ఆంధ్రప్రదేశ్ కేంద్రీయ విశ్వవిద్యాలయం

आंध्रप्रदेश केंद्रीय विश्वविद्यालय

CENTRAL UNIVERSITY OF ANDHRA PRADESH

Jnana Seema, Ananthapuramu, India - 515701

DEPARTMENT OF CHEMISTRY

SCHOOL OF INTERDISCIPLINARY AND APPLIED SCIENCES

Masters Programme
(as per the National Credit Framework 2023)

Vidya Dadati Vinayam
(Education Gives Humility)

M.Sc. Chemistry

Programme Structure
(Effect from Academic Year 2026 - 27)

M.Sc. Chemistry

Department of Chemistry

School of Interdisciplinary and Applied Sciences

CONTENTS

M.Sc. Chemistry
Department of Chemistry
School of Interdisciplinary and Applied Sciences

1. Introduction to the Programme

The Master of Science in Chemistry program at the Central University of Andhra Pradesh offers an advanced and comprehensive education in chemical sciences. This program is designed to equip students with a deep understanding of core areas such as organic, inorganic, physical, and analytical chemistry, along with emerging interdisciplinary fields. Through a balanced integration of theoretical concepts and practical laboratory training, students will develop the expertise required to address scientific and industrial challenges in areas including pharmaceuticals, materials science, environmental chemistry, and chemical research.

This program offers a stimulating academic environment with access to well-equipped laboratories, experienced faculty, and opportunities for research projects and industrial exposure. Graduates of the Master of Science in Chemistry program will be well-prepared for diverse career opportunities or advanced studies in the field of chemical sciences.

2. Eligibility and Admission

Bachelor’s degree in Chemistry (Main) or with Chemistry as one of the major subjects. Candidates should have secured a minimum of 55% marks or 6.0 CGPA (on a 10-point scale) in the qualifying degree examination for the General Category, 50% marks or 5.5 CGPA (on a 10-point scale) for OBC (Non-creamy layer), EWS and 45% aggregate marks or 5.0 CGPA (on a 10-point scale) for SC/ST/PWD candidates. Admission to the programme is through the Common University Entrance Test (CUET-PG).

3. Internship

Students shall complete a summer internship (2 credits) during the first-year summer break, lasting 1-2 months. The internship will be graded in the fourth semester. They are encouraged to take up an internship at industries/ research labs/ institutes/ universities (including CUAP). The evaluation of the internship would be based on external (70%, host institution) and internal (30%, Departmental) assessment.

4. Research Project

Students shall undertake a research project (12 credits) during the 4th semester. The projects can be executed at CUAP or at other Institutes/Universities/Industries. The students' research guides in CUAP will be assigned based on their research interests and academic ranking. The project report shall be submitted in the form of a dissertation at the end of the 4th semester on or before the date notified by the Department. The student shall present the research project work and shall be evaluated through an open presentation.

5. Exit and Lateral Entry

At the end of the first year, the student can avail an exit as PG Dip. in Chemistry, following CUAP guidelines. Candidates who meet the credit requirements are permitted to enter the second year of the M.Sc. Program. Chemistry, following CUAP guidelines.

6. Programme Educational Objectives (Peos)

The M.Sc Chemistry program will enable the student to:

PEO1	understand the core and advanced chemistry concepts thoroughly
PEO2	have societal, health, safety, and cultural issues relevant to the science practices and provide a strong foundation for acquiring advanced knowledge in chemistry
PEO3	acquire critical thinking supported by advanced analytical skills to address chemistry related problems
PEO4	demonstrate the ability to perform accurate quantitative measurements with an understanding of the theory and use of sophisticated instruments, analyze and interpret
PEO5	enhance skills for employability through activities, such as seminars, communication skills, industrial visit, internship, and research project dissertation

7. Programme Specific Objectives (Peos)

Upon successful completion of M.Sc. In the Chemistry programme, the student will be able to:

PSO1	Acquire the knowledge of recent advancements in the scientific field
PSO2	Understand the features of molecules in the organic /inorganic/physical domain
PSO3	Develop computational and experimental skills to explore molecular-level phenomena
PSO4	Apply technical skills in a laboratory environment and secure challenging position in Industry & Academics
PSO5	Enhance employability through laboratory activities, solving problems and cocurricular activities

8. Graduate Attributes

DisciplinaryKnowledge: Content and pedagogical knowledge synchronized with the curriculum frameworks and policies

Communication Skills: Possess clarity in conveying ideas

Critical Thinking: The capacity to apply analytical thought in the teaching and learning process. Problem Solving: Participate in educational problem-solving and apply the knowledge in day-to-day professional endeavors.

Cooperation: Appreciate collaboration among education stakeholders.

ICT Skills: Selecting and integrating appropriate ICT skills for professional development.

Ethics: Doing what is right for society.

M.Sc. Chemistry

Department of Chemistry

School of Interdisciplinary and Applied Sciences

Semester and Course wise Credits Distribution

Semester	Core Course Crdits				DSE Credits		IDE Credits		CCC Credits				SIP Credits		Dissertation Credits		Total Credits
	Code	T	P	Total	Code	Total	Code	Total	Code	T	L/P	Total	Code	Total	Code	Total	
1	CHE101	4	0	4			CHE112 MOOC	3	-		-	-	-	-	-	-	25
	CHE102	4	0	4													
	CHE103	4	0	4													
	CHE104	4	0	4													
	CHE111		4	4													
	CHE113	2		2													
	Total	**18**	**4**	**22**	**-**		**-**	**3**	**-**	**-**	**-**	**-**	**-**	**-**	**-**	**-**	
II	CHE201	4	0	4			CHE212 MOOC	3	CCC213	2	2	4	-	-	-	-	27
	CHE202	4	0	4													
	CHE203	4	0	4													
	CHE204	4	0	4													
	CHE211		4	4													
	Total	**16**	**4**	**20**			**-**	**3**	**-**	**2**	**2**	**4**	**-**		**-**	**-**	
III	CHE301	4	0	4	CHE304	4	CHE312 MOOC	3	CCC313	2	0	2			-	-	25
	CHE302	4	0	4													
	CHE303	4	0	4													
	CHE311		4	4													
	Total	**12**	**4**	**16**		**4**	**-**	**3**	**-**	**2**	**0**	**2**			**-**	**-**	
IV													CHE411	**2**	CHE412	**12**	14
					-	**-**	**-**	**-**	**-**	**-**	**-**	**-**	**-**	**2**	**-**	**12**	
Total Courses	**15**	**-**	**-**	**-**	**1**	**-**	**3**	**-**	**2**	**-**	**-**	**-**	**1**	**-**	**1**	**-**	**23**
Total Credits	**-**	46	12	**58**	**-**	**4**	**-**	**9**	**-**	4	2	**6**	**-**	**2**	**-**	**12**	**91**
Percentage	**-**	50.53	13.18	**63.73**	**-**	**4.39**	**-**	**9.89**	**-**	4.39	2.19	**6.59**	**-**	**2.19**	**-**	**13.18**	**100**

Note: **T:** Theory **P:** Practical **DSE:** Discipline Specific Elective
IDE: Inter-disciplinary Electives **CCC:** Common Compulsory Course **SIP:** Summer Internship Project

Programme Structure

Semester I						
Sl. No.	**Course Code**	**Title of the Course**	**Credit Points**	**Credit Distribution**		
				L*	**T***	**P***
1	CHE101	Inorganic Chemistry I	4	4	0	0
2	CHE102	Organic Chemistry I	4	4	0	0
3	CHE103	Physical Chemistry I	4	4	0	0
4	CHE104	Physical Methods in Chemistry I	4	4	0	0
5	CHE111	**Lab:** Physical Chemistry Laboratory	4	0	0	4
6	CHE112	**IDE-I:** MOOCs	3	3	0	0
7	CHE113	Research Methodology and Publication Ethics	2	2	0	0
Total			**25**	**21**	**0**	**4**

Semester II						
Sl. No.	**Course Code**	**Title of the Course**	**Credit Points**	**Credit Distribution**		
				L*	**T***	**P***
1	CHE201	Inorganic Chemistry II	4	4	0	0
2	CHE202	Organic Chemistry II	4	4	0	0
3	CHE203	Physical Chemistry II	4	4	0	0
4	CHE204	Physical Methods in Chemistry II	4	4	0	0
5	CHE211	Lab: Organic Chemistry Laboratory	4	0	0	4
6	CHE212	**IDE-II:** MOOCs	3	3	0	0
7	CHE213	**CCC-I:** Introduction to AI and ML	2	2	0	0
		Lab: Introduction to AI and ML	2	0	0	2
Total			**27**	**21**	**0**	**6**

Semester III						
Sl. No.	**Course Code**	**Title of the Course**	**Credit Points**	**Credit Distribution**		
				L*	**T***	**P***
1	CHE301	Inorganic Chemistry III	4	4	0	0
2	CHE302	Organic Chemistry III	4	4	0	0
3	CHE303	Physical Chemistry III	4	4	0	0
4	CHE304	Elective	4	4	0	0
5	CHE311	**Lab:** Inorganic Chemistry Laboratory	4	0	0	4
6	CHE312	**IDE-III:** MOOCs (Preferably on Instrumentation Methods in Chemistry)	3	3	0	0
7	CHE313	**CCC-II:** Building Mathematical Ability and Financial Literacy	2	1	1	0
		Total	**25**	**20**	**1**	**4**

Semester IV						
Sl. No.	**Course Code**	**Title of the Course**	**Credit Points**	**Credit Distribution**		
				L*	**T***	**P***
1	CHE411	Research Project	12	0	0	12
2	CHE412	Internship	2	0	0	2
		Total	**14**	**0**	**0**	**14**
		Grand Total	**91**	**62**	**1**	**28**

Note: **L:** Lectures; T: Tutorial; **P:** Practical

Semester-wise Credit Distribution

Semester	Total Credits	Cumulative credit at the end of the semester
1	25	25
II	27	52
III	25	77
IV	14	91

I. Credit Requirement

- The minimum number of credits required to be earned by a student for the award of the degree is **91**.
- Students may earn credits in excess of 95 by opting for additional courses; however, the upper limit shall not exceed **96 credits**.

II. Assessment Pattern

- **Theory Courses**:
  - **Internal (40%)** – Formative evaluation comprising two best out of three tests (each test carrying a maximum of 15 marks, totalling 30 marks), along with seminar/assignments/attendance (10 marks).
  - **External (60%)** – Summative evaluation through the semester-end examination.

III. Laboratory Components:

- **Internal (60%)** – Continuous assessment through lab work and internal examination.
- **External (40%)** – Summative evaluation through the semester-end practical examination.

IV. End-Semester Examination:

- Maximum Marks: **60**
- Duration: **3 Hours**

Important Information to Students

- **i.** The minimum duration for completion of the programme is four semesters (two academic years) and the maximum duration is eight semesters (four academic years) or as per amendments made by the regulatory bodies from time to time.
- **ii.** A student should attend at least 75% of the classes, seminars, practicals in each course of study.
- **iii.** All theory courses in the programme carry a Continuous Internal Assessment (CIA) component to a maximum of 40 marks and Semester End Examination (SEE) for a maximum of 60 marks. The minimum pass marks for a course is 50%.
- **iv.** All lab components carry a Continuous Internal Assessment (CIA) component to a maximum of 60 marks and Semester End Practical Examination (SEE) for maximum of 40 marks. The minimum pass marks for a course in 50%.
- **v.** A student should pass separately in both CIA and the SEE, i.e., a student should secure 16 (50%) out of 40 marks for theory and 30 (50%) out of 60 marks in the lab components in CIA. A student should secure 30 (50%) out of 60 marks for theory and 20 (50%) out of 40 marks for lab components in the SEE.
- **vi.** There are 3 CIA tests for each course per semester from which the best 2 performances are considered for the purpose of calculating the marks in CIA. A record of the continuous assessment is maintained by the academic unit. A record of the continuous assessment is maintained by the academic unit.
- **vii.** Each CIA contains 15 marks, out of the best 2 tests scores are considered for 30 marks. Remaining 10 marks awarded for assignments, class presentations and class participation and punctuality of the student.
- **viii.** A student failing to secure the minimum pass marks in the CIA is not allowed to take the semester end examination of that course. S/he has to redo the course by attending special classes for that course and get the pass percentage in the internal tests to become eligible to take the end semester examination.
- **ix.** Semester-end examination shall consist of objective type questions, descriptive type questions, short answer questions and case studies or any other recommended by the Board of Studies (BoS).
- **x.** Students failing a course due to lack of attendance should redo the course.
- **xi.** Re-evaluation is applicable only for SEE papers and shall not be entertained for other components such as lab/practical /thesis/ dissertation/ internship etc.
- **xii.** An on-campus elective course is offered only if 10 or 50% of the students registered, whichever is higher.

SEMESTER WISE
DETAILED SYLLABUS

SEMESTER-I

Course Code: CHE 101 No. of Credits: 4	Course Title: Inorganic Chemistry I

Course Outcomes		Level
CO-1	Gain knowledge in solid state chemistry and its applications	Knowledge
CO-2	Understand the chemistry of main group elements - rings, chains and clusters	Understand
CO-3	Apply the theories of coordination chemistry to understand the metal- ligand bonding	Apply
CO-4	Analyze the stability of complexes in solution	Analyze
CO-5	Understand reaction mechanisms in inorganic complexes	Understand

CO	Program Outcomes				
	1	2	3	4	5
1	1	2	2	2	3
2	2	1	3	3	3
3	2	2	3	3	3
4	2	1	2	3	3
5	3	2	1	2	3

Course Outline:

Unit-I:

Synthesis and Reactions of Inorganic Solids: Introduction- Crystalline and amorphous solids, crystal systems, Close packing of atoms and ions HCP and FCC, packing efficiency, types of packing voids, unit cell, density and radius ratio calculations. Structures of ionic crystals – AX and AX_2 type crystal structures (NaCl, CsCl, ZnS, fluorite, antifluorite, TiO_2, SiO_2, CaC_2 etc. including unit cell calculation) – Spinel, perovskite and layer structures. Lattice energy - Born-Lande equation and its derivations and applications, Born-Mayer and Kapustinskii equations –. Stoichiometric and non-stoichiometric defects. Band theory, n- and p- type semiconductors and superconductors. Solid state synthesis and reactions in solid state **-** Introduction – law of diffusion, diffusion mechanisms, thermal decomposition of solids -Type I and Type II reactions. Different types of solid-state synthetic methods.

Unit-II:

The Chemistry of the Main Group Elements: Inorganic Rings, chains, and cages- Catenation and Heterocatenation, Heterocyclic ring system- Borazines, Phosphazines- Monomer and Polymer, S-N ring compounds, Homocyclic rings of P, S and Se. Silicate minerals and its classification based on structure. Boranes: Polyhedral skeletal electron pair theory, styx number - boron cage compounds-closo, nido, arachno, carboranes; cage compounds of S and P. Metal cluster: metal-metal bonding and reactivity of di-, tri- and polynuclear clusters, Metal cluster and metal carbonyl structure based on PSEPR theory.

Unit-III:

Theories and studies of coordination compounds: Crystal field theory – Splitting of d orbitals under various geometries - factors affecting splitting, CFSE, evidences for CFSE (Structural and thermodynamic effects), spectrochemical series, Jorgensen relation, site preferences, Jahn Teller distortion – Dynamic and Static effects. Application of CFT – Magnetic properties, spectral properties and Kinetic properties, Limitations of CFT, Ligand field Theory - nephelauxetic effect - MO theory – sigma – and pi- bonding in complexes and evidences for π-bonding – angular overlap model.

Unit-IV:

Studies of Coordination Compounds in Solution: Detection of complex formation in solution – Stability constants – stepwise and overall formation constants – simple methods (Potentiometric, pH metric and photometric methods) of determining the formation constants - factors affecting stability – Irving-William series - statistical and chelate effects – forced configurations.

Unit-V:

Reaction mechanisms in coordination chemistry: Labile and inert complexes -Types of ligand substitution reactions: Dissociative mechanism (D), Associative mechanism (A) interchange mechanism (I) - acid hydrolysis, factors affecting acid hydrolysis, base hydrolysis, conjugate base mechanism (SN1-CB), evidences of conjugate mechanism, anation reaction - reactions without metal ligand bond cleavage. Substitution reactions in square planar complexes- mechanism, trans effect-theories and applications, Interconversion between stereoisomers; Redox reactions Redox Reactions-Electron transfer reactions (complementary and non-complementary types, inner sphere and outer sphere processes), Marcus-Hush theory.

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20. G.E. Rodger, Inorganic and Solid State Chemistry, Cengage Learning India, Edition, 2002.

Course Code: CHE 102 No. of Credits: 4	Organic Chemistry-I

Course Outcomes		Level
CO-1	Demonstrate the utility of UV-visible, IR and fluorescence spectroscopy in structural characterization	Apply
CO-2	Elucidate the structure of organic compounds based on ^{1}H and ^{13}C NMR spectroscopy	Evaluate
CO-3	Explicate the applications of two-dimensional NMR spectroscopic techniques for structural elucidation	Understand
CO-4	Identify the fragmentation patterns of compounds and solve the structure of compounds using mass spectrometry	Evaluate
CO-5	Structural elucidation of unknown compounds using UV-vis, IR, Mass and NMR techniques	Apply

CO	Program Outcomes				
	1	2	3	4	5
1	2	1	3	3	2
2	2	1	3	3	2
3	2	1	3	3	1
4	2	1	3	3	1
5	2	1	2	3	1

Course Outline:

Unit-I:

Physical Organic Chemistry: Thermodynamic stability – general relationship between thermodynamic stability and reaction rates – electronic substituent effects on reaction interCHEiates – Principles of microscopic reversibility –substituent effects – solvent effects – methods of determination of reaction mechanism - kinetic methods – primary and secondary kinetic isotopic effect – non kinetic methods – isotope labeling, crossover experiment, trapping of interCHEiates, stereochemical studies. Linear free energy relationships: Curtin-Hammett, Hammett plot, steric and polar effects – Taft parameters. Solvent effects-Grunwald-Weinstein plots.

Unit-II:

Aromaticity: Criteria for aromaticity – Huckel's theory of aromaticity- energy, structural and electronic criteria for aromaticity – relationship among them. Craig's rule – non-benzenoid aromatic compounds. Aromatic, antiaromatic and homoaromatic compounds. Five-, six-, seven- and eight- membered rings and other systems. Aromaticity in annulenes, polycyclic compounds, charged rings - aromatic cations and anions, fused rings. Heteroaromatic systems. Aromaticity in sydnones and fullerenes.

Unit-III:

Nucleophilic Substitution: Aliphatic nucleophilic substitution: S_N1, S_N2, borderline, S_Ni mechanisms and their Stereochemical aspects. Factors affecting the rates of S_N1, S_N2 and S_Ni and neighbouring group participation. Mechanisms of Rearrangement of Carbocations, Non-classical Carbocations. Substitution vs elimination reaction. Aromatic electrophilic and nucleophilic substitutions: Mechanism, factors influencing ipso substitution and directive effect.

Unit-IV:

Stereochemistry: Configuration, conformation of cycloalkanes: four, five and six-membered rings, Conformational analysis of substituted cyclohexanes. conformation and reactivity. Conformation of fused and bridged ring systems-decalin, norbornane. anomeric effect. Stereochemistry of molecules with N, S, P chiral centers, allenes, spiranes, biphenyls, molecules with chiral planes, helical chirality. Topicity, prostereoisomerism. stereoselective and stereospecific reactions, enantioselective reactions, determination of enantiomeric and diastereomeric excess, double stereo-differentiation. Introduction to asymmetric synthesis – substrate chirality, chiral auxiliaries, chiral reagents, and chiral catalysts. Resolution – optical and kinetic. chemo-, regio - and stereo-selective transformations, Sharpless asymmetric epoxidation.

Unit-V:

Heterocyclic Compounds: Preparation, properties and reactions of pyrrole, furan, thiophene and pyridine. Preparation, properties and reactions of imidazole, pyrazole, oxazole, isoxazole, thiazole, isothiozole, pyrimidine, pyrazine, pyridazine. Preparation, properties and reactions of triazole and triazine. Fused or condensed heterocyclic compounds: Preparation, properties and reactions of indole, quinoline, isoquinoline, carbozol.

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Course Code: CHE 103 No. of Credits: 4	Physical Chemistry I

Course Outline:

Course Outcomes		Level
CO-1	Know the basic concepts involved in chemical kinetics *i.e.,* reaction rate, order and different types of reactions	Knowledge
CO-2	Understand the rate theory and to derive equations involved in heterogeneous catalysis and enzyme catalysis	Understand
CO-3	Analysis the kinetics of fast chemical reactions by different methods	Analyze
CO-4	Identify the point group of molecules and apply the concept of group theory to predict the spectroscopic properties	Apply

CO	Program Outcomes				
	1	2	3	4	5
1	2	1	1	2	1
2	2	1	3	2	1
3	3	1	3	2	1
4	3	1	3	2	1

Unit-I:

Chemical Kinetics and Rate theories: Introduction- Reaction rates and order and molecularity of reaction, Determination of order – differential method and integration method. Theories of reaction Rates-Collision theory, Statistical mechanics, inclusion of steric factor and Conventional Transition State theory (CTST). Determination of rate constants with various methods in CTST, Comparison of collision theory with CTST, Arrhenius equation-characteristics, Significance of energy of activation, Temperature coefficient and its evaluation. Thermodynamic formulation of CTST and limitations.

Unit-II:

Chemical Dynamics: Potential energy surfaces, Dynamics of Unimolecular reactions – Lindemann-Hinshelwood – Rice Ramsperger Kassel (RRK) theory and Rice Ramsperger Kassel - Marcus (RRKM) theory. Kinetics of chain reactions (H_2-Cl_2 and H_2-Br_2 reactions) using steady-state treatment.
Experimental methods for the study of fast reactions-flow and Shock methods-chemical relaxation methods, T-jump and P-jump methods, Molecular beam methods, Flash photolysis, Introduction to femto-chemistry.

Unit-III:

Chemical Kinetics and Catalysis Heterogeneous catalysis: Unimolecular and bimolecular surface reactions, Inhibition effect, determination of activation energy, Bi-molecular surface Reaction-Langmuir-Hinshelwood and Langmuir-Rideal mechanism. Enzyme catalysis - Michelis-Menten equation, Effect of pH and temperature on enzyme catalysis.

Unit-IV:

Group Theory - Point Group and GOT: Point Group: Fundamentals Concept of Symmetry, Matrix representation of symmetry operations. Concepts of groups, molecular point groups, representation of groups, matrix representation of symmetry operations, reducible and irreducible representations, symmetry criterion of optical activity, symmetry restrictions on dipole moment.
Great Orthogonality Theorem: Interpretation of character tables, determination of symmetry species for translations and rotations. Transition moment integral, vanishing of integrals, symmetry aspects of molecular vibrations, vibrations of polyatomic molecules.

Unit-V:

Applications of Group theory in Chemistry: Applications in spectroscopy: IR spectra- Selection rules for vibrational absorption - Symmetry of normal modes of H_2O, C_2H_4, trans-N_2F_2, $CHCl_3$and NH_3 using Cartesian coordinates and internal coordinates, IR activity. Raman Spectra: Complementary of IR and Raman spectra-determination of the Raman active vibrational modes. Electronic spectra: Selection rules for electronic transition, electronic transitions of simple molecules.
Applications in chemical bonding: Transformation of atomic orbitals: Symmetry adapted linear combinations (SALC), Construction of hybrid orbitals for AB_3(planar), AB_4(Td), AB_5(D3h) and AB_6(Oh) type of molecules.

Ligand field theory: splitting of d orbitals in different environments using group theoretical considerations. MO diagram for water and ammonia, method of descending symmetry.

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12. B. S. Garg, Chemical Applications of Molecular Symmetry and Group Theory, Macmillan Publishers India Ltd, 2012.

Course Code: CHE 104 No. of Credits: 4	**Physical Methods in Chemistry I**

Course Outcomes		**Level**
CO-1	Demonstrate the utility of UV-visible, IR and fluorescence spectroscopy in structural characterization	**Apply**
CO-2	Elucidate the structure of organic compounds based on ^{1}H and ^{13}C NMR spectroscopy	**Evaluate**
CO-3	Explicate the applications of two-dimensional NMR spectroscopic techniques for structural elucidation	**Understand**
CO-4	Identify the fragmentation patterns of compounds and solve the structure of compounds using mass spectrometry	**Evaluate**
CO-5	Structural elucidation of unknown compounds using UV-vis, IR, Mass and NMR techniques	**Apply**

CO	**Program Outcomes**				
	1	**2**	**3**	**4**	**5**
1	3	1	2	2	2
2	3	1	2	2	2
3	3	1	2	2	2
4	3	1	2	2	2
5	3	1	2	2	2

Course Outline:

Unit-I:

UV-Visible, Fluorescence Spectroscopy and ORD-CD: Basics of UV Spectroscopy, factors governing absorption maximum and intensity. Woodward Fieser and Fieser-Kuhn's rules - calculation of λ_{max} for simple organic molecules. Fluorescence - principles Stokes shift, quantum yield and application.
ORD-CD: Circular bireferegence, optical rotary dispersion, circular dichroism – Cotton effect curves – octant rule –axial haloketone rule - Applications of chiroptical properties in configurational assignment.

Unit-II:

Infra-Red Spectroscopy: Principle, instrumentation and sampling technique- Hook's law, vibrational frequency, modes of vibrations, and selection rules. Factors influencing vibrational frequency. Fingerprint and functional group region. Interpretation of the IR spectra of alkane, alkenes, alkynes, aromatic compounds, alcohols, ethers, phenol, carbonyl compounds, amines and heterocyclics– related problems.

Unit-III:

Unit-III NMR Spectroscopy-I: ^{1}H NMR, Spectral parameters –chemical shift & factors affecting chemical shift, intensity (integration), multiplicity, types of coupling & coupling constant. Analysis of first order and second – order spectra – shift reagents - structure determination of organic compounds by ^{1}H NMR spectra. spin-spin coupling involving different nuclei (^{1}H, ^{19}F, ^{31}P, ^{13}C). Examples for different spin systems (AB, AX, AMX, AA'BB', ABX) – Nuclear Overhauser Effect, Effect of quadrupolar nuclei (^{2}H, ^{10}B, ^{11}B) on the ^{1}H NMR spectra, – study of fluxional behavior of molecules.

Unit-IV:

NMR Spectroscopy-II: ^{13}C NMR: chemical shift & factors affecting chemical shift, Proton coupled; off–resonance decoupled; proton decoupled ^{13}C NMR spectra, DEPT techniques. Assignment of chemical shifts, additive effect, characteristic chemical shifts of common organic compounds and functional groups.
NMR of paramagnetic molecules – isotropic shifts, contact and pseudo-contact interactions – An elementary treatment of second order spectra – examples.
2D NMR techniques: H,H-COSY, C,H-COSY, HMBC, NOESY and INDAEQUATE.

Unit-V:

Mass spectroscopy: Instrumentation- methods of ionisation - EI, CI, APCI, ESI, MALDI and FAB. HRMS- Mass analyser – magnetic and electrostatic sector, time of flight and quadrupole. Molecular ion, base peak, multicharged ion, metastable ions and isotope ratio. Fragmentation patterns of saturated, unsaturated and aromatic hydrocarbons, alcohols, phenols, aldehydes, ketones, carboxylic acids, esters, amines, nitro, nitrile and halides. McLafferty rearrangement.
Structural elucidation using UV-Visible, IR, Mass, ^{1}H, ^{13}C NMR and 2D-NMR techniques.

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15. A Derome, Modern NMR Technique, Pergamon, 1983.
16. Farrar and E. D. Becker, Pulsed FT NMR Spectroscopy.
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18. C. P. Slichter, Principles of Magnetic Resonance, Third Edition, Springer-Verlag, 1990.
19. T. C. Farrar and E. D. Becker, Pulse and Fourier Transform NMR, Academic Press, New York, 1971.

Course Code: CHE 111 No. of Credits: 4	Course Title: Physical Chemistry Laboratory

Course Outcomes		Level
CO-1	Understand the instrumentation methods involved in the experiments	Understand
CO-2	Perform or develop working models	Create
CO-3	Gain the required experimental skills for career development	Create
CO-4	Apply QM methods for modeling simple organic/inorganic compounds for structural optimization and reaction modeling	Apply

CO	Program Outcomes				
	1	2	3	4	5
1	2	2	2	3	3
2	3	3	3	3	3
3	3	3	3	3	3

Part A: List of Wet Lab Chemistry (Any 10-12 Experiments):

1. Surface Chemistry
   (a) Verification of adsorption isotherms (Freundlich and Langmuir): charcoal-acetic acid or charcoal-oxalic acid system.
   (b) Kinetics & Determination of surface area by adsorption of acetic acid on Charcoal.
2. Phase Diagram
   (a) Determination of the concentration of the electrolyte using CST of phenol-water system.
   (b) Three Component Liquid Systems: Acetic Acid – Chloroform – Water
3. Partition Coefficient
   (a) Partition coefficient of benzoic acid between benzene and water.
   (b) Molecular formula of copper-ammonia complex by the partition coefficient method.
4. Spectroscopy
   (a) Formation kinetics of Chromium-EDTA complex (Spectrometry).
   (b) Simultaneous Estimation of Manganese and Chromium in a Solution of Dichromate and Permanganate Mixture.
   (c) Photocalorimetric determination of Bimolecular rate constant.
5. Surface Tension
   (a) Determine the surface excess of amyl alcohol.
6. Potentiometry
   (a) Titration of a strong and weak Acid Mixture with a Strong Base-Potentiometry.
   (b) Determination of stability constant of silver diammine complex by potentiometric titrations.
   (c) Dissociation of a weak acid by potentiometric titration.
7. Conductometry
   (a) Verification of Ostwald's dilution law and determination of dissociation constant of weak acid.
   (b) Conductometric titrations of a mixture of acids Vs strong base.
   (c) Van't Hoff's factor of benzoic acid between benzene and water.
   (d) Critical Micelle concentration of surfactant by conductivity measurements.
   (e) Verification of Onsager's Equation and Determination of Equivalent Conductance at Infinite Dilution of Strong Electrolytes.
   (f) Conductometric determination of Nickel using DMG.
8. Kinetics
   (a) Second order rate constant for the alkaline hydrolysis of ethyl acetate by conductivity

measurements.

(b) Arrhenius parameters for the Acid–Catalysed Hydrolysis of Methyl acetate.

9. Viscometry

(a) Determination of molecular weight of a polymer by viscosity measurements.

10. Additional

(a) Specific and molar refraction of a liquid by Refractometry.

(b) Reversibility of a redox process and determination of concentration of a given solution by cyclic voltammetry.

(c) Inversion of Sucrose-Polarimeter.

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2. G.W. Garland, J. W. Nibler, D.P. Shoemaker, Experiments in Physical Chemistry, 8thEdn. McGraw Hill, 2009.
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Course Code: CHE 113 Total Hours: 30	Course Title: Research Methodology and Publication Ethics

Course Outcomes		Level
CO-1	Understand the principles of research, literature survey and writing research paper and thesis writing	Understand
CO-2	Gain knowledge on general terminology including various methods for the research	Remember
CO-3	Improve the numerical aptitude and computational knowledge in the basic of collection and presentation of data	Apply
CO-4	Acquire knowledge of safe laboratory practices by handling laboratory glassware, equipment and chemicals	Apply
CO-5	Analyze the idea about writing research papers and report	Apply

CO	Program Outcomes				
	1	2	3	4	5
1	2	1	2	3	1
2	3	1	3	3	1
3	3	1	3	3	1
4	3	1	3	3	1
5	1	1	2	3	1

Course Outline:

Unit-I:

Ethics in research: Ethics, moral philosophy, nature of moral judgements and reactions. Scientific conduct - ethics with respect to science and research. Intellectual honesty and research integrity. Scientific misconducts - falsification, fabrication and plagiarism. Redundant publications - duplicate and overlapping publications. Selective reporting and misrepresentation of data.

Unit-II:

Literature Survey: Importance of literature survey, planning a literature search, identifying key concepts and key words, locating relevant literature and reliability of a source.
Science Citation Index–Journal Impact factors, h-index, g-index, i10 index, Chemical abstracts–UGC infonet, E-Journals and books–Search engines and databases

Unit-III:

Design of Experiments and Data Presentation: Aim, objectives, expected outcome, and methodology to be adopted. Importance of reproducibility of results. Objectives and basic principles of designs of experiments. Data presentation - using graphs, in tables, schemes and figures. Software for drawing. Bibliography tools.

Unit-IV:

Publication Ethics: Best practices and standards, conflicts of interest, publication misconduct, unethical behaviour and related problems. Authorship and contributorship. Identification of publication misconduct, complaints and appeals.

Unit-V:

Research Communication: General aspects of writing – reporting practical and project work, writing literature survey and reviews, organizing a poster display, oral presentation. Guidelines for manuscript writing - abstract, introduction, methodology, results and discussion, conclusion, acknowledgement, references and citation. Writing research reports. Intellectual property (IP) and intellectual property rights (IPR).

Reference:

1. Bird, A., 2006. Philosophy of science. Routledge.
2. A.I. Vogel, "Quantitative Inorganic Analysis", 3rd Ed., ELBS Longman London
3. J. March, 'Advanced Organic Chemistry; Reactions, Mechanisms and Structure', 6th Ed., Wiley–Interscience, 2016
4. MacIntyre, A., 2017. A short history of ethics: A history of moral philosophy from the Homeric age to the twentieth century. University of Notre Dame Press.
5. Chaddah, P., 2018. Ethics in Competitive Research: Do not get scooped; do not get plagiarized.
6. Bordens, K.S. and Abbott, B.B., 2002. Research design and methods: A process approach. McGraw-Hill.
7. Kothari C.R., 2020. Research methodology methods and Techniques. New Age International Publishers.
8. Thomas, C.G., 2021. Research methodology and scientific writing. Thrissur: Springer.

SEMESTER-II

Course Code: CHE 201 Total Hours: 60	Course Title: Inorganic Chemistry-II

Course Outcomes		Level
CO-1	Gain knowledge on structure and bonding in organometallic compounds	Knowledge
CO-2	Apply organometallic chemistry principles in catalysis	Apply
CO-3	Gain knowledge in bioinorganic chemistry and role of metals in biology	Remember
CO-4	Grasp the basics of metalloenzymes and related assessment	Remember
CO-5	Understand mechanistic aspects of organometallic chemistry and bio-inorganic chemistry	Understand

CO	Program Outcomes				
	1	2	3	4	5
1	2	1	2	1	2
2	1	2	1	2	1
3	3	3	3	3	3
4	2	4	2	4	2
5	2	5	2	5	2

Course Outline:

Unit-I:

Structure and bonding in organometallics: Introduction, nomenclature, types of compounds (ionic/covalent), bond energies and stabilities, ligands and classification-σ-donors, π-donors and σ-donors and π-acceptors, reactivity and trends, metal-carbon bonds of main group metals, structure and bonding in organolithium compounds - metal-carbon bonds of transition metals, trends and properties - 16/18-Electron rule – preparation, structure and bonding of metal carbonyls, alkyls, alkenes, alkynes, aryls, hydrides, dihydrogen and dinitrogen complexes – metallocenes: synthesis and properties, ferrocene - structure and bonding, fluxional molecules. σ–bonded ligands:structure, reactivity and bonding of metal phosphines and nitrosyls – bridging, terminal, bent and linear - Fischer carbenes, Schrock carbenes, carbynes, isolobal analogy, metal-metal bonds, transition metal clusters and quintuple bond.

Unit-II:

Reaction mechanisms and catalysis: Important types of reactions of organometallic compounds: substitution, electrophilic and nucleophilic attack on ligands, carbonylation and decarbonylation, oxidative addition, reductive elimination, insertion, hydride elimination, abstraction, transmetallation. Catalytic applications: hydrogenation of olefins, hydroformylation, Reppe reaction, Wacker process, Monsanto acetic acid synthesis, hydrosilylation, Ziegler-Natta polymerisation, cyclooligomerisation, isomerization, olefin metathesis, Fischer-Tropsch process, and CH functionalization reactions.

Unit-III:

Transport and storage of Metal ions in Biology: A brief introduction to bioinorganic chemistry - Transport and storage of metals: Mechanism – Fe, Cu, Zn and V storage and transport – metallothioeins. Basics of Biomineralization. Sodium and potassium ion pumps - mechanisms of ion-transport across cell membranes – bleomycin - siderophores (e.g. enterobactin and desferrioxamine) - transport of iron by transferring - storage of iron by ferritin - biochemistry of calcium as hormonal messenger - Role of Ca^{2+} in blood clotting.

Unit-IV:

Metalloproteins and Metalloenzymes-I: Introduction and classification of metalloproteins and metalloenzymes - enzyme, cofactor, coenzyme, prosthetic group, holoenzyme, and apoenzyme. Dioxygen transport and storage – structure and functions of hemoglobin and myoglobin - Bohr Effect, importance of 2,3-diphosphoglycerate, CO poisoning, hematin formation, sickle cell anemia, and blue baby syndrome - hemerythrin and hemocyanine.– Electron transfer proteins: – Cytochrome a, b, c, cytochrome c oxidase - Iron-sulphur proteins (Ferredoxins, Rubredoxin and Rieske‟s protein) - Classification of copper proteins and examples: blue copper proteins (azurin and plastocyanin). Vitamin B_{12} and B_{12} co-enzyme.

Unit-V:

Metalloproteins and Metalloenzymes-II: Dioxygen activating enzymes: cytochrome P-450, methane monooxygenases (sMMO, pMMO), catechol dioxygenases, tyrosinase, and galactose oxidase. Protective Metalloenzymes: superoxide dismutase (Fe-SOD, Mn-SOD, Cu-Zn couple SOD and Ni-SOD), catalase, and peroxidases. Non-redox metalloenzyme: carboxypeptidase, carbonic anhydrase, and alcohol dehydrogenase. Bioenergetics and ATP Cycle: Glycolysis (glucose to pyruvate conversion) and glucose storage, oxidative oxidative phosphorylation, cyanide poisoning, chlorophylls, photosystems I and II in cleavage of water, involvement of oxygen evolving complex in oxidation of water to O_2. Nickel and Molybdenum containing Enzymes: Xanthine oxidase, aldehyde oxidase, urease, hydrogenases, biological nitrogen fixation using molybdenum nitrogenase.

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13. N. N. Greenwoodand A. Earnshaw, Chemistry of the Elements, 2nd edition, Elsevier, 2005.
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18. M. Bochmann, Organometallics 2: Complexes with transition metal carbon s-bonds, Oxford Chemistry Primers Series, No.12, 1994.
19. W. Parkins and R. C. Poller, An Introduction to Organometallic Chemistry, Palgrave Macmillan, 1986.
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26. Metalloporphyrin nanoparticles: Coordinating diverse theranostic functions, Shuai Shao, Venugopal Rajendiran, Jonathan F. Lovell, *Coordination Chemistry Reviews* 2019, 379, 99–120.

Course Code: CHE 202 **Total Hours: 60**	**Course Title: Organic Chemistry II**

Course Outcomes		**Level**
CO-1	Synthesize organic compounds based on light CHEiated route	**Understand**
CO-2	Compare the concepts of pericyclic reaction mechanisms for thermal and photochemical reactions	**Remember**
CO-3	Demonstrate the detailed mechanism of various name reactions deals with C-C, C-N and C-O bond formation	**Apply**
CO-4	Make a reaction chart on oxidizing reagents and how to apply in the chemical world and research aspects	**Apply**
CO-4	Demonstrate the use of reducing reagents in synthetic organic chemistry	**Understand**

CO	**Program Outcomes**				
	1	**2**	**3**	**4**	**5**
1	3	1	3	3	2
2	3	1	3	3	2
3	3	1	3	3	1
4	3	1	3	3	1
5	3	1	3	3	1

Course Outline:

Unit-I:

Organic Photochemistry: Thermal vs photochemical reactions. Photochemistry of alkenes, dienes, polyenes and carbonyl compounds. Norrish type I and type II, and Patterno–Buchi reactions. Intramolecular reactions of carbonyl compounds, saturated cyclic and acyclic compounds, α,β and β,γ- unsaturated compounds, cyclohexanone and cyclohexadienones Photochemical rearrangement: di- 🕊-methane, oxa/aza di-🕊-methane, Photo-Fries, Lumiketone and Barton rearrangement. Intermolecular cycloaddition reactions and dimerisation. Photochemistry of aromatic compounds- isomerizations, additions, substitutions oxidation and reduction.

Unit-II:

Pericyclic Reactions: Molecular orbitals and symmetry of polyenes- Frontier orbitals of ethylene, 1,3-butadiene, 1,3,5-hexatriene and allyl systems. Classification of pericyclic reactions. Electrocyclic reactions: Conrotation and disrotation in 4n, 4n+2, allyl systems. Cycloaddition reactions: Effect of stereochemistry (cis and endo rules) and substituents on the rate of cycloadditions. analysis of electrocyclic and cycloaddition reactions: FMO and Woodward-Hoffmann correlation diagrams methods. 1,3-Dipolar cycloadditions and cheleotropic reactions. Sigmatropic rearrangements - [1,2]-sigmatropic shifts involving carbon moieties. [m,n] and [m,m] sigmatropic rearrangements. Claisen, Cope and Sommelet Hauser reactions.

Unit-III:

C-C, C-N, and C-O/S bond formation: C-C bond formation: Aldol, Arndt-Eistert, Bardhan-Sengupta, Barbier, Baylis-Hillman, Benzoin, Michael, Perkin, Robinson annulations, Vilsmeier, and Ullmann Reactions. C-N bond formation: Mannich, Mitsunobu, Ritter, Ugi, Doebner, Buchwald-Hartwig, and Stork enamine reactions. Formation of azides and hydrazines. C-O and C-S bond formation –Fischer esterification, Williamson's ether synthesis, Prins, Darzen, and Mitsunobu reactions.

Unit-IV:

Oxidation: Alkenes to diols: $KMnO_4$, OsO_4, Prevost oxidation and Woodward modifications. Oxidative cleavage of 1,2-diols - periodic acid, LTA. Alkenes to epoxides: using hydroperoxides and peroxyacids, Sharpless asymmetric epoxidation and dihydroxylation. Oxidation of allylic and benzylic compounds: DDQ, chloranil, SeO_2, NBS. Alkenes to carbonyl compounds: ozonolysis.
Alcohols to carbonyl compounds: chromium reagents ($K_2Cr_2O_7$, Jones, Sarrett's, Collins, PCC, PDC), MnO_2 and, $Al(\mathit{i}PrO)_3$. Non-metal based reagents: dimethyl sulfoxide and its variants - Swern oxidation, Moffatt's

oxidation (DCC) and Corey-Kim oxidations, hypervalent iodine oxidants (IBX, DMP)

Unit-V:

Reduction: Nucleophilic metal hydrides: LAH, Red-Al, DIBAL-H, $NaBH_4$, Sodium cyanoborohydride, metal trialkylborohydrides. Electrophilic metal hydrides: BH_3 and AlH_3. Electron transfer reducing reagents: Li/Na in liquid NH_3 or alcohol, tri-n-butyl tin hydride. Non-metallic reducing reagents: diimides, Hantzsch ester, Wolf-Kishner reduction. Radical based reductions: tri-n-butyl tin hydride. Catalytic hydrogenation: heterogeneous - Pd/C, homogeneous – Wilkinsons hydrogenation, Knowels asymmetric hydrogenation.

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15. Francis A. Carey, Robert M. Giuliano, Organic Chemistry, 8th Ed. 2008
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Course Code: CHE 203 Total Hours: 60	Course Title: Physical Chemistry II

Course Outcomes		Level
CO-1	Apply the advanced quantum chemical methods for solving many-electron systems	Apply
CO-2	Solve Schrodinger equation for the simple molecules using perturbation, variation and HF methods	Create
CO-3	Demonstrate the applications of LCAO theory and direct bonding in polyatomic molecules	Apply
CO-4	Understand pulse sequences in magnetic resonance spectroscopy and apply advanced spectroscopy techniques in the experiments	Understand

CO	Program Outcomes				
	1	2	3	4	5
1	2	2	3	2	2
2	3	2	3	2	2
3	3	2	3	2	2
4	2	2	3	2	2

Course Outline:

Unit-I:

Quantum Chemistry: Potential energy of hydrogen-like systems: Wave functions and energy of hydrogen like atoms. angular-radial functions - and their plots. The postulate of spin by Uhlenbeck and Goudsmith-Spin orbitals- Construction of spin orbitals from spin functions. Quantization of angular momentum, quantum mechanical operators corresponding to angular momenta (Lx, Ly, Lz and L^2), commutation relations between these operators. Spherical harmonics as Eigen functions of angular momentum operators Lz and L^2. Ladder operator method for angular momentum. Space quantization. Schrödinger equation for many electron atoms: Helium and Lithium atoms.

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Unit-II:

Approximation Methods Born-Oppenheimer approximation, Perturbation theory, Variational methods, Hartree-Fock equations, Self-consistent field method for solving Hartree-Fock equations, Anti-symmetric wave function, Slater determinant wave function, Molecular Hamiltonian operators.

Valence bond treatment for chemical bonding in molecules - molecular orbitals, Molecular orbital theory for different diatomic molecular systems, photoelectron spectra, SCF-LCAO-MO wave function. Electronic states of diatomic molecules -sp, sp^2 and sp^3 hybrid orbitals. Molecular term symbols, Hückel molecular orbitals, bonding in polyatomic molecules.

Unit-III:

EMR and Origin of spectra: Nature of EMR, Interaction of EMR with matter, Natural line width and intensity of spectral lines, Classical and quantum chemical approach to absorption of radiation by molecules. Energy levels in molecules. Born Oppenheimer approximation, Population of energy levels. LASER – three & four level.

Unit-IV:

Optical Spectroscopy-I: Microwave spectroscopy: Molecular classification and Rotation spectra, Diatomic and polyatomic molecules. Application of Rotation spectra (Bond length, Isotopic mass, dipole moment, isotopic abundance), Non-rigidity of rotor.

Vibrational spectroscopy: Vibrational spectra of diatomics & SHO; anharmonicity & Morse potential; Vibration-rotational spectra of diatomics, polyatomic Molecules-P, Q&R branches, Dispersive IR & FTIR, Vibration spectra of polyatomic molecules. Normal modes of vibrations of polyatomic molecules, Coupling of rotation and vibration, Parallel and perpendicular bands, Breakdown of Born-Oppenheimer Approximation.

Unit-V:

Optical Spectroscopy-II: Raman Spectroscopy: Polarizability and classical theory of Raman spectrum, Rotational Raman spectra. Vibrational Raman spectra, mutual exclusion principle, Surface enhanced Raman spectra, Resonance Raman.
Electronic Spectroscopy: Electronic energy states of molecules. Vibrational structure of electronic bands, Electronic transitions and absorption bands, Selection rules. Electron spectroscopy for chemical analysis (ESCA)-UPS, X-ray photoelectron spectroscopy (XPS), Auger electron spectroscopy (AES), Inductively coupled plasma mass spectrometry (ICP-MS).

Reference:

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14. A. Dau and C. Singh, Quantum chemistry classical to computational, Manakin press, 2017.

Course Code: CHE 204 Total Hours: 60	Course Title: Physical Methods in Chemistry II

Course Outcomes		Level
CO-1	Acquire knowledge on advanced concepts in spectroscopy thereby being able to interpret the spectra and solve the structure of metal complexes	**Remember**
CO-2	Discuss the application of electronic spectroscopy to simple coordination compounds and f-block elements	**Understand**
CO-3	Elucidate the structure of simple organometallic complexes by IR and Raman spectroscopic tools	**Apply**
CO-4	Determine the geometry of inorganic complexes using EPR spectroscopy	**Analyze**
CO-5	Depict the advanced spectroscopic tools like NMR, Mossbauer and NQR and its exploitation to express the structure of inorganic complexes	**Evaluate**

CO	**Program Outcomes**				
	1	**2**	**3**	**4**	**5**
1	2	2	2	2	1
2	2	2	2	2	2
3	3	2	3	2	2
4	3	2	3	2	2
5	2	1	3	1	2

Course Outline:

Unit-I:

Electronic Spectroscopy: Microstates, - terms and energy levels for d^1 - d^9 ions in cubic and square fields – Intensity of bands – group theoretical approach to selection rules - Effect of distortion and spin-orbit coupling on spectra- Orgel and Tanabe-Sugano diagrams – Evaluation of 10Dq and β for octahedral complexes of cobalt and nickel – applications to simple coordination compounds – charge transfer spectra – electronic spectra of $[Ru(bipy)3]^{2+}$. Electronic Spectra of f-block elements. Optical rotatory dispersion, circular dichroism and Magnetic circular dichroism – applications to metal complexes.

Unit-II:

Infrared and raman Spectroscopy: IR spectroscopy- Introduction, selection rules, stretching frequency of some inorganic ions-effect of coordination on the stretching frequency- sulphato, carbonato, sulphito, aqua, nitro, thiocyanato, cyano, thiourea, DMSO complexes. Effect of isotopic substitution on the vibrational spectra of molecules – vibrational spectra of metal carbonyls with reference to the nature of bonding, geometry and number of C-O stretching vibrations, Raman spectroscopy – Introduction, combined applications of IR and Raman spectroscopy in the structural elucidation of N2O, ClF3, NO^{3-}, ClO4, metal carbonyls.

Unit-III:

NMR Spectroscopy: Introduction to hetero-nuclear NMR, Factors influencing coupling constant (gyromagnetic ratio, periodicity, hybridisation, s-character, electronegativity, coordination number, trans influence, inter-bond angles, lone-pair and oxidation state) - structural assessment of simple inorganic compounds using ^{1}H, ^{13}C, ^{15}N, ^{19}F, ^{31}P-NMR spectroscopic techniques – Studies on fluxional molecules, quadrupolar nuclei-effect in NMR spectroscopy, shift reagents and applications. Overview of ^{13}C NMR of metal carbonyls, ^{119}Sn, ^{195}Pt, and other nuclei NMR and satellite spectra.

Unit-IV:

EPR Spectroscopy: Theory of EPR spectroscopy - Spin densities and McConnell relationship – Factors affecting the magnitude of g and A tensors in metal species - Zero-field splitting and Kramers degeneracy – Spectra of VO (II), Mn (II), Fe (II), Co (II), Ni (II) and Cu (II) complexes – Applications of EPR to a few biological molecules containing Cu (II) and Fe (III) ions.

Unit-V:

NQR and Mössbauer Spectroscopy:

NQR spectroscopy - Characteristics of quadrupolar nucleus – effects of field gradient and magnetic field upon quadrupolar energy levels – NQR transitions – applications of NQR spectroscopy. Mössbauer spectroscopy - Isomer shifts – Magnetic interactions – Mossbauer emission spectroscopy – applications to iron and tin compounds.

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4. A. K. Das and M. Das, Fundamental concepts of Inorganic Chemistry, 1st Edition, Volume 7, CBS Publishers & Distributors Pvt. Ltd.,2014.
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13. E. A. V. Ebsworth, Structural Methods in Inorganic Chemistry, 3rd ed., ELBS, Great Britain, 1987.
14. R. A. Scott and C. M. Lukehart, Applications of Physical Methods to Inorganic and Bioinorganic Chemistry, John and Wiley & Sons, LTD, 2007.
15. E. I. Solomon, A. B. P. Lever, Inorganic Electronic Structure and Spectroscopy, Vol.,2 Applications and Case Studies, Wiley-Interscience, 2006.
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17. D.N. Satyanarayana, Electronic Absorption Spectroscopy, Universities Press, 2000.
18. R.B. Jordon, Reaction Mechanisms of Inorganic and Organometallic Systems, 3rd Edition, Oxford University Press, 2007.
19. C.J. Ballhausen and H.B. Gray, Molecular Orbital Theory, Benjamin/Cummings Pub. Co, 1965.
20. N. Figgis and M. A. Hitchman, Ligand Field Theory and Its Applications, 1st Edition, Wiley VCH, 1999.
21. S.F.A. Kettle, Physical Inorganic Chemistry – A Coordination Chemistry Approach, Spectrum Academic Publishers, Oxford University Press, 1996.

Course Code: CHE 211 Total Hours: 60	Course Title: Organic Chemistry Laboratory

Course Outcomes		Level
CO-1	Acquire the knowledge of multistep organic synthesis in microwave-assisted synthesis and photochemical reactions	Understand
CO-2	Organize experiments based on the organic preparations and qualitative analysis	Analyze
CO-3	Use knowledge of the purification techniques	Apply
CO-4	Report the separation of two mixtures present in the organic compounds	Understand
CO-5	Support on estimation of organic compounds *viz* volumetric methods	Evaluate

CO	Program Outcomes				
	1	2	3	4	5
1	2	3	3	3	3
2	2	3	3	3	3
3	2	3	3	3	3
4	2	3	3	3	3
5	2	3	3	3	3

Multistep organic synthesis (any four) - conventional synthesis - microwave assisted synthesis - photochemical reactions. Purification of the compounds using column chromatography and characterization of the compounds using spectroscopic techniques.

Qualitative Analysis: Separation and analysis of organic mixture containing two components.

Estimation of Organic Compounds
(a) Estimation of phenol and aniline - volumetric method.
(b) Estimation of glucose by Betrands method.
(c) Estimation of methyl ketone – iodimetric method
(d) Determination of iodine and saponification value of an oil sample.

References:

1. Vogel, A. R. Tatchell, B. S. Furnis, A. J. Hannaford, P. W. G. Smith, Textbook of Practical Organic Chemistry, Prentice-Hall, 5th Ed, 1996.
2. F. G. Mann, B. C. Saunders, Practical Organic Chemistry, 4th Ed, Pearson Education India, 2009.
3. B. Haynes, Qualitative Organic Analysis, Pearson Education, 2011.
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5. V. K. Ahluwalia, R. Aggarwal, Comprehensive Practical Organic Chemistry, Universities Press, 2004.

SEMESTER-III

Course Code: CHE 301 Total Hours: 60	Course Title: Inorganic Chemistry III

Course Outcomes		Level
CO-1	Gain knowledge on magnetic materials and its properties	**Knowledge**
CO-2	Understand the photochemistry of inorganic complexes	**Understand**
CO-3	Apply nuclear chemistry principles in various fields	**Apply**
CO-4	Grasp the importance of metals in CHEicine	**Remember**
CO-5	Gain knowledge on frontier areas of inorganic chemistry	**Knowledge**

CO	**Program Outcomes**				
	1	**2**	**3**	**4**	**5**
1	1	2	2	1	3
2	2	2	2	2	2
3	2	2	3	2	2
4	1	2	2	2	2
5	2	1	2	1	2

Unit-I:

Magnetic material and its properties: Types of magnetism – Dia –para – ferro and antiferro magnetism. Magnetic properties of free ions –Zeeman effect. Determination of Magnetic moments and their applications to the elucidation of structures of inorganic compounds – quenching of orbital momentum in transition metal complexes - temperature dependent and temperature independent paramagnetism - Spin crossover in coordination compounds. Magnetic properties of lanthanides and actinides.

Unit-II:

Inorgnaic Photochemistry: Elementary ideas on the photosystems I and II - Photochemistry of Cr(III), Co(III), Ru(II), Pt(II) and Pt(IV) complexes – photoaquation – photoanation – photoisomerisation – photo redox reactions – charge transfer photochemistry – photosensitisation – solar energy conversion – photogalvanic cell – water splitting.

Unit-III:

Nuclear Chemistry and its Applications: Natural radioactivity – Detection and measurement of radioactivity: Geiger Muller and ionization counters. Radioactive series including neptunium series – group displacement law – Rate of disintegration and half-life period – Average life period. Artificial radioactivity – induced radioactivity – uses of radioisotopes – hazards of radiations – nuclear energy – nuclear reactors – nuclear fission and fusion – product yields – Spallation – photonuclear and thermo nuclear reactions – energy source of the sun and stars – carbon dating – rock dating. radioactive waste disposal – applications of nuclear science in agriculture – Atomic power projects in India. Nuclear CHEicine- Single Proton Emission Tomography (SPECT) and Positron Emission Tomography (PET).

Unit-IV:

Metals in Medicine: Bioinorganic Chemistry of quintessentially toxic metals. Lead, Cadmium, Mercury, Aluminum, Chromium, Iron, Copper, Plutonium. Detoxification by metal chelation. Metals in CHEicine: Anti-arthritis drugs – Au in rheumatoid arthritis – Li in psychiatry. Metal based anti-cancer agents: Introduction to cancer and treatment - conventional drugs-platinum, titanium, ruthenium and other metal based drugs - evolution of cisplatin - mechanism - advantages and disadvantages of Pt based drugs. MRI imaging: Principles of MRI - development of MRI contrasting agents - types of contrasting agents - Gadolinium and other transition complexes.

Unit-V:

Introduction to frontier topics in inorganic Chemistry: Energy storage materials –Li ion battery, hydrides and hydrogen storage materials – challenges. d-block metal oxides: transparent conducting oxide and applications: ITO, FTO, DSCs, solid state LEDs, OLEDs. Superconductors: origin, theory, high temperature superconductors, materials, applications – Molecular materials - fullerides– one-dimensional metals, molecular magnets, spintronic, inorganic liquid crystals – materials and applications. Inorganic fibers: boron, carbon and silicon fibers and applications. Nanomaterials: fundamentals, characterisation methods and fabrication, self-assembled nanostructures. Bio-inorganic nanomaterials: DNA and nanomaterials. Biomimetic – natural and artificial nanomaterials, bio-nanocomposites.

References:

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2. R. Dutta, Syamal, Elements of Magnetochemistry East-West Press 2010. (Unit I)
3. P. W. Atkins and J. Paula, Physical Chemistry, Oxford Publications, 8th edition, 2009.
4. J. E. Huheey, E. A. Keiter, R. L. Keiter and O. K.CHEhi, Inorganic Chemistry - Principles of Structure and Reactivity, 4th edition, Pearson Education, 2006.
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16. C. E. Housecraft and A.G. Sharpe, Inorganic Chemistry, 4th edition, Pearson, 2012.

Course Code: CHE 302 Total Hours: 60	Course Title: Organic Chemistry -III

Course Outcomes		Level
CO-1	Illustrate the application of organometallic reagents and coupling reactions in the field of synthetic organic chemistry	Understand
CO-2	Demonstrate synthetic route for various compounds through functional group interconversion	Remember
CO-3	Construct synthetic routes to achieve any given target molecules through retrosynthetic analysis	Apply
CO-4	Exemplify the significances of rearrangement transformations in organic synthesis	Apply
CO-5	Illustrate the stereochemistry structural features and biological importance of steroids and prostaglandins	Understand

CO	Program Outcomes				
	1	2	3	4	5
1	2	1	2	3	1
2	3	1	3	3	1
3	3	1	3	3	1
4	3	1	3	3	1
5	1	1	2	3	

Unit-I:

Organometallic reagents in organic synthesis: Main group organometallic reagents - organolithium, organomagnesium, organoboron, organosilicon, organotin. Organotransition metal reagents - organocobalt, organonickel, organoplatinum, organocopper, organozinc, organocadmium and organomercury in organic synthesis. Coupling Reactions: Tsuji-Trost, Heck, Kumada, Sonagashira, Negishi, Stille, Suzuki, Hiyama, Buchwald-Hartwig and Fukuyama coupling reactions.

Unit-II:

Synthetic Strategies-I: Functional Group Interconversions: Functional group interconversions, the importance of the order of events in organic synthesis, chemoselectivity, regioselectivity, and Umpolung concept. The concept of protection and deprotection of functional groups in synthesis. Protection of amino, hydroxy, diol, carbonyl and, double and triple bonds.

Unit-III:

Synthetic Strategies-II: Retrosynthesis: Disconnection Approach - synthons and synthetic equivalents, donor and acceptor synthons, disconnection, alternating polarity disconnection and steps in planning the synthesis. One and two groups C-X and C-C disconnections. disconnection of alcohols, olefins and ketones. Logical and illogical disconnections. Two group disconnection 1,2-, 1,3-, 1,4-, 1,5- and 1,6-dioxygenated skeletons and dicarbonyls. Retro Diels – Alder reactions- Wieland Mischer ketone synthesis- Retrosynthesis of 3, 4, 5, 6 membered carbo and heterocycles. Designing synthesis: Disconnection approach in Epothilone, Juvabione and longifolene.

Unit-IV:

Rearrangements in Organic Synthesis: Mechanistic aspects, nature of migration, migratory aptitude, stereochemical aspects and memory effects. Rearrangements of highly substituted glycols, substituted halides, alcohols, terpenes, 1,2-ketones, haloketones, diazo compounds, amides, azides, hydoxamic esters, nitrogen/phosphorus/sulfur ylides, oximes, peracids, peroxides, phosphorus ylides, 1,2-diphenylhydrazine, phenolic esters, allylaryl/vinyl ethers.

Unit-V:

Steroids and Prostaglandins Steroids: Classification of steroids, biological importance- structure, and stereochemistry of cholesterol, Structural features of bile acids – Sex hormones – androsterone, testosterone, estrone, estradiol, progesterone - Structure of ergosterol.

Prostaglandins (PG): Types of PG's prostaglandins. Functions of prostaglandins. Synthesis of prostaglandins E2, prostacyclin (PGI2). Structural features of prostaglandin D2 (PGD2) and prostaglandin F2α (PGF2α).

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27. Thomas H. Lowry, Kathleen Schueller Richardson, Mechanism and Theory in Organic Chemistry, Harper and Row Publishers
28. Edwin S. Gould, Mechanism and Structure in Organic Chemistry, Holt, Rinehart and Winston Publications, 1959

Course Code: CHE 303 Total Hours: 60	Course Title: Physical Chemistry III

Course Outcomes		Level
CO-1	Enrich the knowledge about the fundamental concepts of thermodynamics (classical/statistical) and electrochemistry	Remember
CO-2	Recognize the electrochemical ideas at equilibrium and dynamics progress	Understand
CO-3	Apply different statistical methods	Apply
CO-4	Identify the different types of fuel cells and discuss their merits and demerits	Create

CO	Program Outcomes				
	1	2	3	4	5
1	1	1	3	2	2
2	3	1	3	2	2
3	2	2	3	2	2
4	3	2	2	2	2

Unit-I:

Classical Thermodynamics: Introduction: Laws of thermodynamics, Entropy- Free Energy-Systems of Variable Compositions - Fugacity and Activity- Fugacity determination (graphical method and van der Waals equation of state) –Variation of Fugacity with respect to Temperature and Pressure - Maxwell's relations – significance, Partial molar properties – Chemical potential. Concept of absolute entropy and residual entropy Thermodynamics of mixing: Thermodynamic functions of mixing, Clausius Inequality, Gibbs-Duhem-Margules equation, Konowaloff's rule, Henry's law, excess thermodynamic functions. Third law of thermodynamics: Nernst heat theorem, development of third law of thermodynamics, determination of absolute entropies using third law, entropy changes in chemical reactions. Thermodynamics of Irreversible Processes: Thermodynamics of irreversible processes with simple examples. phenomenological relations. Onsager reciprocal relations - principle of microscopic reversibility. Electrokinetic phenomena. Thermoelectric phenomena.

Unit-II:

Statistical Thermodynamics: Classical approach: Scope of statistical thermodynamics-probability theorem-starlings' approximation, phase space, microstate and macrostate, configuration, system, assembly and ensemble-different types of ensembles- permutations and combinations, thermodynamic probability, Maxwell-Boltzmann statistics and its limitations. Concept of partition functions and its relation with thermodynamic properties, evaluation of translational, rotational, vibrational and electronic partition functions. Sackur-Tetrode equation-thermodynamic properties of monoatomic gases. Quantum approach: Bose-Einstein Statistics, Bose-Einstein condensate, difference between first order and higher order phase transitions, liquid helium, supercooled liquids. Fermi-Dirac statistics- Application of Fermi-Dirac statistics to electron gas in metal and thermionic emission, Comparison of statistical models. Heat capacity of solids: Dulong - Petit law, Einstein's theory and its modification, Debye's theory of heat capacity of solids.

Unit-III:

Electrochemistry-I: Activity and Activity coefficient of electrolytes, Mean ionic activity coefficient. ionic strength, Debye Huckel theory of strong electrolytes, Debye Huckel theory-relaxation and electrophoretic effects, Debye-Huckel-Onsager equation and its derivation. Debye Falkenhagen effect. Wein effect. Ionic activity coefficients of strong electrolytes-Derivation of Debye-Huckel limiting law. Equilibrium Electrochemistry: EMF phenomena, cell potential and its measurement, reference electrodes. Electrochemical cells, concentration cells and activity coefficient determination, liquid junction potential. Determination of solubility. Redox indicators and redox titrations.

Unit-IV:

Electrochemistry-II: Dynamic Electrochemistry: Electrical double layer, various models of electrical double layer, Electrode polarization. Overpotential, hydrogen and oxygen overvoltage, theories of overvoltage, Butler-Volmer equation for simple electron transfer reactions, Tafel plot and its significance, Corrosion: stability of metals, Porbaus Diagram-Evan diagram-corrosion control and methods for prevention.

Unit-V:

Storage Cells and Electroanalytical Techniques: Storage cells: Lead acid battery, lithium battery, nickel cadmium cell. Fuel Cell. Theory and working of fuel cell. H2- O2 fuel cell, methanol fuel cell, solid oxide fuel cells. Electroanalytical Techniques: Polarography – diffusion current, different current, supporting electrolyte, polarographic maxima, three electrode system. Amperometry – principles, types and applications. Cyclic voltammetry – principles, applications. Stripping voltammetry.

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3. M.C. Gupta, Statistical Thermodynamics, New age international, 2007.
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Course Code: CHE 311 Total Hours: 60	Course Title: Inorganic Chemistry Laboratory

Course Outcomes		Level
CO-1	Identify the familiar and less familiar cations by semi-micro qualitative analysis	Analyze
CO-2	Ensures the students to acquire knowledge and have hands on experience in multistep inorganic compound synthesis and characterize them using spectroscopic techniques	Skills
CO-3	Apply the knowledge for performing experiment scientifically and safely to enrich the understanding about experiments in lab work	Understand
CO-4	Perform the preparation of inorganic complexes and purify them	Apply
CO-5	Gain knowledge on working principle of cyclic voltammetry and differential pulse voltammetry techniques and determine the electrochemical properties of complexes	Knowledge

CO	Program Outcomes				
	1	2	3	4	5
1	1	2	2	2	3
2	2	3	3	2	3
3	3	3	1	2	3
4	3	2	3	3	3
5	2	1	3	1	2

Unit-I: Semi-micro qualitative analysis of a mixture containing two common and two rare – cations (any three salt mixtures)

Unit-II: Preparation of the following compounds and their Characterization (any seven experiments)

1. Tetraaminecopper (II) sulphate
2. Potassium trioxalatochromate (III)
3. Cis- and trans-potassium dioxalatediaquachromate (III)
4. Hexaamminenickel (II) chloride complex
5. Synthesis and study of Tris (oxalato) iron(III) potassium salt by Cyclic Voltammetry (CV) and Differential Pulse Voltammetry (DPV), and determination of the following: the formal reduction potential (Eo'); the number of electrons transferred in the redox process (n); electrochemical reversibility.
6. Synthesis and study of Mn^{III} (Salen)Cl by Cyclic Voltammetry and Differential Pulse Voltammetry (DPV), and determination of the following: the formal reduction potential (Eo'); the number of electrons transferred in the redox process (n); electrochemical reversibility.
7. Preparation and determination of the effective magnetic moment and number of unpaired electrons in Mn(acac)3.
8. Preparation and determination of the aquation rate of [Co(NH3)5Cl]Cl2.
9. Preparation and resolution of the optically active compound $[Co(en)3]^{3+}$.
10. Control synthesis of copperoxalate hydrate complex; kinetic vs. thermodynamic factors
11. Bioanalytical techniques – Monitoring the cleavage of DNA and protein by metal complexes using Gel electrophoresis techniques – Agarose and PAGE (Demo only).

Reference:

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2. J. D. Woollins, , Inorganic experiments, 3rd edition, Wiley-VCH Verlag GmbH @ Co. KGaA, 2012.
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John Wiley and Sons, 2011.
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Course Code: CHE 312 Total Hours: 45	Instrumentation Methods in Chemistry

Course Outcomes		Level
CO-1	Understand fundamental concepts of spectroscopy tools and their instrumentation	Understand
CO-2	Get knowledge on the maintenance of research instruments	Understand
CO-3	Get the hands-on experience of the measurement techniques with various examples	Analyze
CO-4	Characterize or identify the products/outcomes of the experiments using UV-VIS, IR, NMR and Fluorescence Spectroscopy, and Chromatographic Techniques	Apply
CO-5	Utilize the advanced analytical techniques in line with the industrial needs	Apply

CO	Program Outcomes				
	1	2	3	4	5
1	3	3	2	3	3
2	3	3	3	1	3
3	2	2	3	2	3
4	3	2	2	3	3

Unit-I:

Spectrophotometry – I: Sample handling and measurement, Selection of reference. To detect the presence of heavy metal ions. Determine composition of Iron-Phenanthroline complex complex by Job's method. Determination of impurities of paracetamol, diazepam tablet to arrive quantitative information. CT spectrum of amine picrate, Find molecular weight of polymeric materials and composites.

Unit-II:

Spectrophotometry – II: Instrumentation – Major components in a typical IR spectrometer, Software and hardware familiarization, Sample preparation (solid and liquid). regulatory requirement governing the use of IR spectrophotometer. Spectral analysis- baseline subtraction, curve-fitting, multi-peak fitting, deconvolution. Identification of functionality in Aspirin. *T*o find the ratio of cis-trans isomers in a mixture, studying the symmetry of inorganic complexes, beyond mid-IR and multimodal analysis, Microanalysis.

Unit-III:

Chromatographic Techniques: Instrumentation and applications of Column Chromatography, HPLC and GPC, techniques. Sample preparation, Method development, Selection criteria of mobile phase (solvents) for eluting, polar, non-polar compounds and its applications. Software handling, Data analysis and interpretation, Do's and Don'ts on handling the equipment. Isolation and purification of products by chromatographic techniques: TLC & Column Chromatography. Analysis of paracetamol by HPLC, Separation of Enantiomers from Racemic mixtures using chiral column chromatography, Methods for measuring MW by gel permeation chromatography.

Unit-IV:

NMR Spectroscopy: Software familiarization, Frequency matching, Setting Parameters, Preparation of samples, sample submission and trouble shooting. – Applications of NMR to simple molecules like Ethyl alcohol (Pure and Impure), Toluene, Phenol, Acetaldehyde and Diethyl ether.

Unit-V:

Fluorescence Spectroscopy: Instrument Handling: Software and hardware familiarization, Spectra Measurement, Time Course, Fixed Wavelength, and Intensity Monitor. Calibration- Water Raman and sources of error. Photophysical Characterization of luminescent materials, characterization of carbon nanotubes. Complexity in Spectral analysis: Inner Filter Effect, Matrix Effect, Effect of Solvent. Characterization of Anthocyanins in different pH.

References:

1. Rohatgi-Mukherjee, K. K., Fundamentals of Photochemistry, New Age International (P) Ltd. 1978

2. Pavia, D. L., Lampman, G. M. and Kriz G. S., Introduction to spectroscopy, 3rd Ed. Thomson Brooks/Cole, 2001.
3. Saroj Kumar and Naba Kumar, Physical Chemistry Practical, New Central Book Agency, 2012.
4. Turro, N. J. Modern Molecular Photochemistry, 4th Ed. University Science Books, Sausalito, 1991.
5. Lakowicz, J.R. Principles of Fluorescence Spectroscopy, 3rd Ed. Springer Science Business CHEia, LLC, New York,
6. Skoog D. A, West D M, Holler, F J and Crouch S R. Fundamentals of Analytical Chemistry, 8th Edition, Saunders College Publishing, 2004.
7. Gary. D. Christian, Wiley India, Analytical Chemistry, 6th Edition, 2009.
8. David Harvey, Modern Analytical Chemistry, 1st Edition, McGraw Hill, 1999.

SEMESTER-IV

Course Code: CHE 411 Total Hours: NA	Dissertation

Course Outcomes		Level
CO-1	Understanding the nature of research problems and identifying the related area of knowledge	Understand
CO-2	Analyze literature reports in order to identify the methodology to solve the research problem	Apply
CO-3	Analyze data and synthesize research findings	Apply
CO-4	Demonstrate capacity to lead and manage change through collaboration with others	Apply

CO	Program Outcomes				
	1	2	3	4	5
1	2	2	2	2	2
2	3	3	3	3	3
3	3	3	3	3	3
4	3		3	3	3

The student shall pursue a research project for the whole semester under the allotted guide. The project report shall be submitted in the form of dissertation and the evaluation will be based on the performance in the lab and the final presentation of the research work done.