, *Nuclear and Radiochemistry*, 3rd Edn, 1981.
11. Shriver and Atkins, Inorganic Chemistry by Atkins, Overton, Rourke, Weller, and Armstrong, Fifth Edition. South Asia Edition (paperback), Oxford University Press, 2010.
12. J. D. Lee, *Concise Inorganic Chemistry*, 5th Edition, Wiley India Pvt Ltd, 2022.
13. J. W. Steed, J. L. Atwood, Supramolecular Chemistry, 2nd Edition, Wiley India Pvt Ltd, 2013.
14. Jean-Marie Lehn, Supramolecular Chemistry : Concepts and Perspectives, Wiley & Sons, 1995.

PCHTC11401: Organic Chemistry-I Credit- 4

Code	Type	Title	Credits	Hours	L	T	P
PCHTC11401	Core-2	Organic Chemistry – I	4	4	3	1	0

Prerequisite Course/Knowledge (If any): **Fundamentals of Organic Chemistry**

Course Learning Outcomes (CLOs)

After completion of this course successfully, the students will be able to……

CLO-1: Analyze the role of reactive intermediates such as carbocations, carbanions, non-classical carbocation in chemical reactions.
CLO-2: Demonstrate the chirality in organic molecules using chiral units such as center, axial, planar, and helicity.
CLO-3: Analyze influence of conformations in cyclic systems on structures and functions of organic molecules.
CLO-4: Illustrate the reaction mechanism aspects in the context of addition, elimination and substitution reactions.
CLO-5: Assess the structural effects of organic molecules and functional groups on the tendency to participate in various oxidation and reduction reactions.

Mapping of Course learning outcomes (CLOs) with Program learning outcomes (PLOs)

	PLO 1	PLO 2	PLO 3	PLO 4	PLO 5	PLO 6	PLO 7	PLO 8	PLO 9	PLO 10	PLO 11	PLO 12
CLO-1	2	3	3	2	1	2	1	1	1	2	2	3
CLO-2	3	2	1	3	1	3	1	2	3	2	---	3
CLO-3	2	3	3	3	2	3	---	---	3	---	2	2
CLO-4	3	3	3	3	2	2	1	---	2	3	2	3
CLO-5	2	3	2	3	2	2	1	---	3	2	3	2

Detailed Syllabus:

UNIT-I: Aromaticity, Reaction mechanism and intermediates: Criteria of Aromatic, benzenoid & non benzenoid compounds, antiaromatic & homoaromatic compounds; Effect of structure on reactivity: conjugation, resonance, inductive effect, mesomeric effects, hyperconjugation, tautomerism, hybridization and steric effect. Methods of determining reaction mechanisms- kinetic and non-kinetic isotope effects, and reaction profile diagram, Hammet and Taft equations. Intermediates in reaction**:** Generation, structure stability and formation of carbocation, carbanion, non-classical carbocations, free radicals, carbenes and nitrenes. **(14 Hrs)**

UNIT-II: Stereochemistry: Elements of symmetry, chirality, Projection formulae and interconversion, enantiomers, diasteroisomers, geometrical isomerism. Chirality involving atoms other than carbon. Optical activity in the absence of chiral centre: Axial and planar chirality and helicity. Configurational notations of simple molecules, D, L and R, S configurational notations, and E/Z notation. Racemic mixture and their resolution. Topicity: Enantiotopic and diastereotopic atoms, ligands and faces. Conformational analysis of cyclic compounds: cyclohexane, mono-substituted cyclohexanes; disubstituted cyclohexanes. Decalins. Principles of asymmetric synthesis, Enantioselectivity and diastereoselectivity. Stereospecific and stereoselective reactions. Chiral auxiliaries **(18 Hrs)**

UNIT-III: Substitution reactions: The evidence for S_N2, S_N1 reaction, S_Ni reaction, Neighbouring group participation, S_NAr, benzyne and S_N1 mechanism Arenium ion mechanism, ipso attack, orientation in other ring systems, nucleophilic substitution, Benzyne Mechanism; Baldwin Rules for ring closure on saturated and unsaturated carbons. **Elimination and addition reactions:** The E2, E1 and E1cB mechanisms, Hoffman and Saytzeff modes of elimination, orientation of the double bond, reactivity effects of substrate structures, attacking base, the leaving group and the medium, pyrolytic elimination; Mechanistic and stereochemical aspects of addition reactions involving electrophiles, nucleophiles, regio- and chemo selectivity orientation and reactivity; Reactivity of carbonyl group, nucleophilic addition of hetero-atoms (N, O), conjugate addition reactions. **(16 Hrs)**

Unit-IV: Oxidations and reductions in organic synthesis: Mechanism, selectivity, stereochemistry and applications of selenium dioxide, Cr and Mn reagents, periodic acid, Osmium tetroxide, Swern oxidations, Baeyer-Villiger oxidation, ozonolysis, epoxidations using peracids. Mechanism, selectivity, stereochemistry and applications of catalytic hydrogenations using Pd, Pt and Ni catalysts, Wolff-Kishner reduction, dissolving metal reductions, metal hydride reductions using $NaBH_4$, $LiAlH_4$, DIBAL, K-selectride, Sodium cyanoborohydride. Sharpless epoxidation, symmetric dihydroxylation, Asymmetric reductions of prochiral carbonyl compounds and olefins. **(16 Hrs)**

Reference books:

1. Carey B. F. A., Sundberg R.J., (2007). *Advanced Organic Chemistry Part A and Part B, Springer, 5th edition*.
2. Kalsi, P.S., (2010). *Stereochemistry: Conformation and Mechanism*, New Age International (p) Ltd. New Delhi.
3. Morrison, R.T., Boyd, R.N. (2011). *Organic Chemistry*, Prentice- Hall of India, 6th edition, New Delhi.
4. Smith, M. B., March J., (Latest Ed.). *March's Advanced Organic Chemistry*, John Wiley and Sons, 6th edition, New York.
5. Sykes, P., (1997). *A Guide Book to Mechanism in Organic Chemistry*, Prentice Hall, 6th edition.
6. Eliel, E. L.; Wilen, S. H. (2008). *Stereochemistry of carbon compounds*. Wiley, Student edition.
7. Clayden, J.; Greeves, N.; Warren, S., (2012). *Organic Chemistry*, Oxford University press, 2nd edition.
8. Bruice Paula, Y., (2015). *Organic Chemistry*, 7th Edition, Pearson Edition.
9. Nasipuri, D. (Latest edition). *Stereochemistry of Organic Compounds: Principles & Applications*, New Age International Publishers.

PCHTC11402: Physical Chemistry-I Credit - 4

Code	Type	Title	Credits	Hours	L	T	P
PCHTC11402	Core-3	Physical Chemistry – I	4	4	3	1	0

Prerequisite Course/Knowledge (If any): **Fundamentals of Physical Chemistry**

Course Learning Outcomes (CLOs)

After completion of this course successfully, the students will be able to……

CLO-1: Understand the fundamentals of chemical and statistical thermodynamics.
CLO-2: Develop problem-solving ability in quantum chemistry and thermodynamics.
CLO-3: Recognize the role of multidisciplinary streams especially physics & maths knowledge in the development of quantum chemistry & thermodynamics.
CLO-4: Apply the fundamental knowledge in quantum chemistry & thermodynamics to an existing and emerging problems in basic science.
CLO-5: Demonstrate the ability to do some independent calculation and use some computational resources at the end of the course.

Mapping of Course learning outcomes (CLOs) with Program learning outcomes (PLOs)

	PLO 1	PLO 2	PLO 3	PLO 4	PLO 5	PLO 6	PLO 7	PLO 8	PLO 9	PLO 10	PLO 11	PLO 12
CLO-1	3	3	1	3	1	3	3	2	3	3	1	2
CLO-2	3	3	1	3	1	3	2	1	3	3	1	2
CLO-3	3	2	1	3	1	3	2	1	3	3	1	2
CLO-4	3	2	2	3	1	3	3	2	3	3	1	2
CLO-5	3	3	1	2	1	2	2	1	3	3	1	2

Detailed Syllabus:

UNIT I-Equilibrium Thermodynamics: Concept of work and heat, review of laws of thermodynamics, enthalpy and heat capacities- concept of entropy, -residual entropy. Free energy, chemical potential, fugacity, liquids and solutions: Partial molar quantities and its significance, ideal and non-ideal solutions, activity and activity coefficients, chemical equilibrium. **(16 Hrs)**

UNIT II-Statistical Thermodynamics: BE, FD, MB statistics and distribution, partition functions and molecular partition functions, concept of ensembles, thermodynamic properties from partition function, mean energy, Residual entropy, heat capacity of mono and diatomic gases, chemical equilibrium, Einstein and Debye theories of heat capacity of solids. Non-equilibrium thermodynamics, Postulates and methodologies, linear laws, Gibbs equation, Onsager reciprocal theory. **(16 Hrs)**

UNIT III-Quantum Chemistry I: Introduction, limitation of classical mechanics and origin of quantum theory, Lagrange & Hamiltonian equation, need for quantum mechanics, postulates,

operators & operator algebra, Linear, Hermitian and non-Hermitian operators, Commuting and non-commuting operators, eigen values, eigen vectors & commutation relation, orthogonality, The Schrodinger equation, Discussion of Solution of Schrodinger equation to few model system e. g particles in 1D, 2D & 3D box, harmonic oscillator, rigid rotor, hydrogen atom etc. **(16 Hrs)**

UNIT IV-Quantum Chemistry II: Approximation methods, viz variation method, perturbation method, Application of variation method and perturbation theory to the Helium atom, Electron spin & Zeeman effect, spin-orbit coupling, introduction to the methods of self-consistent field, the virial theorem. Hartree and Hartree-Fock self-consistent field model, Electronic configuration of atoms, addition of angular momenta, spectroscopic term symbols, spin-orbit coupling, selection rules for atomic spectra, Electronic configuration of atoms, addition of angular momenta, spectroscopic term symbols, selection rules for atomic spectra. Hückel molecular orbital theory and its application for small molecules. **(16 Hrs)**

Reference books:

1. P. W. Atkins, Physical Chemistry, 9thEdtion Oxford University Press, 2010.
2. L.A. Woodward, Molecular Statistics, Oxford University Press.
3. Y. V.C. Rao, An Introduction to Thermodynamics, Wiley Eastern, 1993.
4. R.S.Berry, S.A.Rice and J.Ross, Physical Chemistry, Oxford, 2001.
5. M. Ladd, Introduction to Physical Chemistry, Cambridge, 1998.
6. J. Rajaram & J.C. Kuriacose, Chemical Thermodynamics: Classical, Statistical and Irreversible. Pearson, 2013
7. D. A. McQuarrie and J. D. Simon Physical Chemistry, A molecular Approach, Viva, 1998.
8. F. W. Sears & G. L. Salinger, Thermodynamics, Kinetic Theory & Statistical Thermodynamics, Narosa, 1986.
9. D. A. McQuairrie: Quantum Chemistry, Oxford University press, Oxford, 1982.
10. Ira N. Levine, Quantum Chemistry 7th Ed, Pearson Education India, 2016.
11. A.K.Chandra, Introductory Quantum Chemistry, 4th Ed, McGraw Hill Education, 2017.
12. Donald A McQuarrie, Statistical Mechanics, Viva Books, 2018
13. David Chandler, Introduction to Modern Statistical Mechanics, OUP USA, 1987.
14. P. W. Atkins, R. Friedman., *Molecular Quantum Mechanics*, 5th Edition, 2010

PCHTC11403: Introduction to Analytical Chemistry Credit -2

Code	Type	Title	Credits	Hours	L	T	P
PCHTC11403	Core-4	Introduction to Analytical Chemistry	2	2	2	0	0

Prerequisite Course/Knowledge (If any): **Fundamentals of Analytical Chemistry**

Course Learning Outcomes (CLOs)

After completion of this course successfully, the students will be able to……

CLO-1: Develop knowledge on working principles of various analytical techniques available for chemical analysis in laboratories.
CLO-2: Summarize the advantages and disadvantages of different calorimetry techniques.
CLO-3: Analyze experimental data using various mathematical and statistical models.
CLO-4: Recognize suitable titration method for quantitative analysis of ions/chemicals
CLO-5: Design a suitable method for separation and analysis of chemicals by chromatography.

Mapping of Course learning outcomes (CLOs) with Program learning outcomes (PLOs)

	PLO 1	**PLO 2**	**PLO 3**	**PLO 4**	**PLO 5**	**PLO 6**	**PLO 7**	**PLO 8**	**PLO 9**	**PLO 10**	**PLO 11**	**PLO 12**
CLO-1	3	2	1	3	1	3	2	1	2	1	2	2
CLO-2	3	3	1	1	2	2	2	2	1	2	2	1
CLO-3	1	3	1	3	3	3	1	1	3	3	3	2
CLO-4	3	3	3	1	3	2	2	2	1	3	3	1
CLO-5	3	3	3	2	2	3	1	1	3	2	3	2

Detailed Syllabus:

UNIT I: Errors analysis: Accuracy and precision, absolute, relative, determinate and indeterminate errors, statistical treatment of random errors, computation rules for significant figures, method of least squares, mean deviations, and standard deviation, The Confidence Limit, test of significance, statistics for small data sets, linear least square method, detection limits, use of spreadsheets/softwares in analytical chemistry. **(10 Hrs)**

UNIT II: Electro- and thermoanalytical Methods: Introduction to gravimetric analysis, Thermogravimetry (TGA), Differential Thermal Analysis (DTA), and Differential Scanning Calorimetry (DSC): definition, theoretical basis, instrumentation, factors affecting the data curve, applications, advantages and disadvantages, Bulk Electrolysis, Electrogravimetry and Coulometry. **(12Hrs)**

UNIT-III: Separation Techniques & other analytical methods: Solvent extraction, distribution coefficient, extraction of metals, thin-layer chromatography (TLC), gas chromatography (GC), liquid chromatography (LC), high performance liquid chromatography (HPLC), ion exchange chromatography, gel permeation chromatography. Chromatography coupled instrumentation. Miscellaneous separation techniques. **(10 Hrs)**

Reference books:

1. Douglas A. Skoog, Donald M. West, F. James Holler and Stanley R. Crouch, (2013). *Fundamentals of Analytical Chemistry*, 9th Edition, Cengage Learning.
2. James W. Robinson, Eileen M. Skelly Frame, George M. Frame II, (2005). *Undergraduate Instrumental Analysis*, Sixth Edition, Marcel Dekker, New York.
3. Donald L. Pavia, Gary M. Lampman, George S. Kriz, James R. Vyvyan, (2009). *Introduction to Spectroscopy*, Fourth Edition, Brooks/Cole Thomson Learning.
4. Gary D. Christian, Purnendu Das gupta, Kevin Schug, (2013). *Analytical Chemistry*, 7th Edition, Wiley.

5. P.M.S. Monk "Fundamentals of Electroanalytical Chemistry" J. Wiley & Sons, New York, 2002.
6. Skoog, D.A., West, D.M., Holler, F.J., and Crouch, S.R., Fundamentals of Analytical Chemistry, Brooks/Cole (2003) 8th ed.

PCHTC11404: Mathematics for chemistry Credit -2

Code	Type	Title	Credits	Hours	L	T	P
PCHTC11404	Core-5	Mathematics for chemistry	2	2	2	0	0

Prerequisite Course/Knowledge (If any): **Fundamentals of Mathematics**

Course Learning Outcomes (CLOs)

After completion of this course successfully, the students will be able to……

CLO-1: understand basic and different areas of mathematics.
CLO-2: nurture a mathematical aptitude, thinking, and inculcate skills to solve problems.
CLO-3: inculcate mathematical reasoning and enable them to understand the mathematical models in chemistry.
CLO-4: prepare the students to apply the mathematics knowledge in learning and understanding other courses in physical and inorganic chemistry better, especially like quantum chemistry and molecular spectroscopy etc.
CLO-5: learn the basics of group theory and its application in chemistry. This knowledge may equip them to learn other courses in M.Sc. Chemistry like spectroscopy and coordination chemistry etc.

Mapping of Course learning outcomes (CLOs) with Program learning outcomes (PLOs)

	PLO 1	PLO 2	PLO 3	PLO 4	PLO 5	PLO 6	PLO 7	PLO 8	PLO 9	PLO 10	PLO 11	PLO 12
CLO-1	2	2	1	1	1	2	2	1	2	1	2	2
CLO-2	2	3	1	1	2	2	2	2	1	2	2	1
CLO-3	1	3	1	3	3	3	1	1	3	3	1	2
CLO-4	3	3	3	1	3	2	2	2	1	3	3	1
CLO-5	3	3	3	2	2	3	1	1	3	2	1	2

Detailed Syllabus:

UNIT-I: Numbers: Real and Complex number algebra. Vector algebra. Functions & Variables: Differential calculus-first- and higher-order derivatives, evaluation of minimum and maximum, limits & continuity. Partial differentiations. Exact and inexact differentials. Numerical differentiation. The

gamma and delta functions. Integral Calculus: Indefinite and definite integrals, improper integrals. Methods of integration. Surface and volume integrals. Numerical integrations.

UNIT-II: Differential Equations: Ordinary first- and second-order differential equations. Partial differential equations. Solution of inexact differential equations by the method of integrating factors. Power series and extended power series solutions. Numerical solutions. Special functions: Hermite, Legendre and Laguerre polynomials, recursion relations. Matrices and Determinants. Eigen values and eigen vectors. Orthogonal transformation. Rank & inverse and direct product of matrix.

Reference books:

1. Mathematics for Physical Chemistry. R. G. Mortimer, Academic Press.
2. Advanced Engineering Mathematics. E. Kreyszig, Wiley.
3. Mathematics for Chemistry and Physics. G. Turrell, Academic Press.
4. Numerical Analysis: A Practical Approach. Melvin J. Maron, Macmillan Publishing Co., Inc. NY & Collier Macmillan Publishers, London.

PCHPC11400: Organic Chemistry Laboratory Credit -2

Code	Type	Title	Credits	Hours	L	T	P
PCHPC11400	Core-6	Organic Chemistry Laboratory	2	4	0	0	4

Prerequisite Course/Knowledge (If any): **B.Sc. Chemistry laboratory**

Course Learning Outcomes (CLOs)

After completion of this course successfully, the students will be able to……

CLO-1: Demonstrate purification of organic liquids using Fractional & Vacuum distillations.
CLO-2: Separate the organic solids and their qualitative analysis and identification of functional groups.
CLO-3: Synthesize the biologically important molecules having carbonyl functionality.
CLO-4: Verify the purity of organic compounds by employing a thin layer chromatography
CLO-5: Apply photo-chemical reaction conditions in organic synthesis.

Mapping of Course learning outcomes (CLOs) with Program learning outcomes (PLOs)

	PLO 1	PLO 2	PLO 3	PLO 4	PLO 5	PLO 6	PLO 7	PLO 8	PLO 9	PLO 10	PLO 11	PLO 12
CLO-1	3	3	1	3	1	2	1	1	-	-	-	1

CLO-2	3	3	1	3	1	2	1	1	1	1	1	2
CLO-3	3	3	3	2	1	3	3	2	1	1	-	1
CLO-4	3	3	1	3	1	3	1	1	1	-	-	1
CLO-5	3	3	3	2	1	2	3	1	1	-	-	1

Detailed Syllabus:

S.No	Practical
1	MSDS role in Chemistry Laboratory-One example of chemical handling using MSDS.
2	To prepare dibenzylideneacetone by Claisen-Schmidt condensation
3	To synthesize aspirin from salicylic acid and conformation of it by TLC with commercial drug Ecosprin and melting point comparison
4	Synthesis of Oil of wintergreen by transesterification/ Fischer esterification process.
5	Identify the R_f value of above synthesized compounds by TLC experiment & demonstration of recrystallization process
6	Synthesis of an Azo dye.
7	Synthesis of a Chalcones *via* grinding method-Green Chemistry protocol
8	Separation of above compounds using Column Chromatography and Medium Pressure Liquid Chromatography (MPLC)
9	Photoreduction of benzophenone to benzopinacol.
10	Preparation of benzopinacolone from benzopinacol.
11	To understand the concept of mutarotation in the given carbohydrate material.
12	To calculate the enantiomeric excess of one of the pure enantiomers in a mixture solution.
13	To prepare *p*-bromoacetanalide by green approach.
14 & 15	Separation and Qualitative analysis of an organic mixture containing two components. Minimum two experiments
16	A two-stage synthesis of Organic molecule (Flavanone or Propranolol)

Reference books:

1. Vogel, A.I. (1996). *Text book of practical organic chemistry*, Pearson, 5th edition, UK.
2. Adams, R.; Johnson, J.R.; Wilcox, C.F. (1970). *Laboratory Experiments in Organic Chemistry*,

The Macmillan Limited, London.

3. Mann and Saunders. (2009). *Practical organic chemistry*, Pearson, 4th edition, UK.
4. Pasto, D.P., Johnson, C., Miller, M. (1992). *Experiments and Techniques in Organic Chemistry*, Prentice Hall, 1st edition, US.
5. Roberts, R.M.; Gilbert, J.C.; Rodewald, L.B.; Wingrove, A.S. (1969). *An introduction to Modern Experimental Organic Chemistry*, Ranehart and Winston Inc., New York.

6. Williamson, K.L., Health, D.C. (1999). *Macroscale and Microscale Organic Experiments, Heath, D.C.* and Co., Lexington, MA.

PCHPC11401: Analytical & Computational Chemistry Laboratory Credit-2

Code	Type	Title	Credits	Hours	L	T	P
PCHPC11401	Core-7	Analytical & Computational Chemistry Laboratory	2	4	0	0	4

Prerequisite Course/Knowledge (If any): **B.Sc. Chemistry laboratory**

Course Learning Outcomes (CLOs)

After completion of this course successfully, the students will be able to……

CLO-1: Apply computational tools to understand the fundamentals of atoms, molecules and solids.
CLO-2: Practice the Linux operating system and Linux commands to operate the Quantum Expresso software.
CLO-3: Develop skills to analyze compounds using various analytical techniques.
CLO-4: Illustrate experimental skills to operate various computational software and analytical instruments.
CLO-5: Develop critical thinking, teamwork, and ethics in conducting analytical experiments in the laboratory.

Mapping of Course learning outcomes (CLOs) with Program learning outcomes (PLOs)

	PLO 1	PLO 2	PLO 3	PLO 4	PLO 5	PLO 6	PLO 7	PLO 8	PLO 9	PLO 10	PLO 11	PLO 12
CLO-1	3	3	1	3	2	2	1	3	3	3	1	2
CLO-2	2	2	---	3	1	2	1	3	3	2	3	3
CLO-3	2	3	2	1	2	3	3	2	1	3	3	---
CLO-4	2	3	3	2	2	2	2	2	2	2	2	2
CLO-5	1	1	---	1	2	3	2	1	---	3	1	1

Detailed Syllabus:

S.No	Practical
1	Determination of internal coordinates of organic molecules and metal complexes in the crystal structures retrieved from CCDC using Mercury software.
2	Computation of HOMO-LUMO orbitals for small molecules using Schrodinger/Gaussian

	software.
3	Conformational analysis of cycloalkane using Materials Science platform of Schrödinger/Gaussian software.
4	Indexing XRD pattern and determination of electron density
5	Morse's potential plot of oxygen molecule by density functional theory using Schrodinger/Gaussian software.
6	Computational drug design through protein-ligand docking using Glide tool of Schrodinger/Autodock software.
7	Estimation of calcium in milk power by complexometric titration.
8	Determination of pKa_1 and pKa_2 of glycine by pH titration.
9	Purification of chlorophyll and β-carotene from spinach by column chromatography.
10	Isolation of limonene from orange peels by steam distillation.
11	Colorimetric monitoring oxidation of methanol and ethanol by $K_2Cr_2O_7$.
12	Analysis of aminoacids in the given mixture by TLC using Ninhydrin test.

Reference books:

1. A. Findary, T. A. Kitchner , Practical physical chemistry, (Longmans, Green and Co.)
2. J. M. Wilson, K. J. Newcombe, A. R. Denko, R. M. W. Richett, Experiments in Physical Chemistry, (Pergamon Press)
3. F. Jensen, Introduction to Computational Chemistry (John Wiley and Sons Ltd.)

Semester-II

PCHTC21500: Inorganic Chemistry-II **Credit -4**

Code	Type	Title	Credits	Hours	L	T	P
PCHTC21500	Core-8	Inorganic Chemistry – II	4	4	3	1	0

Prerequisite Course/Knowledge (If any): **NIL**

Course Learning Outcomes (CLOs)

After completion of this course successfully, the students will be able to……

CLO-1: Understand the basics of coordination chemistry including coordination numbers, geometry, and chelate effect.
CLO-2: Describe the bonding theories VBT, CFT, and MOT in turn describe CFSE, High and low spin complexes, magnetic moment of coordination compounds
CLO-3: Interpret the electronic spectra of coordination compounds explaining color, allowed and forbidden transitions through Orgel and Tanabe-Sugano diagrams.
CLO-4: Design reaction mechanism pathways like associative/dissociative, inner and outer sphere mechanism including electron transfer pathways.
CLO-5: Demonstrate the basics, spectral and magnetic properties of Lanthanides and Actinides

Mapping of Course learning outcomes (CLOs) with Program learning outcomes (PLOs)

	PLO 1	PLO 2	PLO 3	PLO 4	PLO 5	PLO 6	PLO 7	PLO 8	PLO 9	PLO 10	PLO 11	PLO 12
CLO-1	3	3	1	2	2	2	2	1	2	1	---	2
CLO-2	3	3	1	2	2	3	1	1	3	2	1	1
CLO-3	3	3	1	3	2	3	1	2	3	1	2	2
CLO-4	3	3	1	2	2	2	2	1	3	1	1	2
CLO-5	3	3	1	2	1	2	1	1	3	1	1	1

Detailed Syllabus:

UNIT I-Introduction and Theories of transition metal complexes: Structure, bonding and properties of transition metal ligand complexes, coordination number, geometry, isomerism (recapitulation) and optical isomerism, HSAB concept, thermodynamic stability, successive and overall stability constants, Irving-William series, chelate and macrocyclic effect. Applications of valence bond theory to metal complexes with coordination numbers 2 to 9 and its limitations, Crystal field theory, crystal field splitting pattern for various geometries from coordination number 2 to 12, concept of low spin and high spin, crystal field stabilization energy, spectrochemical series, thermodynamic and related aspects of crystal fields, ionic radii, heats of ligation, lattice energies, site

preference energies in spinels. Limitations of CFT, evidences of metal-ligand covalency, Molecular orbital (MO) theory, Construction of MO diagram for various geometries (without pi and with pi bonding) using group theoretical concept. (**25 Hrs)**

UNIT II-Electronic spectra and Magnetism of transition metal complexes: Terms, states and microstates for metal ions, repulsion parameters. Electronic spectra of transition metal complexes, selection rules, correlation diagram, Orgel and Tanabe-Sugano diagrams and Lever plot, charge transfer transitions, Jahn-Teller effect, nephelauxetic series. Dia, para, ferro and antiferromagnetism, quenching of orbital angular moment, spin-orbit coupling. Spectroscopic and magnetic properties of lanthanoids. (**20 Hrs)**

UNIT III-Inorganic reaction mechanisms: 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; inner and outer sphere electron transfer reactions and mechanism, metal complexes for photo-catalytic applications. **(12 Hrs)**

UNIT IV-: **IR, Raman, EPR and MB spectra of coordination complexes:**
Applications of vibrational spectroscopy (IR and Raman) in coordination complexes with aqua, cyano, nitro, nitrito, urea, acetylacetonato ligands. Basic concepts of electron paramagnetic resonance (EPR) and its application in copper and other complexes. Principles of Mossbauer spectra, application in low and high spin iron complexes. **(10 Hrs)**

Reference books:

1. J. E. Huheey, *Inorganic Chemistry*, 3rd Edition. Harper International, 1983.
2. B. Douglas, D. McDaniel, J. Alexander, *Concepts and Models of Inorganic Chemistry*,
1. 3rd Edition. John Wiley. 1994.
2. W. L. Jolly, *Modern Inorganic Chemistry*, 2nd Edition. McGraw-Hill.
3. C. Housecroft and A. G. Sharpe, *Inorganic Chemistry*, 5th Edition, Pearson. 2018.
4. B. N. Figgis, M. A. Hitchman, *Ligand field theory and its applications*, Wiley-VCH, 2000.
5. A. P. B. Lever, *Inorganic electronic spectroscopy*, Elsevier, 1984.
6. F.A. Cotton, *Chemical applications of Group theory*, 3rd Edn, John Wiley & Sons, 1990.
7. K. F. Purcell, J. C. Kotz, *Inorganic chemistry*, 1st Edn, W.B. Saunders company, 1977.
8. M. Weller, T. Overton, J. Rourke, F. Armstrong, ***I****norganic Chemistry***,** 7th Edn, Oxford University Press India, 2018. R. S. Drago, Physical methods in Inorganic chemistry, 1st Edition. Affiliated East-West Press, 2012.
9. M. T. Weller, N. A. Young. *Characterization methods in inorganic chemistry*, Oxford University press, 2017.
10. J.Micheal Hollas, *Basic Atomic and Molecular Spectroscopy*: (Tutorial Chemistry Texts), Royal Society of Chemistry, 2002
11. D.N.Sathyanarayana, *Vibrational Spectroscopy: Theory and Applications*, New Age International, 2005.
12. K. Nakamoto, *Infrared and Raman spectra of Inorganic and coordination compounds*, Wiley publishers, 2008.

PCHTC21501: Organic Chemistry-II Credit- 4

Code	Type	Title	Credits	Hours	L	T	P
PCHTC21501	Core-9	Organic Chemistry – II	4	4	3	1	0

Prerequisite Course/Knowledge (If any): NIL

Course Learning Outcomes (CLOs)

After completion of this course successfully, the students will be able to……

CLO-1: Apply reagents in the stereoselective reactions using mild reagents.
CLO-2: Synthesize organic molecules using popular named reactions.
CLO-3: Categorize the pericyclic reactions and construct various cyclic molecules.
CLO-4: Categorize the photochemical reactions and construct various cyclic molecules.
CLO-5: Apply rearrangement reactions in the organic synthesis.

Mapping of Course learning outcomes (CLOs) with Program learning outcomes (PLOs)

	PLO 1	PLO 2	PLO 3	PLO 4	PLO 5	PLO 6	PLO 7	PLO 8	PLO 9	PLO 10	PLO 11	PLO 12
CLO-1	3	1	3	3	1	3	3	1	1	2	1	2
CLO-2	3	1	3	3	2	1	2	1	1	3	1	1
CLO-3	3	2	3	3	2	3	2	1	2	2	1	1
CLO-4	3	3	3	3	2	2	3	1	1	3	1	2
CLO-5	3	3	3	3	2	3	3	1	2	2	1	2

Detailed Syllabus:

UNIT-I: Reagents in organic synthesis: Lithium diisopropylamide(LDA), Dicyclohexyl Carbodiimide(DCC), Trimethylsilyl iodide, Gilman's reagent, DDQ, Prevost Hydroxylation, Phase transfer catalysts, Phosphorous and Sulphur ylides, Merifield resin, Lawson reagents, IBX, Ceric ammonium nitrate, Tebbe reagent. **(14 Hrs)**

UNIT-II: Named Reactions & Rearrangements in organic synthesis: Pinacol-pinacolone, Wagner-Meerwein, Demjanov, Benzil-Benzillic acid, Favorskii, Neber, Beckmann, Hofmann, Curtius, Schimidt rearrangements, Arndt-Eister syntheses, Mukaiyama aldol reaction, Mitsunobu reaction, Shapiro reaction, Vilsmeier–Haack reaction, Baylis-Hillman reaction, Biginelli reaction. **(14 Hrs)**

UNIT-III: Pericyclic reactions: Thermal and photochemical pericyclic reactions, Conrotation and disrotation; Electrocyclic closure and opening in 4n and 4n+2 systems. Woodward-Hoffmann selection rules for electrocyclic reactions. Explanation for the mechanism of electrocyclic reactions and examples. Cycloaddition reactions: Suprafacial and antarafacial interactions. $\pi^2 + \pi^2$ and $\pi^4 + \pi^2$ cycloadditions. Diels-Alder reaction, Woodward-Hoffmann selection rules for cycloaddition reactions

and examples. Mechanism by orbital symmetry correlation diagrams, Fukui Frontier Molecular Orbital (FMO) theory. Endo-exo selectivity in Diels-Alder reaction and its explanation by FMO theory. Sigmatropic reactions: mechanism of sigmatropic reactions, Cope and Claisen rearrangements.

(18 Hrs)

Unit-IV: Photochemistry: Franck-Condon principle, Jablonski diagram, fluorescence and phosphorescence, Singlet and triplet states, Photosensitization, Quantum efficiency, Photochemistry of carbonyl compounds, Norrish type-I and type-II cleavages, Paterno-Buchi reaction, Photoreduction, Photochemistry of enones and para-benzoquinones, Di π – methane rearrangement, Photodynamic therapy, Photochemical [4+2] cycloaddition using singlet Oxygen; Barton reaction.

(16 Hrs)

Reference books:

1. Carey B. F. A., Sundberg R.J., (2007). *Advanced Organic Chemistry Part A and Part B, Springer, 5th edition*.
2. Jie Jack Li, (2009). *Name Reactions: A collection of Detailed Reaction Mechanism*, Publisher: Springer-verlag.
3. McMurry J., *Organic Chemistry***,** Asian Book Pvt. Ltd, 8th edition, New Delhi.
4. Smith, M. B., March J., (Latest Ed.) *March's Advanced Organic Chemistry*, John Wiley and Sons, 6th edition, New York.
5. Clayden, J.; Greeves, N.; Warren, S., (2012) *Organic Chemistry*, Oxford University press, 2nd edition.
6. Sankaraman, S. (2005).*Pericyclic reactions: Reactions, Applications and Theory*, Wiley-VCH.
7. Kurti, L., Czako, B. (2005). *Strategic Applications of Named Reactions in Organic Synthesis*, Elsevier Publications.
8. Coyle, J. D. (1991), *Introduction to organic photochemistry*, Wiley.
9. Halton, B.; Coxon J. M. (2011), *Organic Photochemistry*, Cambridge University Press.
10. K K Rohotgi and Mukherjee, Fundamentals Of Photochemistry, New Age Publishers.
11. I. Fleming, Pericyclic Reactions, Oxford University Press, 1999.
12. N. J. Turro, V. Ramamurthy and J. C. Scaiano, Modern molecular photochemistry of organic compounds, University Science Books, 2010.
13. B. G. Davis, A. J. Fairbanks., *Carbohydrate Chemistry*- Oxford Chemistry Primers, Oxford Science Publications.

PCHTC21502: Physical Chemistry-II **Credit -4**

Code	Type	Title	Credits	Hours	L	T	P
PCHTC21502	Core-10	Physical Chemistry – II	4	4	3	1	0

Prerequisite Course/Knowledge (If any): **NIL**

Course Learning Outcomes (CLOs)

After completion of this course successfully, the students will be able to……

CLO-1: Understand the fundamentals of electrochemistry, chemical kinetics, and colloid & surface chemistry
CLO-2: Develop problem-solving ability in electrochemistry, kinetics, and surface chemistry
CLO-3: Recognize the role of multidisciplinary streams especially basic physics & mathematics along with the role of colloid & surface science knowledge in the development of chemistry
CLO-4: Apply the fundamental knowledge in electrochemistry, kinetics, and surface chemistry to existing and emerging problem in basic science
CLO-5: Demonstrate the ability to do some independent calculation and use some computational resources at the end of the course

Mapping of Course learning outcomes (CLOs) with Program learning outcomes (PLOs)

	PLO 1	PLO 2	PLO 3	PLO 4	PLO 5	PLO 6	PLO 7	PLO 8	PLO 9	PLO 10	PLO 11	PLO 12
CLO-1	3	3	1	2	2	3	2	1	2	3	1	2
CLO-2	3	3	1	3	1	3	2	1	3	3	1	2
CLO-3	3	3	2	2	2	3	3	1	3	3	1	2
CLO-4	3	3	2	2	1	3	3	1	3	3	2	2
CLO-5	3	3	2	3	2	3	2	1	3	3	1	2

Detailed Syllabus:

UNIT I-Kinetics-I: Reviews of basic chemical kinetics, Complex reactions: reversible, pre-equilibrium, consecutive, chain and photochemical, oscillatory reactions, Reaction in solution, solvent effect, ionic reaction and salt effect, enzyme kinetics - Lindenmann's theory of uni-molecular reactions - laser flash photolysis, flow techniques and relaxation methods. **(14 Hrs)**

UNIT II-Kinetics-II: Molecular reaction dynamics collision and activated complex theory, comparison of results with Eyring and Arrhenius equations - reactive collisions, molecular beam experiments, introduction to potential energy surfaces: treatment of H_2 + H reaction – ionic reactions, salt effect. **(14 Hrs)**

UNIT III-Surface Chemistry: Surface phenomena Growth and structure of surface, surface defects, kinetics of surface adsorption: Langmuir and BET isotherms. Surface & interfaces, Surface

characterisation techniques, colloid chemistry, macromolecular films, surface engineering and catalysis **(8 Hrs)**

UNIT IV-Electrochemistry-I: Equilibrium electrochemistry, Activities in electrolytic solutions, mean activity coefficient, Debye-Huckel treatment of dilute electrolyte solutions, origin of electrode potential, half-cell potential, electrochemical cell, Galvanic & electrolytic cells, Electrolysis, Nernst equation, thermodynamics of electrochemical cell**.** **(14 Hrs)**

UNIT V-Electrochemistry-II: Dynamic electrochemistry, Electrical double layer - electrode kinetics: rate of charge transfer, current density, Tafel equation, Butler-Volmer equation - introduction to polarography, Introduction to electrochemical techniques such as pulse, linear, differential voltammetery, cyclic voltammetry etc, applied electrochemistry & energy science, theory of corrosion and inhibition of corrosion. **(14 Hrs)**

Reference books:

1. K. J. Laidler, Chemical Kinetics, 3rd Edn., Harper International, 1987.
2. G. D. Billing & K. V. Mikkelson, Molecular dynamics and chemical kinetics, John Wiley, 1996.
3. J. I. Sheinfield, J. S. Francisco, W. L. Hasse, Chemical kinetics & dynamics, Prentice Hall, 1998.
4. A. J. Bard & L. R. Faulkner, Electrochemical Methods, Fundamental and Applications, JohnWiley, 1980.
5. Bockris & Reddy, Electrochemistry, Vol. 1 & 2, Plenum, 1973
6. H. V. Keer, Solid State Chemistry, Wiley Eastern, 1993.
7. A. K. Cheetam & P. Day, Solid State Chemistry Techniques, Oxford, 1987.
8. Arthur W. Adamson, Physical Chemistry of Surfaces, 6th Edition, Wiley India Pvt Ltd, 2011
9. Southampton Electrochemistry Group, Instrumental Methods in Electrochemistry, Woodhead Publishing, 2001.
10. J. M. Berg, J. L. Tymoczko, L. Stryer, *Biochemistry*, W.H. Freeman & Co Ltd, 5th Edi., 2002.

PCHTC21503: Chemistry of Life Credit -2

Code	Type	Title	Credits	Hours	L	T	P
PCHTC21503	Core-11	Chemistry of Life	2	2	2	0	0

Prerequisite Course/Knowledge (If any): **Basics of Inorganic chemistry and Organic chemistry**

Course Learning Outcomes (CLOs)

After completion of this course successfully, the students will be able to……

CLO-1: Explain the role of metal ions in biological systems and biochemical reactions.
CLO-2: Outline the effects of functional groups of biomolecules on metal-mediated biological reactions.
CLO-3: Categorize biomolecules based on their biological functions and chemical structures.
CLO-4: Synthesis of biomolecules and development of synthetic scheme of biomolecules.

Mapping of Course learning outcomes (CLOs) with Program learning outcomes (PLOs)

	PLO 1	PLO 2	PLO 3	PLO 4	PLO 5	PLO 6	PLO 7	PLO 8	PLO 9	PLO 10	PLO 11	PLO 12
CLO-1	3	2	3	1	2	2	3	1	2	---	1	2
CLO-2	3	3	3	1	1	1	3	1	2	1	2	2
CLO-3	3	3	3	2	2	3	---	1	2	3	3	1
CLO-4	3	2	2	1	2	1	2	---	3	2	1	3

Detailed Syllabus:

UNIT I: Bioinorganic chemistry I: Porphyrins, Dioxygen transport and storage: haemoglobin, myoglobin, hemerythrin and hemocyanine and their electronic structural properties. Electron Transfer protein and photosynthesis: Cytochromes, Fe-S Clusters and blue-copper, metal in photosystems I and II. The role of metalloenzymes: peroxidase, catalase and cytochrome P-450, carboxypeptidase A, carbonic anhydrase, vitamin B_{12} and nitrogenase. metal complexes in medicine. **(16 Hrs)**

UNIT II: Bioorganic chemistry: Biopolymers-DNA, RNA and Proteins- structures of monomers, bonding, sequencing, and hierarchy of structural organization. Chemical synthesis of DNA. Chemical synthesis of peptides- solution phase and solid phase peptide synthesis methods. Applications of PNAS. Representative examples of structure, synthesis and reactions of carbohydrates. Chemical structures and biological significance of fatty acids. **(16 Hrs)**

Reference books:

1. S. J. Lippard, J. M. Berg, *Principles of Bioinorganic Chemistry*, University Science Books. 1994.

2. I. Bertini, H. B. Gray, S. J. Lippard, J. A., Valentine, *Bioinorganic Chemistry*, University Science Books. 1994.
3. A. K. Das, *Bioinorganic Chemistry*, Books & Allied Limited. 2013.
4. W. Kaim; *Bioinorgnic Chemistry*, 2nd Edition, John Wiley. 2013.
5. R. M. Roat-Malone, *Bioinorganic Chemistry*, John Wiley, 2002.
6. David Van Vranken and Gregory A, Introduction to Bioorganic Chemistry and Chemical Biology. Garland Science (Taylor & Francis), 2012.
7. I. L. Finar, *Advanced Organic Chemistry*, Vol. 2 ELBS, New Delhi, 1975.

PCHTC21504: Chemical applications of Group Theory Credit -2

Code	Type	Title	Credits	Hours	L	T	P
PCHTC21504	Core-12	Chemical applications of Group Theory	2	2	1	1	0

Prerequisite Course/Knowledge (If any): **NIL**

Course Learning Outcomes (CLOs)

After completion of this course successfully, the students will be able to……

CLO-1: Understand the basic concepts of symmetry and its mathematical expression.
CLO-2: Apply these mathematical notations into objects and molecules.
CLO-3: Analyze infrared, Raman, and electronic spectra of simple molecules.
CLO-4: Understand orbital symmetry and energy levels and in the conjugated alkenes.
CLO-5: Apply the knowledge of group theory into different fields such as asymmetric synthesis, spectroscopy, photochemistry, crystallography, and even to other branches of science like physics and biology.

Mapping of Course learning outcomes (CLOs) with Program learning outcomes (PLOs)

	PLO 1	PLO 2	PLO 3	PLO 4	PLO 5	PLO 6	PLO 7	PLO 8	PLO 9	PLO 10	PLO 11	PLO 12
CLO-1	3	3	3	3	3	3	3	3	3	-	3	3
CLO-2	3	3	3	2	2	3	3	1	3	1	1	3
CLO-3	3	2	3	3	3	3	3	3	3	-	2	3
CLO-4	3	3	3	3	2	3	3	3	-	-	3	3
CLO-5	2	4	3	2	1	2	3	2	3	1	2	2

Detailed Syllabus:

UNIT I-Group Theory: Groups, sub-groups, classes and their properties, postulates of group, construction of group multiplication table, symmetry elements and operations, general relations

among symmetry elements and operations, molecular symmetry and point groups, matrix representation of symmetry elements, representation of groups, character, reducible and irreducible representations, Great Orthogonality theorem, properties of irreducible representations, Mulliken's symbols for irreducible representations, character tables, applications of character tables in IR, Raman and electronic spectroscopy. **(16 Hrs)**

UNIT II-Applications of Group Theory:

Group theory & quantum mechanics, wave functions as basis for irreducible representations, direct products, time dependent perturbation theory; Selection rules in spectroscopy; Symmetry-adapted linear combinations (SALC); linear combination of atomic orbitals (LCAO), application of LCAO in organic chemistry. **(16 Hrs)**

Reference books:

1. F. A. Cotton. *Chemical applications of group theory*, 3rd edition, Wiley India edition, 2003.
2. R. L. Carter, Molecular Symmetry and Group Theory, Wiley India, 2004.
3. K. Veera Reddy, *Symmetry and spectroscopy of molecules*, 2nd edition, New Age International Publishers, 2009.
4. B. S. Garg, *Chemical applications of molecular symmetry and group theory*, 1st edition, Macmillan Publishers Indian Ltd, 2012.
5. Mark Ladd, *Symmetry of Crystals and Molecules*, Oxford University Press, 2014.
6. L. H. Hall, *Group Theory and Symmetry in Chemistry*, McGraw Hill Book Company, 1969.

PCHPC21500: Inorganic Chemistry Laboratory Credit -2

Code	Type	Title	Credits	Hours	L	T	P
PCHPC21500	Core-13	Inorganic Chemistry Laboratory	2	4	0	0	4

Prerequisite Course/Knowledge (If any): **B.Sc. Chemistry laboratory**

Course Learning Outcomes (CLOs)

After completion of this course successfully, the students will be able to……

CLO-1: Understand the safety and precautionary measures in handling chemicals.
CLO-2: Demonstrate the rudimentary principle related to inorganic synthesis
CLO-3: Synthesize the given list of compounds using standard procedure in a pure form.
CLO-4: Analyze compounds using various analytical techniques and arrive at the conclusion of the correct chemical structure.
CLO-5: Design and synthesize either the same compound by different synthetic strategy or a new compound.

Mapping of Course learning outcomes (CLOs) with Program learning outcomes (PLOs)

	PLO 1	PLO 2	PLO 3	PLO 4	PLO 5	PLO 6	PLO 7	PLO 8	PLO 9	PLO 10	PLO 11	PLO 12
CLO-1	3	2	2	2	3	3	3	3	3	3	--	3
CLO-2	3	2	3	3	3	3	3	3	--	3	--	
CLO-3	3	1	3	3	3	3	3	3	--	3	3	3
CLO-4	3	3	3	3	3	1	3	3	3	3	3	3
CLO-5	3	3	3	3	3	1	3	3	3	3	--	2

Detailed Syllabus:

(Any 7 experiments from serial number 1-9 and any 2 experiments from serial number 10 will be conducted)

S.No	Practical
1	Preparation and characterization of cobalt ammine complexes Lab 1: Synthesis of $[Co(NH_3)_6]Cl_3$, Lab 2: Synthesis of $[Co(NH_3)_5Cl]Cl_2$, Lab 3: UV, IR and conductometric characterization of complexes
2	Synthesis of transition metal complex $[Ni(PPh_3)_2Br_2]$ and its magnetic study Lab 4: Synthesis of $[Ni(PPh_3)_2Br_2]$ Lab 5: Measurement of magnetic susceptibility of the complex

3	Estimation of Copper and Zinc in Brass by Gravimetric and Volumetric analysis Lab 6: Estimation of copper by volumetric method Lab 7: Estimation of copper by Gravimetric method
4	Synthesis of Jacobson Type Catalyst and its catalytic study Lab 8: Synthesis of Salen and Mn(Salen)Cl Lab 9: Catalytic activity of Mn(Salen)Cl on cyclohexene
5	Preparation and chiral resolution of tris(ethylenediamine)cobalt(III) chloride, $[Co(en)_3]Cl_3$. Lab 10: Synthesis of $[Co(en)_3]Cl_3$. Lab 11: Chiral resolution into its optical isomers
6	Lab 12: Preparation of tris(ethylenediamine)nickel(II)chloride dihydrate$[Ni(en)_3]Cl_2.\ 2H_2O$ Lab 13: Dichloridobis(ethylenediamine)nickel(II) dihydrate$[Ni(en)_2Cl_2].\ 2H_2O$ from $[Ni(en)_3]Cl_2.\ 2H_2O$.
7	Lab 14: Preparation of *cis* and *trans* –bis(glycinato) copper (II) monohydrate
8	Lab 15: Preparation $[Al(8\text{-}HQ)_3]$ and their fluorescence properties
9	Lab 16: Preparation and characterization of Ferrocene
10	Additional Experiments: 1) Determination of Composition of the Cu-EDTA complex by Job's Method 2) Preparation and characterization of nitro- and nitrito-pentamminecobalt(III) chloride 3) Preparation and characterization of tris(acetylacetonato) manganese(III) 4) Preparation and characterization of metal-phorphyrins 5) Preparation and characterization of tris(acetylacetonato) chromium(III) 6) Preparation and magnetic studies of $[Ni(NCS)_2(PPh_3)_2]$ 7) Preparation and thermochromic properties of Copper(II), N,N-diethylenediamine complex.

Reference books:

1. Text book of Quantitative Analysis, A.I. Vogel 4thedn (1992)
2. Electronic Spectroscopy by A.B. P. Lever.
3. Inorganic Synthesis (Vol. Series)

PCHPCC21501: Physical Chemistry Laboratory Credit -2

PCHTC21501	Core-14	Physical Chemistry Laboratory	2	4	0	0	4

Prerequisite Course/Knowledge (If any): **B.Sc. Chemistry laboratory**

Course Learning Outcomes (CLOs)

After completion of this course successfully, the students will be able to……

CLO-1: Understand the fundamentals of doing experimental physical chemistry
CLO-2: Develop problem-solving & troubleshooting ability in experimental physical chemistry
CLO-3: Recognize the role of multidisciplinary streams starting with basic science to understanding the key role of instruments in doing experimental physical chemistry
CLO-4: Apply the fundamental knowledge in experimental physical chemistry to existing and emerging problem in basic science
CLO-5: Demonstrate the ability to do some independent calculation and use some computational resources at the end of the course

Mapping of Course learning outcomes (CLOs) with Program learning outcomes (PLOs)

	PLO 1	PLO 2	PLO 3	PLO 4	PLO 5	PLO 6	PLO 7	PLO 8	PLO 9	PLO 10	PLO 11	PLO 12
CLO-1	3	3	2	2	1	3	2	1	2	3	1	2
CLO-2	3	3	1	3	2	3	3	1	2	3	1	2
CLO-3	3	3	1	2	1	3	3	1	2	3	1	2
CLO-4	3	3	3	2	1	3	3	1	2	3	1	2
CLO-5	3	3	2	2	1	3	2	1	3	3	1	2

Detailed Syllabus:

(Any twelve of the following experiments will be conducted)

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S.No	Practical
I.	**Potentiometric Titration (Electrodics)** 1. Potentiometric titration of Zn^{2+} or Cd^{2+} or Pb^{2+} with potassium ferrocyanide and determination of composition of Zn(II) or Cd(II) or Pb(II) -ferrocyanide complex (three different experiments as the metal ion only changed). 2. Determination of standard reduction potential using quinhydrone electrode. 3. Redox-titration: Determination of concentration of reductant or oxidant by

	potentiometric method.
II.	**Conductometric Titration (Ionics)** 4. Solubility product of sparingly soluble salt by conductance measurements. 5. Determination of Equilibrium constant & equivalent conductance at infinite dilution of a weak / strong electrolyte. 6. Conductometric determination of critical micelle concentration of any given surfactant.
III.	**Chemical Kinetics** 7. Saponification of ethyl or methyl acetate using conductometric methods a) Determination of rate constant & order of reaction with respect to reactants b) Influence of ionic strength on the rate constant (Salt effect) c) Effect of Temperature on rate constant (Arrhenius Equation) Above practical is equivalent to 3 different experiments 8. Determination of rate constant of Inversion of sucrose by polarimeter & verification of the effect of catalyst on the rate constant.
IV.	**Thermodynamics, Phase rule, Surface Chemistry** 9. Heat of neutralisation of a strong acid by a strong base. 10. Adsorption of acetic acid or iodine on charcoal. 11. Three component liquid system (acetic acid, benzene, water). 12. Determination of dimerization constant of benzoic acid in organic medium.
V.	**Miscellaneous experiments (pH, Colorimetry etc.)** 13. Determination of Composition & stability constant of given complex such as Fe (III)- Salicylic acid complex by Job's method using colorimetry. 14. Determination of ionic product of water by pH metric method. 15. Determination of hydrolytic constant of given salts such as ammonium chloride by pH metric method. 16. Determination of pKa of dibasic or tribasic acids by pH-metric methods.

Reference books:

1. A.Findar, T.A.Kitchner, Practical Physical Chemistry (Longmans, Green and Co).
2. J.M.Wilson, K.J.Newcombe, A.R.Denko, R.M.W.Richett, Experiments in Physical Chemistry, (Pergamon Press).
3. B.Viswanathan, P.S.Raghavan Practical Physical Chemistry (Viva Books).
4. Saroj Maity, Naba Ghosh, Physical Chemistry Practical (NCBA).

Semester-III

PCHTC31505: Molecular Spectroscopy Credit -4

Code	Type	Title	Credits	Hours	L	T	P
PCHTC31505	Core-15	Molecular Spectroscopy	4	4	3	1	0

Prerequisite Course/Knowledge (If any): **NIL**

Course Learning Outcomes (CLOs)

After completion of this course successfully, the students will be able to……

CLO-1: Understand the basic principles of light-matter interactions and learn quantum mechanical methods to analyze the interactions
CLO-2: Apply selection rules in microwave, infrared, Raman, UV-Vis spectroscopy/ Rotational, Vibrational & Electronic spectroscopy
CLO-3: Describe the principles of ESCA, PES, AUGER spectroscopy.
CLO-4: Understand the basic physical concepts of nuclear magnetic resonance.
CLO-5: Understand theories of various NMR techniques.

Mapping of Course learning outcomes (CLOs) with Program learning outcomes (PLOs)

	PLO 1	PLO 2	PLO 3	PLO 4	PLO 5	PLO 6	PLO 7	PLO 8	PLO 9	PLO 10	PLO 11	PLO 12
CLO-1	3	3	1	2	1	2	2	1	2	3	1	2
CLO-2	3	3	1	2	1	3	2	1	2	3	1	2
CLO-3	3	3	2	3	1	3	2	1	2	3	1	2
CLO-4	3	3	2	3	1	3	3	1	2	3	1	2
CLO-5	3	3	1	3	1	3	3	1	3	3	1	2

Detailed Syllabus:

UNIT I-Rotational, Vibrational & Electronic spectroscopy: Electromagnetic radiation, interaction of electromagnetic radiation with matter, quantum mechanical approach - transition probabilities: Einstein coefficients - pure vibrational and rotational spectra, selection rules, vibrational and rotational spectra of polyatomic molecules, normal modes, anharmonicity, selection rules – Raman effect: classical and quantum theory of Raman effect, rotational and vibrational Raman spectra. Franck-Condon principle, Electronic Spectra of atoms/molecules, Born-Oppenheimer Approximation, Rotational fine structures Fortrat Diagram, Pre-dissociation, Transition moments, assignment of electronic transitions of N_2, H_2O and formaldehyde using group theory, solvent effect, ESCA, PES, AUGER techniques. **(32 Hrs)**

UNIT II-Introduction to NMR:-Origin of magnetic moments in matter, electronic and nuclear moments, interaction with magnetic field, Larmor equation - conditions for magnetic resonance absorption, relaxation mechanism and time, line widths and line shapes, chemical shift, ring currents, diamagnetic anisotropy, spin-spin splitting, high resolution NMR spectra of simple molecules, first and second order treatment of AB systems - FT techniques. **(16 Hrs)**

UNIT III- Advanced NMR techniques: Charge density calculations, computation of ^{13}C-chemical shift values using table, theories of vicinal and germinal coupling, long range coupling, 1D and 2D NMR and Nuclear Overhauser Effect, 2-D NMR, DEPT, INADEQUATE, SEFT, SPI, COSY, NOESY, ROESY, HMBC, HSQC, Introduction of dynamic and solid state NMR. **(16 Hrs)**

Reference books:

1. P. W. Atkins, *Physical Chemistry*, Oxford, London, 7th edition, 2006.
2. D. L. Pavia, G. M. Lampman and G. S. Kriz, *Introduction to Spectroscopy*, 2ndEdn, Saunders
3. C. N. Banwell, *Fundamentals of Molecular Spectroscopy*, 4th Edition Tata McGraw Hill, 2016.
4. A. Carrington and Machlachlon, *Magnetic Resonance*, Harper & Row, 1967.
5. G. M. Barrow, *Introduction to Molecular Spectroscopy*, McGraw Hill, 1964.
6. D. H. Williams and I. Fleming, *Spectroscopic methods in organic chemistry*, Tata McGraw Hill, 1998.
7. J. Micheal Hollas, *Modern Spectroscopy*, 4th Edition, Wiley India Pvt Ltd, 2010
8. Harald Gunther, *NMR Spectroscopy: Basic Principles, Concepts and Applications in Chemistry*, 2nd Edition, Wiley India Pvt Ltd, 2010
9. J. Micheal Hollas, Basic Atomic and Molecular Spectroscopy: (Tutorial Chemistry Texts), Royal Society of Chemistry, 2002.
10. D. N. Sathyanarayana, Vibrational Spectroscopy: Theory and Applications, New Age International, 2005.
11. J. Keeler, *Understanding NMR Spectroscopy*, Wiley India Pvt Ltd, 2nd Edi., 2013.
12. D. N. Satyanarayana, *Handbook of Molecular Spectroscopy*, IK International publishing house, 2015.
13. D. N. Satyanarayana, *Introduction to Magnetic Resonance Spectroscopy*, IK International publishing house, 2013.
14. E. B. Becker, *High resolution NMR*, Academic Press, 2nd Edi., 1980.
15. R. S. Drago, *Physical Methods for Chemists*, East-west Press Pvt Ltd, 2nd Edi., 2016.

PCHTC31506: Organic Spectroscopy Credit – 3

Code	Type	Title	Credits	Hours	L	T	P
PCHTC31506	Core-16	Organic Spectroscopy	3	3	2	1	0

Prerequisite Course/Knowledge (If any): **NIL**

Course Learning Outcomes (CLOs)

After completion of this course successfully, the students will be able to……

CLO-1: Describe the applications of UV-Visible spectroscopy in the identification of conjugation in organic compounds.
CLO-2: Apply IR spectroscopy to identify the various functional groups in organic molecules.
CLO-3: Evaluate the structure of organic compounds using ^{1}H, ^{13}C, and 2D-NMR Spectroscopy.
CLO-4: Describe the basic principles and applications of organic-mass spectrometry.
CLO-5: Apply UV-Visible, IR, NMR, and mass spectrometry in structure elucidation of organic compounds.

Mapping of Course learning outcomes (CLOs) with Program learning outcomes (PLOs)

	PLO 1	PLO 2	PLO 3	PLO 4	PLO 5	PLO 6	PLO 7	PLO 8	PLO 9	PLO 10	PLO 11	PLO 12
CLO-1	3	3	1	3	1	2	1	2	3	2	1	2
CLO-2	3	3	1	3	1	2	1	2	3	2	1	2
CLO-3	3	3	3	3	1	3	1	1	3	3	3	2
CLO-4	3	3	3	3	1	3	1	2	3	3	3	2
CLO-5	3	3	3	3	3	3	2	3	3	3	3	2

Detailed Syllabus:

UNIT-I: Introduction to spectroscopic techniques: Application of UV – Visible and IR spectroscopy to organic structure elucidation. Electromagnetic spectrum, absorption of energy by organic compounds; Effect of solvent on UV spectrum, red shift & blue shift, Woodward – Fisher rules and theoretical λ_{max} calculations; IR spectrometer instrument & basic principles, Organic functional group identification through IR spectroscopy. **(14 Hrs)**

UNIT-II: Application of NMR Spectroscopy. Basic principles. Introduction to NMR techniques. CW and FT NMR techniques. ^{1}H NMR Spectral parameters – intensity, chemical shift, multiplicity, coupling constant. Analysis of first order and second - order spectra. Structure determination of organic compounds by ^{1}H NMR spectra. Multinuclear ^{1}H NMR &^{13}C NMR: Proton coupled, off resonance decoupled, proton noise decoupled ^{13}C NMR spectra. Assignment of chemical shifts, additively effect, characteristic chemical shifts of common organic compounds and functional groups, DEPT & SEFT spectra. 2D NMR techniques ^{1}H – ^{1}H COSY, ^{1}H – ^{13}C COSY – HMBC, and NOESY. **(24 Hrs)**

UNIT-III: Application of mass spectrometry: Basic principles, mass analyzers, ionization methods: EI, PI, CI, FAB, MALDI, ES. Liquid chromatography and mass spectrometry, types of ions and fragmentations, even electron rule, nitrogen rule, isotope abundance, McLafferty rearrangement.
Organic structure elucidation, techniques of ion production, ion and daughter ions, molecular ion and isotope abundance. Nitrogen rule energetics of fragmentation, metastable ions, common fragmentation pathways, fragmentation pattern of common chemical classes. Illustrative examples from macromolecules and supramolecules. **(10 Hrs)**

Reference books:

1. R. M. Silverstein and F. X. Webster, Spectrometric identification of organic compounds, 6thEdn, Wiley.
2. W. Kemp, Organic Spectroscopy, 3rdEdn., MacMillon, 1994.
3. Pavia, Lampman and Kriz, Introduction to Spectroscopy, 3rdEdn., Brooks/Cole.
4. D. H. Williams and Ian Fleming, Spectroscopic methods in organic chemistry, Tata McGraw Hill,1998.
5. W. Kemp, Introduction to multinuclear NMR.
6. P. S. Kalsi, Spectroscopy of Organic Compounds, 6th edition, New age international, 2004.

PCHTC31507: Organometallic Chemistry **Credit – 4**

Code	Type	Title	Credits	Hours	L	T	P
PCHTC31507	Core-17	Organometallic Chemistry	4	4	3	1	0

Prerequisite Course/Knowledge (If any): **NIL**

Course Learning Outcomes (CLOs)

After completion of this course successfully, the students will be able to……

CLO-1: Understand the basics of Organometallic (OM) chemistry. Illustrate organometallic complexes with phosphines, carbenes, alkyl, alkene, and alkyne as ligands.
CLO-2: Evaluate Pi-Conjugated systems as ligands, synthesis, and reactivity of metallocenes,fluxionality and dynamic NMR
CLO-3: Explain the structure, bonding, reactivity, and spectral study of metal carbonyls, carbonyl clusters and isolobal analogy.
CLO-4: Devise special reactions of organometallic chemistry: Oxidative addition, reductive elimination and migratory insertion.
CLO-5: Design the catalytic cycles, mechanistic studies and apply metal-catalyzed reactions for industrial applications.

Mapping of Course learning outcomes (CLOs) with Program learning outcomes (PLOs)

	PLO 1	PLO 2	PLO 3	PLO 4	PLO 5	PLO 6	PLO 7	PLO 8	PLO 9	PLO 10	PLO 11	PLO 12
CLO-1	3	3	2	2	2	3	2	1	3	1	---	1
CLO-2	3	3	1	2	2	3	2	2	2	1	1	1
CLO-3	3	3	1	2	2	3	2	1	3	1	---	2
CLO-4	3	3	2	2	2	2	3	2	2	1	1	1
CLO-5	3	3	3	2	2	3	3	2	3	1	3	2

Detailed Syllabus:

UNIT I- Organometallic Chemistry of Main Group elements: Organometallic compounds of ***s***-and ***p***-block elements such as Li, Be, Mg, Al and Si as well as compounds of Zn and Hg. Organometallic clusters with low and high nuclearity and their structure predictions using Capping rule and Wade-Mingos-Lauher rules, metal-metal bond, isolobal analogy. **(14 Hrs)**

UNIT II-Organometallic Chemistry of Transition metals: Metal carbonyls, metal alkyl, alkene and alkynes, metal carbene types- Fischer, Schrock and intermediate carbenes such as Grubbs carbenes and their applications. Metal carbynes of Fischer and Schrock. Complexes containing η^5-cyclopentadienyl ligands: ferrocene and other metallocenes: structure, bonding and reactions.

Ferrocene derivatives in asymmetric catalysis, OMCs containing η^3- η^{4-} η^6- η^7- η^8- and η^9 ligands, Hydride, dihydrogen complexes and fluxionality. **(20 Hrs)**

UNIT III-Unique reactions of Organometallic Complexes: Oxidative addition, reductive elimination, β- hydride elimination, α- hydrogen abstraction and migratory insertion. **(5 Hrs)**

UNIT IV-Catalysis: Homogeneous and Heterogeneous catalysis. Olefin hydrogenation: Wilkinson catalyst, iridium and ruthenium based catalysts, directing effects in hydrogenation and asymmetric hydrogenation. hydrocyanation and hydrosilylation of alkenes. Hydroformylation: cobalt catalysts, rhodium-phosphine catalysts, *n*/*iso* ratio of products, enantioselective hydroformylation. Monasanto acetic acid process, Cativa and Wacker processes. metathesis: Grubb's and Schrock Catalysts, ring opening metathesis (ROM), ring closing metathesis(RCM), enyne metathesis (EM). Olefin polymerization: Ziegler-Natta and metallocene based catalysts. Coupling reactions: Industrial applications, different catalysts for coupling. Suzuki-Miyaura, Heck, Sonagashira, Stille, Kumada, Negishi, Hiyama and Buchwald-Hartwig C-N cross coupling reactions. **(25 Hrs)**

Reference Books:

1. R. H. Crabtree, *The organometallic chemistry of transition metals*, 7th Edn. Wiley, 2019.
2. Ch.Elsenbroich, A. Salzar, *Organanometallics*, 2nd Edn, VCH Publishers Inc, NY, 1992.
3. B. D. Gupta, A. J Elias, *Basic Organometallic chemistry*, 2nd Edn, University Press, 2013.
4. J. E. Huheey, E. A. Keiter & R. L. Keiter, *Inorganic Chemistry: Principles of Structure and Reactivity, Pearson Education*, 4th Edn. 1992.
5. R. Whyman, *Applied organometallic chemistry and catalysis*, Oxford University Press, 2001.
6. C. E. Housecraft and A. G. Sharpe, Inorganic Chemistry, Pearson, 5th Edn. 2018.
7. J. P. Collman, L.S. Hegedus, J. R. Norton, R. G. Finke, P*rinciples and applications of organotransition metal chemistry*, University Science Books, 1987.
8. K. F. Purcell and J. C. Kotz, *Inorganic chemistry,* W.B. Saunders Company,1977.

PCHTC31508: Organic Chemistry-III **Credit – 4**

Code	Type	Title	Credits	Hours	L	T	P
PCHTC31508	Core-18	Organic Chemistry-III	4	4	3	1	0

Prerequisite Course/Knowledge (If any): **NIL**

Course Learning Outcomes (CLOs)

After completion of this course successfully, the students will be able to……

CLO-1: Synthesis of organic molecules using enolate chemistry.
CLO-2: Develop organic synthetic strategies using the disconnection approach.
CLO-3: Assess the reactivity patterns of enolates and their mechanisms
CLO-4: Synthesis of heterocyclic compounds with mono and di heteroatoms.
CLO-5: Classification of organic molecules from the nature.

Mapping of Course learning outcomes (CLOs) with Program learning outcomes (PLOs)

	PLO 1	PLO 2	PLO 3	PLO 4	PLO 5	PLO 6	PLO 7	PLO 8	PLO 9	PLO 10	PLO 11	PLO 12
CLO-1	3	1	3	3	1	3	3	1	1	2	1	1
CLO-2	3	2	3	3	2	3	3	1	2	3	3	2
CLO-3	3	2	3	3	2	2	2	1	1	2	2	1
CLO-4	3	3	3	3	2	3	3	2	2	3	2	2
CLO-5	3	3	3	3	2	3	3	1	3	2	3	3

Detailed Syllabus:

UNIT-I: Enolate of carbonyl compounds: Kinetic and thermodynamic control, Potential energy diagrams, methods of determining mechanisms, isotopes effects. Enolates: Regio- and stereo-selectivity in enolate generation. "O" versus "C" alkylation, effect of solvent; Thermodynamically and kinetically controlled enolate formations via different bases; Various transition state models to explain stereoselective enolate formation; Enamines; Regioselectivity in generation, Application in controlling the selectivity of alkylation. **(12 Hrs)**

UNIT-II: Heterocycles in Chemistry: Introduction to heterocycles; Nomenclature; Single heteroatom heterocycles Furan, pyrrole, thiophene, indole, pyridine, quinoline, isoquinoline synthesis, reactivities and application. Synthesis and reaction of five membered heterocycles containing two heteroatoms, imidazole, oxazole, thiazole; Benzo-fused five-membered and six membered heterocycles. **(16 Hrs)**

Unit-III: Natural product chemistry: Alkaloids: Natural occurrence, General structural features, Isolation and their physiological action, Hoffmann's exhaustive methylation, Emde's modification, Structure elucidation and synthesis of Hygrine and Nicotine. Medicinal importance of Nicotine, Hygrine, Quinine, Morphine, Cocaine, and Reserpine. **Terpenes:** Occurrence, classification, isoprene rule; Elucidation of structure and synthesis of Citral, Neral, α-terpineol and limonene Biosynthesis of

acyclic and monocyclic terpenes from acetyl CoA. **Steroids:** Structure of common steroids such as cholesterol and steroidal hormones; Chemical synthesis of hormones using cholesterol. **(16 Hrs)**

Unit-IV: Synthetic strategies: Synthon, Synthetic equivalent, Functional group interconversion (FGI), Functional group addition, Functional group elimination. Criteria for selection of target; Linear and convergent synthesis; Retrosynthetic analysis and synthesis involving chemo selectivity, regioselectivity, reversal of polarity and cyclizations; Criteria for disconnection of strategic bonds; One group and two group C-X disconnections in 1,2-, 1,3-, 1,4 difunctional compounds. Protection and deprotection of functional groups in synthetic strategy: Protection of alcohols by silyl ethers and ester formations and their deprotection; Protection of 1, 2 diols- by acetal, ketal and their deprotection. **(20 Hrs)**

Reference books:

1. Finar, I.L. (2006). *Organic Chemistry: Stereochemistry and the Chemistry of Natural Products.* Dorling Kindersley Pvt. Ltd., 6th edition, India.
2. Bhat, S. V., Nagasampagi, B. A., Meenakshi, S. (2009). *Natural Product Chemistry & Applications*, Narosa Publishing House, New Delhi.
3. I. L. Finar, *Advanced Organic Chemistry*, Vol. 2 ELBS, New Delhi, 1975.
4. McMurry J., *Organic Chemistry***,** Asian Book Pvt. Ltd, 8th edition, New Delhi.
5. Morrison, R.T., Boyd, R.N. (2011). *Organic Chemistry*, Prentice- Hall of India, 6th edition, New Delhi.
6. Clayden, J.;Greeves,N.;Warren,S., (2012). *Organic Chemistry*, Oxford University press, 2nd edition.
7. Warren S.; Wyatt, P. (2008). *Organic Synthesis-The Disconnection Approach*, Wiley 2nd edition.
8. R. H. Thomson, Chemistry of Natural Products - Wiley, New York, 1996.
9. Coyle, J. D. (1991), *Introduction to organic photochemistry*, Wiley.
10. Smith, M. B.; March, J. (2007), *March's Advanced Organic Chemistry*, Wiley 6th edition.

PCHTD31500: MOOC Course (NPTEL; SWAYAM) / Other Department Elective Credit -3

Code	Type	Title	Credits	Hours	L	T	P
PCHTD31500	Generic Elective Course-01	MOOC Course (NPTEL; SWAYAM) / Other Department Elective	3	3	2	1	0

Students have to take one Open elective course from other departments in the University, preferably of 3 credits. Students are encouraged to take the opportunity to learn other aligned or non-aligned subjects as Open electives. Students can choose options to improve their language proficiency, IT proficiency, personality development, etc. MOOC Course (NPTEL; SWAYAM) can also be considered based on the interest of students.

Since these courses from other departments/platforms, Mapping of Course learning outcomes (CLOs) with Program learning outcomes (PLOs) are not undertaken.

PCHTS31500: Literature Survey and Seminar **Credit-2**

Code	Type	Title	Credits	Hours	L	T	P
PCHWS31500	Skill Enhancement Course-01	Literature Survey and Seminar	2	4	0	0	4

Prerequisite Course/Knowledge (If any): NIL

Course Learning Outcomes (CLOs)

After completion of this course successfully, the students will be able to……

CLO-1: Able to understand literature types and select the topic
CLO-2: Analyse and identify new research problems in chemistry.
CLO-3: Plan the new synthetic scheme or protocol based on the literature search.
CLO-4: Present experiments and analyze the data.
CLO-5: Prepare the power point presnetation based on the literature search

Mapping of Course learning outcomes (CLOs) with Program learning outcomes (PLOs)

	PLO 1	PLO 2	PLO 3	PLO 4	PLO 5	PLO 6	PLO 7	PLO 8	PLO 9	PLO 10	PLO 11	PLO 12
CLO-1	3	3	2	3	1	2	3	2	1	3	1	3
CLO-2	3	3	2	2	1	2	3	2	1	3	1	2
CLO-3	3	3	3	3	2	3	3	2	3	3	3	3
CLO-4	3	3	1	3	2	3	1	2	3	2	3	2
CLO-5	2	2	3	3	---	1	3	2	1	3	3	3

Students have to consult respective faculty members and select topics of their interest. One student should work on a single topic based on the choice of interest. Guide allotment for the Literature survey and seminar will be based on choice cum merit.
Once guide allotment is declared, the student has to survey literature with the help of guide during the semester and submit a report and give a presentation individually at the end of the course. Research presentation carries 20% of the marks. Students will be periodically assessed for their literature survey work by the individual faculty member or group of faculty members and 20% of the marks will be credited for this continuous assessment.

The final presentation of the research topic, presentation, and comprehensive viva carries 60% marks.

Semester-IV

PCHRC41500: Research training & Project report **Credit-20**

Code	Type	Title	Credits	Hours	L	T	P
PCHRC41500	Research	Research training & Project report	20	40	0	2	38

Prerequisite Course/Knowledge (If any): **NIL**

Course Learning Outcomes (CLOs)

After completion of this course successfully, the students will be able to……

CLO-1: Understand and identify new research problems in chemistry.
CLO-2: Collect literature in the identified research area using scientific resources.
CLO-3: Design the new synthetic scheme or protocol based on the literature search.
CLO-4: Execute experiments to collect and analyze the data.
CLO-5: Prepare the research report based on the obtained results.

Mapping of Course learning outcomes (CLOs) with Program learning outcomes (PLOs)

	PLO 1	PLO 2	PLO 3	PLO 4	PLO 5	PLO 6	PLO 7	PLO 8	PLO 9	PLO 10	PLO 11	PLO 12
CLO-1	3	2	2	3	3	3	3	3	3	3	3	3
CLO-2	3	2	1	3	3	2	3	3	3	--	3	2
CLO-3	3	3	3	3	3	3		3	2	--	3	2
CLO-4	3	3	3	3	3	3	1	3	2	1	--	2
CLO-5	3	2	3	2	2	2	2	1	3	1	2	3

Detailed Syllabus:

Individual faculty members will float a stipulated number of projects. Students have to consult respective faculty members and select projects. More than one student can work under a single project based on the nature of the project. Guide allotment for the MSc project will be based on choice cum merit.

Once guide allotment (either single or more than one guide) is declared, the student has to submit a research proposal and give a presentation, either individually or one member from the group. Research proposal & presentation carries 20% of the marks. Students will be periodically assessed for their project work by the individual faculty member or group of faculty members and 20% of the marks will be credited for this continuous assessment.

The final submission of the research project i.e. small thesis, presentation, and comprehensive viva carries 60% marks.

Note:

1. Student should submit 3 copies of the final research project copy in hard binding format with all declarations and signatures.
2. For referencing any ACS journal pattern should be followed.