M.Sc. Chemistry & Ph.D Chemistry

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 behavior 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 = 23

Code	Type	Title	Credits	Hours	L	T	P
PCHTCC1001	Core -1	Inorganic Chemistry – I	4	4	3	1	0
PCHTCC1002	Core-2	Organic Chemistry – I	4	4	3	1	0
PCHTCC1003	Core-3	Physical Chemistry – I	4	4	3	1	0
PCHTCC1004	Core-4	Introduction to Analytical Chemistry	3	3	2	1	0
PCHTCC1005	Core-5	Mathematics for Chemistry	2	2	1	1	0
PCHPCC1006	Core-6	Organic Chemistry Laboratory	3	6	0	2	4
PCHPCC1007	Core-7	Analytical & Computational Chemistry Laboratory	3	6	0	2	4
Total			**23**	29	12	9	8

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

Semester-II — No. of credits = 24

Code	Type	Title	Credits	Hours	L	T	P
PCHTCC2008	Core-8	Inorganic Chemistry – II	4	4	3	1	0
PCHTCC2009	Core-9	Organic Chemistry – II	4	4	3	1	0
PCHTCC2010	Core-10	Physical Chemistry – II	4	4	3	1	0
PCHTCC2011	Core-11	Chemistry of Life	4	4	3	1	0
PCHTCC2012	Core-12	Chemical applications of Group Theory	2	2	1	1	0
PCHPCC2013	Core-13	Inorganic Chemistry Laboratory	3	6	0	2	4
PCHPCC2014	Core-14	Physical Chemistry Laboratory	3	6	0	2	4
Total			**24**	30	13	9	8

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

Semester-III — No. of credits = 25

Code	Type	Title	Credits	Hours	L	T	P
PCHTCC3015	Core-15	Molecular Spectroscopy	4	4	3	1	0
PCHTCC3016	Core-16	Spectroscopic Identification of Organic Compounds	4	4	3	1	0
PCHTCC3017	Core-17	Organometallic Chemistry	4	4	3	1	0
PCHTCC3018	Core-18	Organic Chemistry-III	4	4	3	1	0
PCHTDS3080	Generic Elective Course-01	MOOC Course (NPTEL; SWAYAM) / Other Department Elective	3	3	2	1	0
PCHPAE3041	Ability Enhancement Compulsory Course-01	Research Orientation & instrumentation	6	12	0	4	8
Total			**25**	**31**	**14**	**9**	**8**

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

Semester-IV — No. of credits = 12

Code	Type	Title	Credits	Hours	L	T	P
PCHRDS4061	Discipline Specific Elective-014	Research training & Project report	12	24	0	6	18
Total			**12**	**24**	**0**	**6**	**18**

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

Semester-wise distribution of courses

Semester	I	II	III	IV	Total
Core Course	23	24	16	---	**63**
Ability Enhancement Compulsory Course	---	---	06	---	**06**
Discipline Specific Elective	---	---	---	12	**15**
Generic Elective Course	---	---	03	---	**03**
Total	**23**	**24**	**25**	**12**	**84**

Total No. of Credits = 84

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

Semester-I

PCHTCC1001: Inorganic Chemistry-I **Credit 4**

Code	Type	Title	Credits	Hours	L	T	P
PCHTCC1001	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: Understand the fundamentals and applications of VSEPR, VBT, and MO theories governing the inorganic chemistry.
CLO-2: Understand the structure, bonding, and properties of electron-deficient clusters and cages of boron, silicon, and phosphorus compounds.
CLO-3: Categorize inorganic solids into different classes based on its structure, chemical property, and applications.
CLO-4: Apply the knowledge of radioactivity and nuclear reactions into various applications such as radio-dating, reaction mechanisms, and nuclear energy.
CLO-5: Apply basic concepts into other branches of chemistry and other allied subjects.

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- Periodic Table and Bonding: Arrangement of elements in the Periodic Table, periodic properties. Bonding and structure: Types of bonds, orbital symmetry and overlaps, concept of VB and MO theory, concept of hybridization, bond energy and covalent radii, concept of resonance, molecular dipole moment, Fajan's rules. **(12 Hrs)**

UNIT II-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 and layered structures. Lattice energy, Born-Lande equations and modifications. Defects (0D, 1D, 2D, 3D) in ionic solids and associated theories. Band theory, semiconductors and its type & superconductors. **(15 Hrs)**

UNIT III-p block elements: Boron hydrides (small boranes and their anions, B1−B4), boron nitride, borazines, carboranes, metalloboranes, metallocarboranes. Diamond, graphite, fullerenes, silicates, silicones, zeolites, organo-silicon compounds. Phosphorus allotropes, Berry's pseudo rotation, phosphorus-nitrogen compounds, organo-phosphorus compounds, hydrides, oxides and oxy acids of nitrogen, phosphorus, sulphur and halogens, sulphur-nitrogen and inter-halogen compounds, pseudohalogens ,poly halide anions, noble gas compounds. **(30 Hrs)**

UNIT IV- Nuclear Chemistry Nuclear chemistry: radioactive decay and equilibrium. nuclear reactions, Q value, cross sections, types of reactions, chemical effects of nuclear transformations; fission and fusion, fission products and fission yields; radioactive techniques, tracer technique. **(7 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.

PCHTCC1002: Organic Chemistry-I Credit- 4

Code	Type	Title	Credits	Hours	L	T	P
PCHTCC1002	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 the chemical reactions.

CLO-2: Demonstrate chirality in organic molecules using units such as center, axial, planar

, and helicity.

CLO-3: Predict E/Z and R/S configuration in organic molecules by applying concepts of stereochemistry

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 types of organic 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-kintetic, isotope effects, and reaction profile diagram, Hammet and Taft equations. Criteria of aromatic, benzenoid & non benzenoid compounds, antiaromatic & homoaromatic compounds. Intermediates in reaction**:** Generation, structure stability and formation of carbocation, carbanion, non-classical carbocations, free radicals, carbenes and nitrenes. **(16 Hrs)**

UNIT-II: Stereochemistry: Influence of hybridization on structure of organic compounds. 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, DL and RS 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 **(24 Hrs)**

UNIT-III:Substitution reactions: The S_N2, S_N1, mixed S_N1 and S_N2 and SET mechanism, S_Ni mechanism, SE2 and SE1 mechanism; Reactivity effects of substrate structure, attacking nucleophile, leaving group and reaction medium; ambident nucleophile, regioselectivity, S_NAr, benzyne and S_N1 mechanism; Arenium ion mechanism, ipso attack, orientation in other ring systems; Neighbouring group participation. **(08 Hrs)**

UNIT-IV: 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)**

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.

PCHTCC1003: Physical Chemistry-I — Credit - 4

Code	Type	Title	Credits	Hours	L	T	P
PCHTCC1003	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 quantum chemistry, classical and statistical thermodynamics
CLO-2: Develop problem-solving ability in quantum chemistry and thermodynamics
CLO-3: Recognize the role of multidisciplinary streams especially basic physics & mathematics knowledge in the development of quantum chemistry & thermodynamics
CLO-4: Apply the fundamental knowledge in quantum chemistry & thermodynamics to an 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	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, first law of thermodynamics, enthalpy and heat capacities- concept of entropy, second law of thermodynamics, third law of thermodynamics-residual entropy. Free energy, chemical potential, fugacity, liquids and solutions: ideal and non-ideal solutions, chemical equilibrium. **(16 Hrs)**

UNIT II-Statistical Thermodynamics: BE, FD, MB statistics and distribution, partition functions and molecular partition functions, 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, Black body radiation, photoelectric effect, Classical mechanics, Lagrange & Hamiltonian equation, Inadequacy & 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 viral 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. **(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. Physical Chemistry, R.S.Berry, S.A.Rice and J.Ross, 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

PCHTCC1004: Introduction to Analytical Chemistry — Credit -3

Code	Type	Title	Credits	Hours	L	T	P
PCHTCC1004	Core-4	Introduction to Analytical Chemistry	3	3	2	1	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: Thermal 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. **(12 Hrs)**

UNIT-II: 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. **(12 Hrs)**

UNIT-III: Electroanalytical Methods and Electrochemical Sensors: Introduction of electrochemical cells: *Potentiometry:* Types of electrodes: Reference electrode, Indicator electrode, Glass electrode, and Ion-selective electrodes, Liquid memberane electrode, Clark's electrode. *Coulometry:* Different methods, Coulometric titration and Conductometric titrations. *Voltammetry:* Principle, Voltammograms, Equation of Voltagram, Modified Voltametric methods, DPV, Cyclic Voltammetry, Amperometry, and Anodic Stripping Voltammetry. *Electrochemical Sensors:* (a) Ion sensors (B) Oxygen Sensors (C) Glucose Sensors **(12 Hrs)**

UNIT-IV: Separation Techniques: Solvent extraction, thin-layer chromatography, gas chromatography (GC), liquid chromatography (LC), high performance liquid chromatography (HPLC), ion exchange chromatography, gel permeation chromatography. Chromatography coupled instrumentation. **(12 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. A.J. Bard e L.R. Faulkner " Electrochemical methods. Fundamentals and Applications " J. Wiley & Sons, New York, 2001
7. Skoog, D.A., West, D.M., Holler, F.J., and Crouch, S.R., Fundamentals of Analytical Chemistry, Brooks/Cole (2003) 8th ed.

PCHTCC1005: Mathematics for chemistry — Credit -2

Code	Type	Title	Credits	Hours	L	T	P
PCHTCC1005	Core-5	Mathematics for chemistry	2	2	1	1	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 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.

PCHPCC1006: Organic Chemistry Laboratory **Credit -3**

PCHPCC1006	Core-6	Organic Chemistry Laboratory	3	6	0	2	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	Fractional & Vacuum Distillations. Ex. Hexane, Ethyl Acetate, DMF, DMSO
2-3	Separation and Qualitative analysis of an organic mixture containing two components. At least two experiments to be performed
4	Thin Layer Chromatography (TLC)
5	Separation of compounds using Column Chromatography and Medium Pressure Liquid Chromatography (MPLC)
6	Synthesis of Dibenzalpropanone from benzaldehyde and acetone
7	Synthesis of a Chalcones *via* Claisen-Schmidt condensation.
8	Nitration of Salicylic acid using Calcium nitrate.
9	Preparation Aspirin by acetylation.
10	Bromination of Acetanilide: Green Approach
11	Photoreduction of benzophenone to benzopinacol
12	Synthesis of benzopinacol from benzophenone using Photoreduction

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.

PCHPCC1007: Analytical & Computational Chemistry Laboratory **Credit-3**

PCHPCC1007	Core-7	Analytical & Computational Chemistry Laboratory	3	6	0	2	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	Plotting atomic orbitals and hybrid orbitals using Origin software.
3	Conformational analysis of cyclohexane using Materials Science platform of Schrödinger software.
4	Indexing an XRD pattern-Determination of density by X-ray method.
5	Morse's potential plot of oxygen molecule by density functional theory using Quantum ESPRESSO software.
6	Computational drug design through protein-ligand docking using Glide tool of Schrodinger software.
7	Estimation of temporary and permanent hardness of tap water and packed drinking water by complexometric titration.
8	Determination of pKa1 and pKa2 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	Estimation of molar extinction co-efficient of KMnO4 and K2Cr2O7 by colorimetry.
12	Determination of molecular weight of proteins using SDS-PAGE.

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

PCHTCC2008: Inorganic Chemistry-II **Credit -4**

Code	Type	Title	Credits	Hours	L	T	P
PCHTCC2008	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 to transition metal complexes: A brief history of coordination chemistry, nomenclature, coordination numbers, geometry and isomerism, chelate effect and stability constants. **(10 Hrs)**

UNIT II-Theories of transition metal complexes: Valence bond theory, Crystal field theory, crystal field splitting, application of d-orbital splitting to explain magnetic properties, low spin and high spin 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 energies, site preference energies. Molecular Ortbital theory of complexes (quantitative principles involved in complexes without pi and with pi bonding), ligand field theory. **(20 Hrs)**

UNIT III-Electronic spectra and Magnetism of transition metal complexes: Electronic spectra of transition metal complexes, selection rules, correlation diagram, Orgel and Tanabe-Sugano diagrams and Lever plot, charge transfer and d-d transitions, Jahn-Teller effect, nephelauxetic series. Dia, para, ferro and antiferromagnetism, quenching of orbital angular moment, spin-orbit coupling. **(20 Hrs)**

UNIT IV-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; electron transfer reactions. **(10 Hrs)**

UNIT V- Lanthanides and Actinides: Chemistry of lanthanides and actinides: lanthanide contraction, oxidation states, spectral and magnetic properties, use of lanthanide compounds as shift reagents. (**4 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, ***Inorganic Chemistry,*** 7th Edn, Oxford University Press India, 2018.

PCHTCC2009: Organic Chemistry-II — Credit- 4

Code	Type	Title	Credits	Hours	L	T	P
PCHTCC2009	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 the basic oxidation and reduction reactions on organic molecules.
CLO-2: Apply reagents in the stereoselective reactions using mild reagents.
CLO-3: Plan to synthesize molecules using popularly named reactions.
CLO-4: Categorize the photochemical reactions and construct various cyclic molecules.
CLO-5: Apply oxidations, reductions, photochemical 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: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. **(18 Hrs)**

UNIT-II: 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-III: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-IV: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)

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.

PCHTCC2010: Physical Chemistry-II **Credit -4**

Code	Type	Title	Credits	Hours	L	T	P
PCHTCC2010	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: Basic Chemical Kinetics Molecularity, order and rate of reactions, Arrhenius theory - Complex reactions: reversible, pre-equilibrium, consecutive, chain and photochemical, oscillatory reactions, enzyme kinetics - Lindenmann's theory of uni-molecular reactions - laser flash photolysis, flow techniques and relaxationmethods. **(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 **(6 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., HarperInternational, 1987.
2. G. D. Billing & K. V. Mikkelson, Molecular dynamics and chemical kinetics, JohnWiley, 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

PCHTCC2011: Chemistry of Life — Credit -4

Code	Type	Title	Credits	Hours	L	T	P
PCHTCC2011	Core-11	Chemistry of Life	4	4	3	1	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: Demonstrate the applications of enzyme-kinetics in the identification of types of inhibitors.
CLO-4: Categorize biomolecules based on their biological functions and chemical structures.
CLO-5: Demonstrate the steps involved in the structure elucidation of various natural products using chemical, analytical and synthetic methods.

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

Detailed Syllabus:

UNIT I: Bioinorganic chemistry I: Occurrence of elements, specific ligands, and coordination sites in biomolecules. Metal homeostasis in biology: Transport and storage of K^+, Ca^{2+} Iron and copper. Dioxygen transport and storage: haemoglobin, myoglobin, hemerythrin and hemocyanine and their electronic structural properties. Synthetic oxygen carrier and model systems. Electron Transfer protein and photosynthesis: Cytochromes, Fe-S Clusters and blue-copper, metal in photosystems I and II. Enzymes and its classifications. The role of metallo enzymes: peroxidase, catalse and cytochrome P-450, superoxide dismutase and carboxypeptidase A, carbonicanhydrase, vitamin B12 and nitrogenase. Medicinal bioinorganic chemistry. (**28 Hrrs)**

UNIT II: Biophysical chemistry: Chemistry and biology of water, Chemical forces responsible for stability of biomolecules; hydrogen bonding; electrostatic interactions, hydrophobic interactions; stacking interactions; enzymes, catalysis, and kinetics- Michaelis-Menten equation, and Lineweaver–Burk plot; enzyme inhibition and different types of enzyme inhibition. **(8 Hrs)**

UNIT III: Bioorganic chemistry: Biopolymers-DNA, RNA and Proteins- structures of monomers, bonding, and hierarchy of structural organization. Chemical methods involved in sequencing of DNA and Proteins. Chemical and biochemical synthesis of DNA- Phosphoramidite method and replication. Chemical and biochemical synthesis of peptides/proteins- solution phase and solid phase peptide synthesis methods and ribosomal synthesis of proteins. Applications of PNAS. **(12 Hrs)**

UNIT IV: Natural product chemistry: Chemistry of terpenes- general methods, classification and special isoprene rule. Characterization of terpenes- Citral, limonene, carotene. Biosynthesis of acyclic and monocyclic terpenes from acetyl CoA. **:** Chemistry of steroids-Structure of common steroids such as cholesterol and steroidal hormones; Chemical and biochemical synthesis of cholesterol; Chemical synthesis of hormones using cholesterol; Chemistry of alkaloids - structure determination and synthesis of nicotine, morphine, cocaine. **(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. C.R. Cantor & P.R. Schimmel, Biophysical Chemistry, W.H.Freeman& Company, 1980
7. David Van Vranken and Gregory A, Introduction to Bioorganic Chemistry and Chemical Biology. Garland Science (Taylor & Francis), 2012.

8. R.H. Thomson, Chemistry of Natural Products - Wiley, New York, 1996.
9. I. L. Finar, *Advanced Organic Chemistry*, Vol. 2 ELBS, New Delhi, 1975.
10. Bhat, S. V., Nagasampagi, B.A., Meenakshi, S. (2009). *Natural Product Chemistry & Applications*, Narosa Publishing House, New Delhi.

PCHTCC2012: Chemical applications of Group Theory **Credit -2**

Code	Type	Title	Credits	Hours	L	T	P
PCHTCC2012	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

PCHPCC2013: Inorganic Chemistry Laboratory — Credit -3

PCHPCC2013	Core-13	Inorganic Chemistry Laboratory	3	6	0	2	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 twelve of the following experiments will be conducted)

S.No	Practical
1	Preparation of cobalt ammine complexes $[Co(NH_3)_6]Cl_3$, $[Co(NH_3)_5Cl]Cl_2$, $[Co(NH_3)_4Cl_2]Cl$.
2	Preparation of *cis* and *trans* –bis(glycinato) copper (II) monohydrate Determination of percentage weight of copper in $[Cu(glycinato)_2].H_2O$.
3	Preparation of tris(ethylenediamine)cobalt(III) chloride, $[Co(en)_3]Cl_3$.
4	Preparation of tris(ethylenediamine)nickel(II)chloride dihydrate$[Ni(en)_3]Cl_2$. $2H_2O$ and Dichlorobis(ethylenediamine)nickel(II) dihydrate$[Ni(en)_2Cl_2]$. $2H_2O$ from $[Ni(en)_3]Cl_2$. $2H_2O$.
5	Preparation of lanthanum hexacyanoferrate (III) pentahydrate, $La[Fe(CN)_6].5H_2O$. Calculating the percentage of $[Fe(CN)_6]^{3-}$
6	Estimation of iodine in iodised common salt using Iodometry.
7	Colorimetry: Simultaneous determination of chromium and manganese in a solution by visible spectroscopy.
8	Analysis of Brass (Gravimetric and Volumetric).
9-12	Qualitative analysis of binary mixture (Group analysis of Cations and Anions along with less common metals).
13	Preparation of Silicon based linear and cyclic polysiloxane polymers and its characterization by Infrared spectra.
14	Preparation and characterization of Ferrocene
15	Preparation and characterization of tris(acetylacetonato) aluminum(III)

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)

PCHPCC2014: Physical Chemistry Laboratory **Credit -3**

PCHPCC2014	Core-14	Physical Chemistry Laboratory	3	6	0	2	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)

Note: In the given module any two experiments will be conducted.

S.No	Practical
1	**Potentiometric Titration (Electrodics)** I. Determination of standard redox potential of standard redox couple. II. 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). III. Potentiometric titration of mixture of halides. IV. Determination of standard reduction potential of quinhydrone electrode. V. Potentiometric titration of mixture of acids (strong & weak) with strong base. VI. Redox-titration: Determination of concentration of reductant or oxidant by potentiometric method.
2	**Conductometric Titration (Ionics)** I. Solubility product of sparingly soluble salt by conductance measurements. II. Determination of Equilibrium constant & equivalent conductance at infinite dilution of a weak electrolyte.

	III. Determination of equivalent conductance at infinite dilution of strong electrolyte. IV. Verification of Ostwald's dilution law. V. Conductometric determination of mixture of acids using strong electrolyte. VI. Conductometric determination of critical micelle concentration of any given surfactant.
3	**Chemical Kinetics** I. 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) (**This practical is equivalent to three different experiments**). II. Kinetics of iodination of acetone by spectrophotometry or by colorimetry method a)Acetone effect; b)Iodine effect; c)Acid effect (**This practical is also can be split into at least two separate experiments**). III. Kinetics of alkaline hydrolysis of dye such as crystal violet or similar such compounds by spectrophotometry or colorimetry method. IV. Determination of rate constant of Inversion of sucrose by polarimeter & verification of the effect of catalyst on the rate constant. V. Kinetics of catalytic decomposition of hydrogen peroxide.
4	**Thermodynamics, Phase rule, SurfaceChemistry** I. Vapour pressure measurements and enthalpy of vaporisation of solvent such as water. II. Heat of neutralisation of a strong acid by a strong base. III. Adsorption of acetic acid or iodine on charcoal. IV. Critical micelle concentration of given surfactant by surface tension measurements. V. Three component liquid system (acetic acid, benzene, water). VI. Two component simple eutectic system (Examples: o-nitrophenol & naphthalene, acetamide & Benzoic acid, p-nitrotoluene & diphenylamine etc.). Determination of dimerization constant of benzoic acid in organic medium.
5	**Miscellaneous experiments (pH, Colorimetry etc.)** I. Determination of Composition & stability constant of given complex such as Fe (III)- Salicylic acid complex by Job's method using colorimetry. II. Verification of Beer-Lambert's law & determination of concentration of unknown solution.

	III. Determination of ionic product of water by pH metric method. IV. Determination of hydrolytic constant of given salts such as ammonium chloride by pH metric method. V. Determination of pKa of dibasic or tribasic acids by pH-metric methods. VI. Determination of strength of individual acids (E.g. HCl & acetic acid) in a mixture by pH metric method.

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

PCHTCC3015: Molecular Spectroscopy **Credit -4**

Code	Type	Title	Credits	Hours	L	T	P
PCHTCC3015	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, NMR, EPR, Mossbauer spectroscopy and NQR.
CLO-4: Differentiate various resonance techniques used in the analysis of molecules.
CLO-5: Apply the fundamental knowledge of molecular spectroscopy to existing and an emerging problem in basic science

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 times, line widths and line shapes, 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-Other Resonance Spectroscopy Methods:- NMR of ^{1}H, ^{11}B, ^{19}F, ^{31}P and other active nuclei. NMR of simple molecules and metal complexes. NMR of paramagnetic complexes- Contact shifts. Electron paramagnetic resonance (EPR): Hyperfine splitting, *g* value, ESR of organic free radicals, zero-field splitting and Kramer's degeneracy, Line widths in Solid state EPR. The principles of Mossbauer spectroscopy. Origin of isomer shifts, quadrupole splitting and h. f. s. Nuclear quadrapole resonance (NQR). **(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.

A. Carrington and Machlachlon, *Magnetic Resonance*, Harper & Row, 1967.

4. G. M. Barrow, *Introduction to Molecular Spectroscopy*, McGraw Hill, 1964.
5. D. H. Williams and I. Fleming, *Spectroscopic methods in organic chemistry*, Tata McGraw Hill, 1998.
6. J. Micheal Hollas, *Modern Spectroscopy*, 4th Edition, Wiley India Pvt Ltd, 2010
7. Harald Gunther, *NMR Spectroscopy: Basic Principles, Concepts and Applications in Chemistry*, 2nd Edition, Wiley India Pvt Ltd, 2010
8. 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.
11. J.Micheal Hollas, Basic Atomic and Molecular Spectroscopy: (Tutorial Chemistry Texts), Royal Society of Chemistry, 2002
12. D.N.Sathyanarayana, Vibrational Spectroscopy: Theory and Applications, New Age International, 2005

PCHTCC3016: Spectroscopic Identification of Organic Compounds **Credit – 4**

Code	Type	Title	Credits	Hours	L	T	P
PCHTCC3016	Core-16	Spectroscopic Identification of Organic Compounds	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: 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: Structure elucidation. Application of UV – Visible and IR spectroscopy to organic structure elucidation. Electromagnetic spectrum, absorption of energy by organic compounds, types of spectroscopic methods to organic structure elucidation. Woodward – Fisher rules, Octant rule, Application of ORD – CD to stereochemical assignments. Organic functional group identification through IR spectroscopy. **(16 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. **(16 Hrs)**

UNIT-III: 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. **(12 Hrs)**

UNIT-IV: 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. **(20 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.

PCHTCC3017: Organometallic Chemistry — Credit – 4

Code	Type	Title	Credits	Hours	L	T	P
PCHTCC3017	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 1: Introduction, history, classification of ligands, 18-electron rule, metal carbonyls: synthesis, structure, π- bonding and infrared spectroscopy and reactions of metal carbonyls. Organometallic complexes (OMCs) with alkyl group, alkene and alkyne as ligands, synthesis, reactions and bonding models. OMC of neutral spectator ligands: phosphines, multidentate phosphines, chiral phosphines and NHCs. **(20 Hrs)**

UNIT II-Organometallic Chemistry 2: Brief about organometallic compounds of ***s***-and ***p***-block elements. Complexes containing η^5- cyclopentadienyl ligands: ferrocene and other metallocenes: structure, bonding and reactions. OMCs containing η^{4}- η^6- η^7- and η^8 ligands. Multinuclear carbonyl clusters, metal-metal bond, Mingo's rules, isolobal analogy. Hydride, dihydrogen complexes and fluxionality. (**15 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. **(24 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.

PCHTCC3018: Organic Chemistry-III — Credit – 4

Code	Type	Title	Credits	Hours	L	T	P
PCHTCC3018	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: Summarize photochemical intermediates involved in organic reactions.
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: Write the synthetic schemes based on photochemistry, enolates, and heterocyclics.

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: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)**

UNIT-II: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 chemoselectivity, 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)**

UNIT-III: Enolate of carbonyl compounds: Kinetic and thermodynamic control, Potential energy diagrams, methods of determining mechanisms, isotopes effects, regionand stereo-selective reactions. Enolates: Regio- and stereo-selectivity in enolate generation. "O" versus "C" alkylation, Effect of solvent, Counter cation and Electrophiles; Symbiotic effect; Thermodynamically and kinetically controlled enolate formations; Various transition state models to explain steroselectiveenolate formation; Enamines; Regioselectivity in generation, Application in controlling the selectivity of alkylation. **(12 Hrs)**

UNIT-IV: 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)**

Reference books:

1. Finar, I.L. (2006). *Organic Chemistry: Stereochemistry and the Chemistry of Natural Products.* Dorling Kindersley Pvt. Ltd., 6th edition, India.
2. McMurry J., *Organic Chemistry***,** Asian Book Pvt. Ltd, 8th edition, New Delhi.
3. Morrison, R.T., Boyd, R.N. (2011). *Organic Chemistry*, Prentice- Hall of India, 6th edition, New Delhi.

4. Clayden,J.;Greeves,N.;Warren,S., (2012). *Organic Chemistry*, Oxford University press, 2nd edition.
5. Warren S.; Wyatt, P. (2008). *Organic Synthesis The Disconnection Approach*, Wiley 2nd edition.
6. Coyle, J. D. (1991), *Introduction to organic photochemistry*, Wiley.
7. Halton, B.; Coxon J. M. (2011), *Organic Photochemistry*, Cambridge University Press.
8. Smith, M. B.; March, J. (2007), *March's Advanced Organic Chemistry*, Wiley 6th edition.

PCHTGE3080: MOOC Course (NPTEL; SWAYAM) / Other Department Elective Credit -3

Code	Type	Title	Credits	Hours	L	T	P
PCHTGE3080	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.

PCHPAE3041: Research Orientation & instrumentation Credit-6

PCHPAE3041	Ability Enhancement Compulsory Course-01	Research Orientation & instrumentation	6	12	0	4	8

Prerequisite Course/Knowledge (If any): **MSc Chemistry laboratory courses in Semester-I and Semester-II**

Course Learning Outcomes (CLOs)

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

CLO-1: Understand the fundamentals of research methodology of chemical sciences
CLO-2: Apply the research and publication ethics
CLO-3: Demonstrate the applications of Intellectual Property Rights (IPR)
CLO-4: Employ sophisticated instruments to study the chemical compounds
CLO-5: Develop critical thinking and orientation towards research projects.

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

Detailed Syllabus:

UNIT-I: Research methodology: Research, Definition, Need of research, Identification of the problem, Laboratory Methods of research: Qualitative and Quantitative, Research evaluation methods. Research and publications ethics. Publication misconduct. Structuring the M.Sc. thesis and thesis writing. **(16 Hrs)**

Unit-II: IPR and Innovations: Introduction to Intellectual Property Rights (IPR). International treaties and conventions. Types of IPRS such as patents, designs, copyrights. IP Policy statements of India, US and Europe. Patent search, drafting and filing of patent application. Case Studies. IP as a career option, types of roles, and recruiters. **(16 Hrs)**

Unit-III: Instrumentation: Hands-on experience of advanced instruments such as UV-visible Spectrophotometer, FT-IR Spectrometer, polarimeter, RP-HPLC, MPLC, Electrochemical work-station, Raman spectrometer, Lyophilizer, Fluorescence Spectrometer, Photochemical reactor. basic instruments such as rotary evaporator, pH meter, Melting-pint apparatus, Vacuum oven and Furnace. **(32 Hrs)**

Unit-IV: Defining M.Sc project problem: Concerned students and faculties finalize the M.Sc research project and related activities. **(32 Hrs)**

Reference books:

1. J. Anderson, B. H. Dursten and M. Poole, Thesis and Assignment Writing, Wiley Eastern.
2. D. C. Harris Quantitative Chemical Analysis, 2007, W. H. Freeman and Company
3. R. Panneerselvan, Research Methodology, PHI, New Delhi.
4. Michael M. Marda, Research Methods of Science, 1st Ed., Cambridge University Press, New York.
5. Acharya, N. K., (2001). *Textbook on intellectual property rights,* Asia Law House.
6. Ganguli, P. (2001). *Intellectual Property Rights; Unleashing the Knowledge Economy*, Tata McGraw-Hill.
7. Watal Jayashree, *Intellectual Property Rights in the WTO and developing countries*, Oxford University Press, Oxford.
8. Guru Manjula, Rao, M.B., (2003). *Understanding Trips: Managing Knowledge in Developing Countries*, Sage Publications.

Semester-IV

PCHRDS4061: Research training & Project report **Credit-8**

Code	Type	Title	Credits	Hours	L	T	P
PCHRDS4061	Discipline Specific Elective-01	Research training & Project report	12	24	0	6	18

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. The student allotment to the guide will be done at the end of Semester II.

The following evaluation pattern will be followed for the Research training & Project report

Examination	Items	Marks
Internal	M.Sc thesis assessment committee (Three member committee):	
	(i) Supervisor	60
	External evaluation:	
	(i) one faculty within the department	30

	(ii) one faculty outside the department/university	30
Total internal marks		120
End semester	All the faculties in the department are involved in the assessment	
	Presentation	90
	Viva-voce examination	90
	Total end semester marks	180

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.

Ph.D. Chemistry

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

Name of the Academic Program Ph.D Chemistry

Qualification Descriptors (QDs)

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

QD-1: Demonstrate commendable knowledge and skills in advanced and interdisciplinary areas of chemistry.

QD-2: Employ sophisticated techniques and sound research methodologies to achieve the comprehensive solutions for specific problems.

QD-3: Apply disciplinary knowledge and transferable skills to the interdisciplinary areas of chemistry to solve the unsolved problems.

QD-4: Develop international standards in writing, communications, team-work, and ethics to disseminate results of research work.

QD-5: Prepares future researchers, scientists, team-leaders, and scientific intellectuals in the the chosen area of chemistry.

QD-6: Demonstrate abilities to analyze the conditions in a given area of chemistry to create employment opportunities for chemists and society.

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

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

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

Name of the Academic Program Ph.D Chemistry

Program Learning Outcomes (PLOs)

After the completion of Ph.D Chemistry programme, the student will be able to:

PLO-1: Justify the need for conducting research work for the wellbeing of society and the world.

PLO-2: Develop skills to recognize the unsolved problem in the chosen area of the research field.

PLO-3: Design methodology to provide an amicable and elegant solution to research problems.

PLO-4: Synthesize new and novel compounds/drugs/materials useful for mankind.

PLO-5: Interpret results based on true observations of data derived from experimentation.

PLO-6: Create new knowledge in chemistry that is useful for science/public communities.

PLO-7: Write research articles/reviews/communications of international standards.

PLO-8: Develop abilities to handle sophisticated instruments and computational software.

PLO-9: Relates philosophy, integrity, and ethics in the publication of research work.

PLO-10: Prepares future academicians, scientists, researchers, and job creators**.**

PLO-11: Generates highly skilled, intelligent, and cleaver manpower for society.

PLO-12: Create global leaders in the chosen area of the research field of science and technology.

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

Ph.D Chemistry_ Course Structure
Department of Chemistry
Central University of Karnataka, Kalaburagi

Semester-I **No. of credits = 12**

Code	Type	Title	Credits	Hours	L	T	P
DCHTCC1001	Core-1	Research Methodology	4	4	3	1	0
DCHTCC1002	Core-2	Research and publication ethics	2	2	1	1	0
DCHTDS1061	Discipline Specific	Research Specific Course	2	2	2	1	0
DCHPAE1041	Ability Enhancement Compulsory Course	Research preparation and Instrumentation	4	8	0	2	6
Total			**12**	16	7	5	6

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

Distribution of courses

Semester	I
Core Course	06
Discipline Specific Elective	02
Ability Enhancement Compulsory Course	04
Total	**12**

Semester-I

DCHTCC1001: Research Methodology **Credit 4**

Code	Type	Title	Credits	Hours	L	T	P
DCHTCC1001	Core-1	Research Methodology	4	4	3	1	0

Prerequisite Course/Knowledge (If any): **General aptitude**

Course Learning Outcomes (CLOs)

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

CLO-1: Describe research, identification of research problems, and preparation of proposals.
CLO-2: Practice ethics in all the domains of research.
CLO-3: Analyze the results using mathematical and statistical tools
CLO-4: Develop skills to use ChemDraw, Origin Lab, Schrödinger, and Quantum Expresso, etc. in the research work
CLO-5: Outline writing of research publication, presentation, and Ph.D. thesis.

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

Detailed Syllabus:

UNIT I: Research methodology: Research, Definition, Need of research, Identification of the problem, Research evaluation methods, Various indexes (h-index, i-index, etc.). Laboratory Methods of research: Qualitative and Quantitative. Preparations of Research proposal/Synopsis. Literature survey (Chemical abstracts, Scopus, Scifinder etc.). Research report, articles, review, and references. Structuring the Ph.D. thesis and thesis writing. Research specific ethics lectures. **(16 Hrs)**

UNIT II: Data and Errors analysis: Data: Types (primary and secondary data), collection methods; presentation (graphical and diagrammatical); relevance, limitations and cautions; Data Processing: checking, editing, coding, transcriptions, classifications and tabulation. Data Analysis: meaning and methods; quantitative and qualitative analysis. Theoretical Distribution: normal, Poisson, binomial with application in various area/disciplines. Errors analysis: Accuracy and precision, absolute, relative, determinate and indeterminate errors. **(16 Hrs)**

UNIT III: Statistics: Introduction, Probability theories, Conditional probability, Poisson distribution, Binomial distribution and Properties of normal distributions, Estimates of Means and Proportions, Chi-Square test, Association of attributes, t-Test, Anova, Standard deviation, Co-efficient of variations, Correlation and regression analysis, Mathematical and statistical analysis using software tools MATLab, SPSS, PsiLAB etc. **(16 Hrs)**

UNIT IV: Computer applications: Computer basics, Data representation, Computer generation and classification, Computer languages, Operating systems, Computer networks.
Spreadsheet tool: Introduction to spreadsheet and its features and functions, Using formulae and functions, Generating charts/graphs and other features (Tools: Microsoft Excel, Libre office, Open office etc.)
Presentation tool: Introduction to presentation tool and its features and functions, Preparation of presentations (Microsoft PowerPoint, Libre office, Open Office etc.). **(16 Hrs)**

Reference books:

1. J. Anderson, B. H. Dursten and M. Poole, Thesis and Assignment Writing, Wiley Eastern.
2. D. C. Harris Quantitative Chemical Analysis, 2007, W. H. Freeman and Company
3. R. Panneerselvan, Research Methodology, PHI, New Delhi.
4. Michael M. Marda, Research Methods of Science, 1st Ed., Cambridge University Press, New York.
5. C. C. Kothari and Gourav Garg, Research Methodology, 3rd Ed., New Age Internationa.
6. S. K. Muthu, Probability and Error for Physical Science, Orient Lougman.
7. P. R. Majhi and P. K. Khatua, Research Methodology, Himalaya Publication House.

DCHTCC1002: Research and publication ethics Credit-2

Code	Type	Title	Credits	Hours	L	T	P
DCHTCC1002	Core-2	Research and publication ethics	2	2	1	1	0

Prerequisite Course/Knowledge (If any): **General aptitude**

Course Learning Outcomes (CLOs)

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

CLO-1: Understand philosophy and ethics in research.
CLO-2: Practice intellectual honesty and research integrity
CLO-3: Discuss scientific misconducts, conflicts of interest and predatory publishers and journals
CLO-4: Demonstrate the use of plagiarism software like Turnitin, Urkund, and other open-

source software tools

CLO-5: Judge the quality of the publications using Indexing databases

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

Detailed Syllabus:

OVERVIEW: This course has total 6 units focusing on basics of philosophy of science and ethics, research integrity, publication ethics. Hands-on-sessions are designed to identify research misconduct and predatory publications. Indexing and citation databases, open access publications, research metrics (citations, h-index, Impact Factor, etc.) and plagiarism tools will be introduced in this course.

Pedagogy: Class room teaching, guest lectures, group discussions, and practical sessions.

Evaluation: Continuous assessment will be done through tutorials, assignments, quizzes, and group discussions. Weightage will be given for active participation. Final written examination will be conducted at the end of the course.

Course structure: The course comprises of six modules listed in table below. Each module has 4-5 units.

MODULES	UNIT TITLE	TEACHING HOURS
Theory		
RPE 01	Philosophy and Ethics	4
RPE 02	Scientific Conduct	4
RPE 03	Publication Ethics	7
Practice		
RPE 04	Open Access Publishing	4
RPE 05	Publication Misconduct	4
RPE 06	Databases and Research Metrics	7
	Total	**30**

SYLLABUS IN DETAIL

THEORY

- **RPE 01: PHILOSOPHY AND ETHICS (3 Hrs)**
  1. Introduction to philosophy: definition, nature and scope, concept, branches
  2. Ethics: definition, moral philosophy, nature of moral judgments and reactions

- **RPE 02: SCIENTIFICCONDUCT (5 Hrs)**
  1. Ethics with respect to science and research
  2. Intellectual honesty and research integrity
  3. Scientific misconducts: Falsification, Fabrication, and Plagiarism (FFP)
  4. Redundant publications: duplicate and overlapping publications, salami slicing
  5. Selective reporting and misrepresentation of data

- **RPE 03: PUBLICATION ETHICS (7 Hrs)**
  1. Publication ethics: definition, introduction and importance
  2. Best practices / standards setting initiatives and guidelines: COPE, WAME, etc.
  3. Conflicts of interest
  4. Publication misconduct: definition, concept, problems that lead to unethical behavior and vice versa, types
  5. Violation of publication ethics, authorship and contributorship
  6. Identification of publication misconduct, complaints and appeals
  7. Predatory publishers and journals

PRACTICE

- **RPE 04: OPEN ACCESS PUBLISHING (4 Hrs)**
  1. Open access publications and initiatives
  2. SHERPA/RoMEO online resource to check publisher copyright & self-archiving policies
  3. Software tool to identify predatory publications developed by SPPU
  4. Journal finder/journal suggestion tools viz. JANE, Elsevier Journal Finder, Springer Journal Suggested, etc.

- **RPE 05: PUBLICATION MISCONDUCT (4 Hrs)**

  (A) Group Discussions (2 hrs.)
  1. Subject specific ethical issues, FFP, authorship
  2. Conflicts of interest
  3. Complaints and appeals: examples and fraud from India and abroad

  (B) Software tools (2 hrs.) :Use of plagiarism software like Tumitin, Urkund and other open source software tools

- **RPE 06: DATABASES AND RESEARCH METRICS (7 Hrs)**

  (A) Databases (4 hrs.)
  1. Indexing databases
  2. Citation databases: Web of Science, Scopus, etc.

  (B) Research Metrics (3 hrs.)
  1. Impact Factor of journal as per Journal Citation Report, SNIP, SIR, IPP, Cite Score
  2. Metrics: h-index, g index, i10 index, altmetrics

References

Bird, A. (2006). *Philosophy of Science*. Routledge.
MacIntyre, Alasdair (1967) *A Short History of Ethics.* London.
P. Chaddah, (2018) Ethics in Competitive Research: Do not get scooped; do not get plagiarized, ISBN:978-9387480865
National Academy of Sciences, National Academy of Engineering and Institute of Medicine. (2009). *On Being a Scientist: A Guide to Responsible Conduct in Research: Third Edition*. National Academies Press.
Resnik, D. B. (2011). What is ethics in research & why is it important. *National Institute of Environmental Health Sciences*, 1–10. Retrieved from https://www.niehs.nih.gov/research/resources/bioethics/whatis/index.cfm
Beall, J. (2012). Predatory publishers are corrupting open access. Nature, 489(7415), 179–179. https://doi.org/10.1038/489179a
Indian National Science Academy (INSA), Ethics in Science Education, Research and Governance(2019), ISBN:978-81-939482-1-7. http://www.insaindia.res.in/pdf/Ethics_Book.pdf

DCHTDS1061: Research Specific Course — Credit- 2

Code	Type	Title	Credits	Hours	L	T	P
DCHTDS1061	Discipline-Specific	Research Specific Course	2	2	3	1	0

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

Course Learning Outcomes (CLOs)

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

CLO-1: Understand the research work.
CLO-2: Identify the cutting-edge areas in related topics.
CLO-3: Develop knowledge to solve unsolved problems
CLO-4: Explain the advantages of the research work
CLO-5: Evaluate the experimental and computational skills

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

Detailed Syllabus:

Faculty research specific course can be undertaken through offline-mode or Online MOOC course (NPTEL/SWAYAM). Intention of the course is to introduce the students to cutting-edge research area of chemistry and interdisciplinary subjects. Following course are offering by the faculties at Department of Chemistry, Central University of Karnataka.

1. Chemistry and biology of peptides
2. Proteomics in Mass Spectroscopy
3. Advanced organic synthesis
4. Green Chemistry
5. Chemistry of Natural Products
6. Introduction to Nanoscience
7. Applied Electrochemistry
8. Chemical Crystallography
9. Coordination chemistry
10. Organometallic Catalysis

DCHPAE1041: Research preparation and Instrumentation **Credit 4**

Code	Type	Title	Credits	Hours	L	T	P
DCHPAE1041	Ability Enhancement Compulsory Course	Research preparation and Instrumentation	4	8	0	2	6

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

Course Learning Outcomes (CLOs)

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

CLO-1: Comply with laboratory safety and security
CLO-2: Develop skills to operate various high-end research equipment.
CLO-3: Apply various computational tools and software in day to day research
CLO-4: Analyze the data using mathematical and statistical tools
CLO-5: Illustrate IP creation, management, entrepreneurship, and content related to patents

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

Detailed Syllabus:

Unit-I: Laboratory Safety and Security: Safety rules, Chemical safety, Workplace Hazardous Material Information System (WHMIS), Material Safety Data Sheets (MSDS), Science laboratory safety signs, Emergency procedures, First aid, Rules specific for the organic chemistry laboratories, Waste management. Major safety concerns in research Labs. Policies regarding safety. Introduction to the basic concepts of green chemistry. Demonstration of hands-on training of conducting laboratory experiments through representative examples. **16 Hrs**

Unit-II: Instrumentation: Hands-on experience of basic instruments such as rotary evaporator, pH meter, Melting-pint apparatus, Liquid chromatography, TLC, Vacuum oven, Furnace and advanced instruments such as UV-visible Spectrophotometer, FT-IR Spectrometer, polarimeter, RP-HPLC, MPLC, Electrochemical work-station, Raman spectrometer, Lyophilizer, Fluorescence Spectrometer, Photochemical reactor. **16 Hrs**

Unit-III: Computational Laboratory: Hands-on training on the operation and use of 'Chemdraw' Software, Molecular analysis of crystals using Mercury software, performing literature survey using 'SciFinder', plotting the graphs and statistical analysis of the data using 'Origin' Software, molecular docking studies using Schrödinger maestro tool, density functional theory (DFT) of molecules using Schrödinger material suite tool and analysis of 3D-structure of biomolecules using 'PyMOL' software. Basic of MATLab, Comsole, Python.

16 Hrs

Unit-IV: Legal aspects of Laboratory discoveries: Introduction to Intellectual Property Rights (IPR). International treaties and conventions. Types of IPRS such as patents, designs, copyrights. IP Policy statements of India, US and Europe. Patent search, drafting and filing of patent application. Case Studies. IP as a career option, types of roles, and recruiters. **16 Hrs**

References

1. Techniques and experiments for organic chemistry, Ault A., University Science Books, 1998.
2. Green Chemistry: Theory and Practice. P.T. Anastas and J.C. Warner. Oxford University Press.
3. IPR Handbook for Pharma Students and Researchers, Parikshit Bansal, PharmaMed Press, 2008.
4. World Intellectual Property Organization, WIPO
   http : //www.wipo.int/edocs/pubdocs/en/intproperty/489/wipopub489.pdf
5. A course Book in International Intellectual Property, Doris Estelle Long and Anthony D'Amato.-St Paul, Minn.: West Publishing Co., 2000.