M.Sc. Chemistry Programme (CBCS) Curriculum

Department of Chemistry
School of Basic and Applied Sciences
Central University of Tamil Nadu
Thiruvarur 610 005

CENTRAL UNIVERSITY OF TAMIL NADU

VISION

To develop enlightened citizenship of knowledge society for peace and prosperity of individuals, nation and the world, through promotion of innovation, creative endeavors, and scholarly inquiry and to be a global destination of higher education and research.

MISSION

- To serve a beacon of change, through multi-disciplinary learning, for creation of knowledge community, by building a strong character and nurturing a value-based transparent work ethics, promoting creative and critical thinking for holistic development and self-sustenance for the people of India.
- The University seeks to achieve this objective by cultivating an environment of excellence in teaching, research and innovation in pure and applied areas of learning.

OBJECTIVES AND GOALS

- To disseminate and advance knowledge by providing instructional and research facilities in such branches of learning as it may deem fit
- To make special provisions for integrated courses in humanities, social sciences, science and technology in its educational programmes
- To take appropriate measures for promoting innovations in teaching-learning process and inter-disciplinary studies and research
- To educate and train manpower for the development of the country
- To establish linkages with industries for the promotion of science and technology
- To pay special attention to the improvement of the social and economic conditions and welfare of the people, their intellectual, academic and cultural development

DEPARTMENT OF CHEMISTRY

The Department of Chemistry started functioning from the year 2010 with five-year integrated M.Sc. Chemistry programme. The Department has the distinction of starting the first two-year P.G. program in Science at CUTN. Besides, state-of-the-art P.G. and research laboratories were established. The Department is committed to excellence in chemistry by establishing research programmes for meeting scientific and technological challenges faced by the ever changing, science centered world of the 21st century.

The Department offers M.Sc., Integrated M.Sc., Post Graduate Diploma in Chemical Lab Technician (PGDCLT) and Ph.D. programmes. The Department provides ample opportunity for the students to accumulate a thorough fundamental knowledge of all fields of Chemistry. Meticulous lecture courses in the general areas of inorganic, organic and physical chemistry are conducted regularly in addition to the state-of-the-art laboratory courses which provides hands-on experience to the students at all levels.

The Department's primary focus is to instill the necessary spark and provide the scientific impetus so that the students can virtually experience the jiggling and wiggling of atoms and molecules. To enable students to have a glimpse of contemporary research, both in terms of academia and industry, the final year students in Chemistry will be completely engaged in project works. We aim to produce highly sought after and knowledgeable graduates for careers in academia, industry, and research institutes.

VISION AND MISSION OF THE DEPARTMENT

VISION

The Department envision establishing itself as a place of excellence for chemistry education and research programmes globally.

MISSION

- To bridge the gap between academia and industry by regularly updating the curriculum on par with recent developments in science and encourage doing in house projects
- To educate and invoke the students to deliver their maximum outputs in competitive examinations and meet industrial competences.
- To develop chemists with excellent analytical and synthetic skills through the curriculum with more laboratory components and industrial visits/internships.

1. THE PROGRAMME

The two-year M.Sc. Chemistry programme offered under CBCS by the Department of Chemistry, CUTN has four semesters, which include 19 courses in total with an overall credit of 82.

2. COURSE FEATURES

The 19 courses embrace core, elective (Department selective), skill enhancement courses, apart from research methodology and online MOOCs courses. In addition, an internship and research project courses are included in the curriculum.

3. 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 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. The admission into the programme is done through the Common University Entrance Test (CUET-PG).

4. EXAMINATION

The assessment of a student pursuing M.Sc. Chemistry programme shall be based on his/her performances in the Continuous Internal Assessment (CIA) and the End Semester Examinations (ESE). The distribution of marks for CIA and ESE are 40% and 60%, respectively. Irrespective of the score obtained by a student in the CIA, he/she must score a minimum of 50% in the ESE for passing a course.

4.1. CONTINUOUS INTERNAL ASSESSMENT (CIA)

The 40% marks for CIA shall be based on the students' performance in the following

(i) Periodical assessment tests (30%)
(ii) Assignment and seminar presentations (10%)

4.2. END SEMESTER EXAMINATION (ESE)

The ESE (maximum marks 60%) will be conducted by the University at the end of each semester (odd and even). The student must register for the first semester examination in order to be eligible for registration in the following semester examinations. A student shall register for subsequent semester examinations only after registering for the previous semester examinations.

4.3. QUESTION PAPER PATTERN

The question paper comprises of three sections, with maximum marks of 60% and allowed time of 3 hours.

SECTION A (10 X 1 = 10) Answer ALL the questions

Ten Multiple Choice Questions, two questions from each unit. Four choices of answers in each question.

SECTION B (5 x 3 = 15) Answer any FIVE questions

Five questions to be answered from the given choice of seven questions.

SECTION C (5 x 7 = 35) Answer ALL the questions

Answer all questions choosing either (a) or (b) from each question. One question from each unit.

5. PRACTICAL COURSE ASSESSMENT

The assessment of practical courses will be done on the basis of the students' performance in the laboratory, regular attendance, the number of experiments performed, on-time submission of observation and record notes, and written/viva-voce examinations.

6. ATTENDANCE

In each semester, the minimum attendance for a student to get eligible for appearing in the end semester examination is 75%. Upon failing the minimum requirement, the student shall abide by the University norms for eligibility.

7. INTERNSHIP

Students shall undergo summer internship (4 credits) after II-semester for a period of minimum 2 months. They are encouraged to take up internship at industries/ research labs/ institutes/ universities (including CUTN). The evaluation of the internship would be based on external (70%, host institution) and internal (30%, Departmental) assessment.

8. RESEARCH PROJECT

Students shall undertake a research project (12 credit) during the 4^{th} semester. The students' research guide will be allotted based on research interest and academic ranking. The project report shall be submitted in the form of a dissertation at the end of the 4^{th} semester on or before the date notified by the Department. The student shall present the research project work and shall be evaluated.

9. REVISION OF CURRICULUM

The Department of Chemistry shall revise and amend the regulations in the curriculum based on the feedback received from the stakeholders.

PROGRAMME EDUCATIONAL OBJECTIVES (PEOs)

The M.Sc. Chemistry programme 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, analyse and interpret.
PEO5: enhance skills for employability through activities, such as, seminar, communication skills, industrial visit, internship, and research project dissertation.

GRADUATE ATTRIBUTES

Disciplinary Knowledge: Content and pedagogical knowledge synchronised with the curriculum frameworks and policies
Communication Skills: Possess clarity in conveying the ideas
Critical Thinking: Capacity to apply analytical thought in the teaching and learning process
Problem Solving: Participate in the educational problem solving and applying the knowledge in the day-to-day professional endeavours.
Cooperation: Appreciate collaboration and cooperation among stakeholders of education.
ICT Skills: Selecting and integrating appropriate ICT skills for professional development.
Ethics: Doing what is right to society
Self-Directed Learning: Developing autonomy and self-regulation in teaching learning and professional development.
Reasoning: Ability to interpret and draw the conclusion from qualitative/quantitative data with open-mindedness
Creativity: Ability to produce new ideas
Societal and Environmental Concern: Performing an act or solving a problem with respect to societal and environmental concern
Lifelong Learning: Understands the need for learning and practices it throughout life

PROGRAMME OUTCOMES (POs)

On successful completion of M.Sc. programme, the student will be able to

PO1: Think critically and analyse problems.
PO2: Prepare and present scientific and technical information resulting from laboratory outputs.
PO3: Design methodologies, analyse, and evaluate innovative scientific research problems.
PO4: Pursue higher education / become an employee / entrepreneur.
PO5: Work independently as well as in a team.

POs	PEO1	PEO2	PEO3	PEO4	PEO5
PO1	3	3	3	3	3
PO2	3	2	3	3	2
PO3	2	3	3	2	2
PO4	3	3	3	3	3
PO5	3	2	2	3	3

PROGRAMME SPECIFIC OUTCOMES (PSOs)

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

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

COURSE STRUCTURE

No	Course Code	Course Title	Course Type	Credit	Hours / week	Marks	
						Int	Ext
SEMESTER – I							
1	CHE2011	Inorganic Chemistry-I	Theory	4	4	40	60
2	CHE2012	Organic Chemistry-I	Theory	4	4	40	60
3	CHE2013	Physical Chemistry-I	Theory	4	4	40	60
4	CHE2014	Organic Chemistry Laboratory	Practical	4	7	100	
5	CHEEXX	Elective	Theory	4	4	40	60
Total				**20**	**23**		
SEMESTER – II							
6	CHE2021	Inorganic Chemistry-II	Theory	4	4	40	60
7	CHE2022	Organic Chemistry-II	Theory	4	4	40	60
8	CHE2023	Physical Chemistry-II	Theory	4	4	40	60
9	CHE2024	Physical Methods in Chemistry-I	Theory	4	4	40	60
10	CHE2025	Physical Chemistry Laboratory	Practical	4	7	100	
11		Skill Enhancement Course	Theory	2	3	40	60
Total				**22**	**26**		
SEMESTER – III							
12	CHE2031	Physical Methods in Chemistry-II	Theory	4	4	40	60
13	CHE2032	Organic Chemistry-III	Theory	4	4	40	60
14	CHE2033	Physical Chemistry-III	Theory	4	4	40	60
15	CHE2034	Research Methodology (Regular / MOOCS course)*	Theory	4	4	40	60
16	CHEEXX	Elective	Theory	4	4	40	60
17	CHE2035	Inorganic Chemistry Laboratory	Practical	4	7	100	
18	CHE2036	Internship#	Practical	4	#	100	
Total				**28**	**27#**		
*The student shall attend the online course during any one of the semesters from I to III. #Students must undergo summer internship at the end of semester II for a period of minimum 2 months. They are encouraged to take up internship at industries/research labs/ institutes/ universities (including CUTN).							
SEMESTER – IV							
19	CHE2101	Research Project*	Project	12	*	100	
Total				**12**			
*Throughout the semester							

TOTAL CREDIT		
1	Theory	54
2	Practical	12
3	Internship	04
4	Project	12
Total		**82**

Semester: I **Course Type: Theory** **Course Code: CHE2011**
Credit: 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	Grasp the basic principles and their application in coordination chemistry and reaction mechanism	**Apply**
CO4	Predict reaction mechanisms in inorganic complexes	**Analyze**
CO-5	Understand the natural and artificial radioactivity	**Understand**

Unit-I Synthesis and Reactions of Inorganic Solids

Weak Chemical forces: van der Waals forces, Hydrogen bonding, Close packing of atoms and ions HCP and BCC types of packing voids, radius ratio – derivation – its influence on structures. Lattice energy – Born-Lande equation - Kapustinski equation, Madelung constant. Structures of ionic crystals – A.X. and AX2 type crystal structures (NaCl, CsCl, ZnS, fluorite, antifluorite, TiO_2, SiO_2, CaC_2 etc.) – Spinel, perovskite and layer structures. Properties - Stoichiometric and non-stoichiometric defects. Band theory, n- and p- type semiconductors and superconductors and its types. Reactions - Fick's law of diffusion and its derivation, types of diffusion mechanisms, thermal decomposition of solids -Type I and Type II reactions - Synthetic methods. Energy storage materials –Li ion battery, hydrides and hydrogen storage materials – Molecular materials - fullerides– one-dimensional metals, molecular magnets, inorganic liquid crystals.

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 J.T. effect, Jahn Teller effect and chelation, 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

Electron transfer reactions – Inner sphere (ISET) and outer sphere (OSET) electron transfer processes. Role of bridging ligand with ISET reaction – tunneling transfer – multiple bridging in the activated complex in the ISET process. Complimentary and non-complimentary E.T. reactions. Cross reactions and Marcus Hush theory. Reaction mechanism of coordination compounds – Reaction Mechanism: Kinetics and mechanism of reactions in solution – labile and inert complexes – Types of ligand substitution reactions – mechanism; Dissociative mechanism (D), Associative mechanism (A) interchange mechanism (I), Substitution Reaction in octahedral complexes – general mechanism, general rate law for A,D and I - distinction between D, Id, IA pathways, replacement of coordinated water, mechanism of acid hydrolysis, base hydrolysis – DCB mechanism – direct and indirect evidences in favour of the mechanism. Ligand substitution reactions without cleavage of M-L Bond - Anation Reactions. Substitution in square planar complexes – General mechanism, Trans effect, influences of entering and leaving groups. Application of trans effect – synthesis of isomers of Pt(II) complexes – theories of trans effect and cis-trans isomerisation. reaction. Application of substitution reactions in the synthesis of Platinum and Cobalt complexes. isomerisation and racemisation reactions of complexes – reactions of four and six-coordinate complexes – interconversion between stereoisomers.

Reference Books:

1. J. E. Huheey, E. A. Keiter, R. L. Keiter and O. K.Medhi, Inorganic Chemistry - Principles of Structure and Reactivity, 4th edition, Pearson Education, 2006.
2. P. W. Atkins and, J. Paula, Physical Chemistry, Oxford Publications, 8thedition, 2009.
3. B. Douglas, D. McDaniel and J. Alexander, Concepts and Models of Inorganic Chemistry, 3rd edition, John Wiley & Sons, 2010.
4. F. A. Cotton and G. Wilkinson, Advanced Inorganic Chemistry, 3rd ed. Wiley-Eastern Company, New Delhi, 1990.
5. L.V. Azaroff, Introduction to Solids, McGraw hill, New York. 1960.
6. A. R. West, Solid State Chemistry and Its Applications, John Wiley & Sons, 1984.
7. K. Chakrabarty, Solid State Chemistry, New Age Publishers, 1996.
8. H. V. Keer, Principles of the Solid State, Wiley Eastern Limited, 1993.
9. D.M. Adams, Inorganic Solids: An Introduction to Concepts in Solid State Structural Chemistry, Wiley, 1974.
10. C.N.R. Rao and K.J. Rao, Phase Transitions in Solids, McGraw Hill, 2010.
11. M. C. Day, J. Selbin, Theoretical Inorganic Chemistry, East West Press. 2nd Ed, 1985.
12. S. F. A. Kettle, Physical Inorganic Chemistry – A Coordination Chemistry Approach, Spectrum Academic Publishers, Oxford University Press, 1996.
13. F. Basolo, R. G. Pearson, Mechanism of Inorganic Reactions, John Wiley, New York,1967.
14. G. L. Miessler and D. A. Tarr, Inorganic Chemistry, 3rd edition, Pearson, 2004.
15. C. E. Housecraft and A.G. Sharpe, Inorganic Chemistry, 4th edition, Pearson, 2012.
16. K. F. Purcelland, J. C. Kotz, Inorganic Chemistry, Cengage Learning, 2012.
17. M. C. Day Jr., J. Selbin, Theoretical Inorganic Chemistry, Literary Licensing, L.C., 2012.
18. G. Wilkinson, R. D. Gillarsand J. A. McCleverty, Comprehensive Co-ordination Chemistry, Pergamon Press, 1987.
19. G. Wulfberg, Inorganic Chemistry, University Science Books, 2000.
20. D.M. Adam, Inorganic Solids: An introduction to concepts in solid-state structural chemistry, John Wiley & Sons, 1974.

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

C.O.	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

Semester: I **Course Type: Theory** **Course Code: CHE2012**
Credit: 4 **Course Title: Organic Chemistry-I**

Course Outcomes		Level
CO-1	Relate thermodynamic stability and reaction rates	**Understand**
CO-2	Predict the aromaticity of organic compounds based on applying various rules	**Apply**
CO-3	Demonstrate the detailed mechanism of nucleophilic and electrophilic substitution reactions	**Understand**
CO-4	Sketch the importance of stereochemistry to predict the reactivity based on various stereochemical factors	**Apply**
CO-5	Learn the preparation and properties of various heterocyclic compounds including fused ring compounds	**Remember**

Unit-I Physical Organic Chemistry

Thermodynamic stability – general relationship between thermodynamic stability and reaction rates – electronic substituent effects on reaction intermediates – 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 intermediates, stereochemical studies. Linear free energy relationships: 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 stereochemistry. Factors affecting the rates of S_N1, $S_N2$and S_Ni and neighbouring group participation. Mechanisms of Rearrangement of Carbocations, Bridged (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, 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

Nomenclature, five and six membered heterocycles, Heterocyclic compounds with one heteroatom: Preparation, properties and reactions of pyrrole, furan, thiophene and pyridine. Heterocyclic compounds with two heteroatoms: Preparation, properties and reactions of imidazole, pyrazole, oxazole, isoxazole, thiazole, isothiozole, pyrimidine, pyrazine, pyridazine. Heterocyclic compounds with three hetero atoms: Preparation, properties and reactions of triazole, triazine. Fused or condensed heterocyclic compounds: Preparation, properties and reactions of indole, quinoline, isoquinoline, carbozole.

Reference Books:

1. E. V. Anslyn, D. A. Dougherty, Modern Physical Organic Chemistry, University Science Books, 2004
2. Raj K. Bansal, Heterocyclic Chemistry, 4th Ed., Anshan Limited, 2008.
3. Alan R. Katritzky, Christopher A. Ramsden, John A. Joule, Viktor V. Zhdankin Handbook of Heterocyclic Chemistry, Elsevier Publication, 2010.
4. I. L. Finar, Organic Chemistry, Vol II, 6th Ed, Pearson Education, 2002.
5. R. T. Morrison, R. N. Boyd, Organic Chemistry, 7th Ed, Pearson Education, 2010.
6. J. Clayden, N. Greeves, S. Warren, Organic Chemistry, 2nd Ed, Oxford University Press, 2014.
7. Michael B. Smith, March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure, 8nd Ed., Wiley Publications, 2019
8. Graham Solomons, T. W. Fryhle, C. B. Snyder, S. A., Organic Chemistry, 12th Ed, Wiley, 2016.
9. J. E. McMurry, Fundamentals of Organic Chemistry, 7th Ed, Cengage Learning India Edition, 2013.
10. I. L. Finar, Organic Chemistry, Vol I, 6th Ed, Pearson Education, 2002.
11. P. Sykes, A Guidebook to Mechanism in Organic Chemistry, 6th Ed., Orient Longman, New Delhi, 1988.
12. Francis A. Carey and Richard J. Sundberg, Advanced Organic Chemistry, Part A: Structure and Mechanisms, Springer, 5th Ed. 2007
13. Daniel E. Levy, Arrow Pushing in Organic Chemistry-An easy approach to understanding reaction mechanisms, Wiley Publications, 2008
14. Robert B. Grossman, The Art of Writing Reasonable Organic Reaction Mechanisms, 2nd Ed, Springer, 2003
15. L. G. Wade, Organic Chemistry, 6th Ed. Pearson, 2006
16. Francis A. Carey, Robert M. Giuliano, Organic Chemistry, 8th Ed. 2008
17. Peter Vollhardt, Neil Schore, Organic Chemistry-Structure and Function, 6th Ed. W. H. Freeman and Company, 2011
18. Thomas H. Lowry, Kathleen Schueller Richardson, Mechanism and Theory in Organic Chemistry, Harper and Row Publishers
19. Edwin S. Gould, Mechanism and Structure in Organic Chemistry, Holt, Rinehart and Winston Publications, 1959

C.O.	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

Semester: I **Course Type: Theory** **Course Code: CHE2013**
Credit: 4 **Course Title: Physical Chemistry-I**

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**

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 & 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

I.R. 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, I.R. activity.

Raman Spectra: Complementary of I.R. 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(D_3h) 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

Reference Books:

1. W. J. Moore and R. G. Pearson, Kinetics and Mechanism, Wiley, New York, 1988.
2. F. Daniels and R. A. Alberty, Physical Chemistry, 8h Edition, Wiley, New York, 1994.
3. P. W. Atkins, Physical Chemistry 8th Edn., Wiley, New York, 2006.
4. J. Rajaram, J.C. Kuriakose, Kinetics and Mechanisms of Chemical Transformations, Macmillan India, 2000.
5. K. J. Laidler, Chemical kinetics, 3rd Edn. Harper & Row, 1987.
6. C. Kalidas, Chemical Kinetic Methods: Principles of Fast Reaction Techniques and Applications, New Age International, 2005.
7. D.A. McQuarrie, J. D. Simon, Physical chemistry: A Molecular Approach, University Science Books,1997.
8. F. A. Cotton: Chemical Applications of Group Theory, Wiley Eastern, 1985.
9. P. K Ghosh and P. K Shukla: Atomic Electronic Structure, Prentice Hall of India,1994.
10. V. Ramakrishnan and M. S. Gopinathan: Group Theory in chemistry, Vishal Publication, 1986.
11. D. M. Bishop, Group theory and Chemistry, Dover, 1989.
12. B. S. Garg, Chemical Applications of Molecular Symmetry and Group Theory, Macmillan Publishers India Ltd, 2012

C.O.	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

Semester: I **Course Type: Practical** **Course Code: CHE2014**
Credit: 4 **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 separation of two mixture present in the organic compounds	**Understand**
CO-5	Support on estimation of organic compounds *viz* volumetric methods	**Evaluate**

Students are expected to try various approaches in organic synthesis and characterization. The assessment is based on the practical skills in the lab, originality and the written report at the end of the course. Topics include but are not restricted to the below points.

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.

Reference Books

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.
4. P. B. Cranwell, L. M. Harwood, C. J. Moody, Experimental Organic Chemistry, 3rd Ed, Wiley-Blackwell, 2017.
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C.O.	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

Semester: II **Course Type: Theory** **Course Code: CHE2021**
Credit: 4 **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 magnetic properties of inorganic compounds and photochemistry	**Understand**

Unit-I Structure and bonding in organometallics

16/18-Electron rule – Preparation, Structure, Bonding – spectra of metal alkyls, aryls, hydrides, dihydrogen and dinitrogen complexes - metallocenes - electronic structure and bonding in ferrocene - synthesis, physical and spectroscopic properties of metallocenes – fluxional molecules. σ–bonded ligands: metal- phosphines, Nitrosyls – bridging and terminal nitrosyls, bent and linear: structures, reactivity and bonding. Carbenes: N-heterocyclic carbenes, Fischer carbenes, Schrock carbenes, carbynes. Isolobal analogy, metal-metal bonds, transition metal clusters. Quintuple bond. Template synthesis of macrocyclic ligands.

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; Catalysis: Hydrogenation of olefins, hydroformylation, Wacker process, Ziegler-Natta polymerisation, cyclooligomerisation, Isomerization reactions, olefin metathesis, Monsanto acetic acid synthesis, Fischer-Tropsch process, hydrosilylation, carbonylation, and C.H. 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. Metals at the Center of Photosynthesis: Primary Processes in Photosynthesis – Photosystems I and II - Light Absorption (Energy Acquisition) – Exciton transport (Direct Energy Transfer) – Charge separation and electron transport – Manganese catalyzed oxidation of water to O_2.

Unit-IV Metalloporphyrins and Metalloenzymes

Dioxygen transport and storage - hemoglobin and myoglobin: electronic and spatial structures - hemerythrin and hemocyanine – synthetic Oxygen carriers, model systems - blue copper proteins (Cu) - iron-sulfur proteins (Fe) - cytrochromes electron transport chain - carbon monoxide poisoning - iron enzymes - peroxidase, catalase and cytochrome P-450, copper enzymes - superoxide dismutase, carboxypeptidase, carbonicanhydrase, vitamin B_{12} and B_{12} coenzymes, nitrogen fixation. Essentials of trace elements and chemical toxicology: Trace elements in

biological system. Metal ion toxicity - classes of toxic metal compounds – detoxification. Metals in medicine: Anti arthritis drugs – Au and Cu in rheumatoid arthritis – Li in psychiatry – Pt, Au and metallocenes in anti-cancer drugs- metals in radio-diagnosis and magnetic resonance imaging.

Unit-V Nuclear Chemistry II

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 medicine- Single Proton Emission Tomography (SPECT) and Positron Emission Tomography (PET).

Reference Books:

1. P. Powell, Principles of Organometallic Chemistry, 2nd ed., Springer, 1998.
2. K. F. Purcell and J. C. Kotz, Inorganic Chemistry, Saunders Golden Sunburst Series, W.B. Saunders Company, Philadelphia, 1987.
3. J. E. Huheey, E. A. Keiter, R. L. Keiterand, O. K. Medhi, Inorganic Chemistry - Principles of Structure and Reactivity,4th edition, Pearson Education, 2006.
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6. B. D. Gupta, and A. J. Elias, Basic Organometallic Chemistry: Concepts, Syntheses, and Applications of Transition Metals, 1st edition, Universities Press, CRC Press, 2010.
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11. C. E. Housecraftand A.G. Sharpe, Inorganic Chemistry, 4thedition, Pearson, 2012.
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18. S. E. Kegley, and A. R. Pinhas, Problems and Solutions in Organometallic Chemistry, University Science Books, Oxford University Press, 1986.
19. B. Douglas, D. H. McDaniel and J. J. Alexander, Concepts and Models of Inorganic Chemistry, 2nd edition, John Wiley & sons, New York, 2006.
20. M. Bochmann, Organometallics 1: Complexes with transition metal-carbon s-bonds; Oxford Chemistry Primers Series, No. 13,1994.
21. M. Bochmann, Organometallics 2: Complexes with transition metal carbon s-bonds, Oxford Chemistry Primers Series, No.12, 1994.
22. W. Parkins and R. C. Poller, An Introduction to Organometallic Chemistry, Palgrave Macmillan, 1986.
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C.O.	**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

Semester: II **Course Type: Theory** **Course Code: CHE2022**
Credit: 4 **Course Title: Organic Chemistry-II**

Course Outcomes		Level
CO-1	Synthesize organic compounds based on light mediated route	**Understand**
CO-2	Compare the concepts of pericyclic reaction mechanism 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	To demonstrate the use of reducing reagents in the synthetic organic chemistry	**Understand**

Unit-I Organic photochemistry

Thermal vs photochemical reactions. Photochemistry of alkenes, dienes and polyenes. 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-pi-methane, oxa/aza di-pi 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: 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 and secondary effects. Analysis of Electrocyclic reactions: FMO and Woodward-Hoffmann correlation diagrams methods. Cycloaddition reactions: Effect of stereochemistry and substituents on the rate of cycloadditions, analysis of cycloaddition reactions. 1,3-Dipolar cycloadditions and cheleotropic reactions. Sigmatropic rearrangements - [1,2]-sigmatropic shifts involving carbon moieties. [m,n] and [m,m] sigmatropic hydrogen shifts. 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

Alcohols to carbonyl compounds-chromium(VI) oxidants, dimethyl sulfoxide - Swern oxidation, manganese(IV) oxide, silver carbonate, hypervalent iodine(III) and (V) reagents, ceric ammonium nitrate (CAN), N-oxyl radical. Alkenes to epoxides by H_2O_2, hydroperoxides and peroxyacids. Prevost oxidation and Woodward modifications. Oxidative cleavage of 1,2-diols - periodic acid. Oxidation of allylic and benzylic C-H bonds - NBS, DDQ, chloranil-T, SeO_2, and TEMPO. PCC, Oppenauer and Corey-Kim oxidation.

Unit-V Reduction

Catalytic hydrogenation - homogeneous and heterogeneous catalytic reductions. Dissolving metal reductions. Non-metallic reductions - Wolff-Kishner, diimide reductions, and Hantzsch ester. Metal hydride reductions - Nucleophilic metal hydrides, Sodium cyano borohydride, Li and Na borohydrides, $LiAlH_4$, DIBAL-H and Red-Al. Electrophilic metal hydrides - BH_3 and AlH_3. Hydrogenolysis - use of tri-n-butyl tin hydride. Reduction using SmI_2. Noyori and Knowels asymmetric hydrogenation.

Reference Books:

1. V. Ramamurthy, Organic Photochemistry, CRC Press, 1997.
2. J. M. Coxon, B. Halton, Organic Photochemistry, Cambridge University Press, 1987
3. G. R. Chatwal, Organic Photochemistry, Himalaya Publishing House, 1998.
4. S. Sankararaman, Pericyclic Reactions, Wiley VCH, 2005.
5. Ian Fleming, Pericyclic Reactions, Oxford University Press, 2015.
6. R. T. Morrison, R. N. Boyd, Organic Chemistry, 7th Ed, Pearson Education, 2010.
7. J. Clayden, N. Greeves, S. Warren, Organic Chemistry, 2nd Ed, Oxford University Press, 2014.
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C.O.	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

Semester: II **Course Type: Theory** **Course Code: CHE2023**
Credit: 4 **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 H.F. 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**

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.

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

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 I.R. & 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

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 Books:

1. I. N. Levine: Quantum Chemistry, Prentice Hall India, 1994.
2. S. N. Datta: Lecture on Chemical bonding and quantum chemistry, 1998.
3. D. A. McQuairrie: Quantum Chemistry, Oxford University press, Oxford, 1982.
4. P. W Atkins: Molecular Quantum Mechanics, Clarendon Press, Oxford, 1983.
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14. A. Dau and C. Singh, Quantum chemistry classical to computational, Manakin press, 2017.

C.O.	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

Semester: II **Course Type: Theory** **Course Code: CHE2024**
Credit: 4 **Course Title: 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**

Unit-I UV-Visible, Fluorescence Spectroscopy and ORD-CD

Basics of U.V. Spectroscopy, factors governing absorption maximum and intensity. Woodward Fieser and Fieser-Kuhn's rules - calculation of λmax 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 assignments.

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 I.R. spectra of alkane, alkenes, alkynes, aromatic compounds, alcohols, ethers, phenol, carbonyl compounds, amines and heterocyclics– related problems

Unit-III NMR Spectroscopy-I

^{1}H NMR, Spectral parameters – intensity, chemical shift, multiplicity, coupling constant, factors affecting chemical shift. Analysis of first order and second – order spectra – shift reagents - structure determination of organic compounds by ^{1}H NMR spectra. Chemical shifts and coupling constants (spin-spin coupling) involving different nuclei (^{1}H, ^{19}F, ^{31}P, ^{13}C) interpretation. Examples for different spin systems – 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: Proton coupled; off–resonance decoupled; proton noise decoupled ^{13}C NMR spectra, DEPT techniques. Assignment of chemical shifts, additively effect, characteristic chemical shifts of common organic compounds and functional groups.

NMR of paramagnetic molecules – isotropic shifts contact and pseudo-contact interactions – Lanthanide shift reagents. An elementary treatment of second order spectra – examples.

2D NMR techniques: H,H-COSY, C,H-COSY, HMBC, NOESY and INADEQUATE.

Unit-V Mass spectrometry

Instrumentation – methods of ionisation - E.I., CI, APCI, ESI, MALDI and FAB. 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-COSY techniques

Reference Books:

1. R. M. Silverstein and F. X. Webster, Spectrometric identification of organic compounds, John Wiley and Sons. Inc., 6th edition, 1997.
2. W. Kemp, Organic Spectroscopy, 3rd edition, MacMillan, 1994.
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14. A Derome, Modern NMR Technique, Pergamon, 1983.
15. Farrar and E. D. Becker, Pulsed FT NMR Spectroscopy.
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C.O.	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

Semester: II **Course Type: Practical** **Course Code: CHE2025**
Credit: 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 Q.M. methods for modelling simple organic/inorganic compounds for structural optimization and reaction modelling	**Apply**

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.

Part B: List of Computational Chemistry Experiments (Any 3-4 Experiments)

1. Calculation of electrostatic charges of atoms in organic molecules using population analysis.
2. Calculation of Resonance energy of aromatic compounds.
3. Calculation of dimerization energy of carboxylic acids.
4. Perform the conformational analysis of butane using potential energy scan.
5. Find the transition state of simple organic reactions and plot the reaction profile.
6. Determination of heat of hydration of organic molecules.
7. Find the Gibbs free energy of simple gaseous phase reactions and calculate equilibrium constant.
8. Calculation of pKa of simple organic molecules and compare it with experimental values.
9. Docking studies involving protein ligand interactions.
10. Calculation of electrophilicity index in hard-soft acids and bases.

Reference Books:

1. J. B. Yadav, Advanced Practical Physical Chemistry, Goel Publishing House, 2001.
2. G.W. Garland, J. W. Nibler, D.P. Shoemaker, Experiments in Physical Chemistry, 8thEdn. McGraw Hill, 2009.
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7. D.C. Young, Computational Chemistry: A Practical Guide for Applying Techniques to Real World Problems, John Wiley & Sons, 2001.
8. D. Rogers Computational Chemistry Using the PC, 3rdEdn, John Wiley & Sons,2003.
9. A.R. Leach, Molecular Modelling: Principles and Applications, 2ndEdn, Longman, 2001.
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C.O.	**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
4	3	3	3	3	3

Semester: III **Course Type: Theory** **Course Code: CHE2031**
Credit: 4 **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 I.R. 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**

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

I.R. 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 I.R. and Raman spectroscopy in the structural elucidation of N_2O, ClF_3, NO^{3-}, ClO_4, metal carbonyls.

Unit-III NMR and NQR Spectroscopies

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. NQR spectroscopy - Characteristics of quadrupolar nucleus – effects of field gradient and magnetic field upon quadrupolar energy levels – NQR transitions – applications of NQR spectroscopy.

Unit-IV EPR and Mössbauer spectroscopies

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 V.O. (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. Mössbauer spectroscopy - Isomer shifts – Magnetic interactions – Mossbauer emission spectroscopy – applications to iron and tin compounds.

Unit-V Magnetic and photochemical properties of Inorganic complexes

Types of magnetism – Dia –para – ferro and antiferro magnetism. Magnetic properties of free ions – first order Zeeman effect – Determination of Magnetic moments and their applications to the elucidation of structures of inorganic compounds – temperature dependent and temperature independent paramagnetism - Magnetic properties of lanthanides and actinides. Spin crossover in coordination compounds. Inorganic and organometallic photochemistry – principles- Unimolecular charge-transfer photochemistry of cobalt(III) complexes – mechanism of CTTM, photoreduction – ligand-field photochemistry of chromium(III) complexes – Adamson's rules, photoactive excited states, V-C model – photophysics and photochemistry of ruthenium – polypyridine complexes, emission and redox properties.

Reference Books:

1. R. S. Drago, Physical Methods for Chemistry, 2nd Ed, Saunders College Publishing, 1992.
2. A. B. P. Lever, Inorganic Electronic Spectroscopy, 2nd Sub Ed, Elsevier Science, 1986.
3. J. E. Huheey, E. A. Keiter and R. L. Keiter and O. K. Medhi, Inorganic Chemistry – Principles of Structure and Reactivity, 4th Edition, Pearson Education, 2006.
4. A. K. Das and M. Das, Fundamental concepts of Inorganic Chemistry, 1st Edition, Volume 7, CBS Publishers & Distributors Pvt. Ltd.,2014.
5. G. Wulfberg, Inorganic Chemistry, University Science Books, 2000.
6. K. Nakamoto, Infrared and Raman Spectra of Inorganic and Coordination Compounds, Part B: Applications in Coordination, Organometallic, and Bioinorganic Chemistry, Wiley-Interscience; 5th edition, 1997.
7. J. Ferraudi, Elements of Inorganic Photochemistry, Wiley, New York, 1988.
8. E. A.V Ebsworth, D. W. H. Rankin and S. Cardock- Structural Methods in Inorganic Chemistry, 1987.
9. A. I. Jonathan, Luzyanin, K, NMR Spectroscopy in Inorganic Chemistry - Oxford University Press, 2020.
10. A. W. Adamson, P. D. Fleischauer, Concepts of Inorganic Photochemistry, Wiley, 1975.
11. A. Earnshaw, Introduction to Magnetochemistry, Academic Press, 1968.
12. D. Bahnemann, A. O. T. Patrocinio, Springer Handbook of Inorganic Photochemistry, Springer Cham, 2022.
13. F. A. Cotton and G. Wilkinson, Advanced Inorganic Chemistry, 3rd ed., Wiley-Eastern Company, New Delhi, 1990.
14. P. J. Wheatley, The Determination of Molecular Structure, 2nd Ed, Dover Pubns, 1981.
15. J. and R. G. Wilkins Lewis, Modern Coordination Chemistry Principles and Methods, Interscience Publishers, Inc., 1967.
16. E. A. V. Ebsworth, Structural Methods in Inorganic Chemistry, 3rd ed., ELBS, Great Britain, 1987.
17. R. A. Scott and C. M. Lukehart, Applications of Physical Methods to Inorganic and Bioinorganic Chemistry, John and Wiley & Sons, LTD, 2007.

18. E. I. Solomon, A. B. P. Lever, Inorganic Electronic Structure and Spectroscopy, Vol.,2 Applications and Case Studies, Wiley-Interscience, 2006.
19. B. P. Lever, Inorganic Electronic Spectroscopy, 2nd Sub Edition, Elsevier Science, 1986.
20. D.N. Satyanarayana, Electronic Absorption Spectroscopy, Universities Press, 2000.
21. R.B. Jordon, Reaction Mechanisms of Inorganic and Organometallic Systems, 3rd Edition, Oxford University Press, 2007.
22. C.J. Ballhausen and H.B. Gray, Molecular Orbital Theory, Benjamin/Cummings Pub. Co, 1965.
23. N. Figgis and M. A. Hitchman, Ligand Field Theory and Its Applications, 1st Edition, Wiley VCH, 1999.
24. S.F.A. Kettle, Physical Inorganic Chemistry – A Coordination Chemistry Approach, Spectrum Academic Publishers, Oxford University Press, 1996.

C.O.	**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

Semester: III **Course Type: Theory** **Course Code: CHE2032**
Credit: 4 **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**

Unit-I Organometallic Reagents and Catalysts

Application of organometallic compounds of lithium, magnesium, boron, silicon and tin in organic synthesis. Applications of organoplatinum, organonickel, organocobalt, organocopper, organozinc, organocadmium and organomercury in organic synthesis.

Coupling Reactions: Mechanism and applications of Buchwald-Hartwig cross coupling, Kumada, Fukuyama, Heck Reaction, Hiyama, Sonogashira, Stille, Suzuki, Tsuji-Trost, Negishi, Enzymes and whole cell mediated biotransformations

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. Control of relative stereochemistry and enatioselectivity in carbonyl condensations. Retro Diels – Alder reactions- Pericyclic reactions- Wieland Mischer ketone synthesis- Reterosynthesis of 3, 4, 5, 6 membered heterocycles containing two nitrogens. Designing synthesis: Disconnection approach in Epothilone, Juvabione and longifolene.

Unit-IV Rearrangement and Transformation Reactions

Classification of rearrangements. General mechanistic consideration, nature of migration, migratory aptitude, stereochemical aspects and memory effects in rearrangements. Rearrangement to electron deficient carbon - pinacol-pinacolone, Wagner-Meerwein, benzillic acid, Wolf, Rupe and Demjanov rearrangements. Rearrangement to electron deficient nitrogen - Hofman, Curtius, Schmidt, Lossen and Beckmann rearrangements. Rearrangement to electron deficient oxygen - Baeyer-Villiger rearrangement. Rearrangement to electron rich carbon - Fovorskii, Wittig, Neber and Stevens rearrangements. Aromatic rearrangement - Fries, Claisen and benzidine rearrangements.

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 E_2, prostacyclin (PGI_2). Structural features (synthesis not required) of prostaglandin D_2 (PGD_2) and prostaglandin $F_{2\alpha}$ ($PGF_{2\alpha}$).

Reference Books:

1. B. D. Gupta, Basic Organometallic Chemistry: Concepts, Syntheses and Applications, University Press, 2011
2. Robert H. Crabtree, The Organometallic Chemistry of the Transition Metals, Wiley, 2014
3. Norio Miyaura, S.L. Buchwald, Metal Catalyzed Cross-Coupling Reactions and More, 2003.
4. G. Denis Meakis, Functional Groups: Characteristics and Interconversions, Oxford Science Publications, 1996
5. Jie Jack Li, Name Reactions: A Collection of Detailed Mechanisms and Synthetic Applications, 5th Ed, Springer, 2014
6. Christian M. Rojas, Molecular Rearrangements in Organic Synthesis, John Wiley & Sons, Inc, 2015
7. S. Warren, P. Wyatt, Organic Synthesis: The Disconnection Approach, Wiley, 2008
8. P. Wyatt, S. Warren, Organic Synthesis: Strategy and Control, Wiley-Blackwell, 2007
9. R. O. C. Norman, J. M. Coxon, Principles of Organic Synthesis, 3rd edn, 1993
10. W. Carruthers, I. Coldham, Modern Methods of Organic Synthesis, 4th edn, Cambridge University Press, 2015
11. E. J. Corey, X. M. Cheng, The Logic of Chemical Synthesis, Wiley-India Private Ltd, 2011.
12. K. C. Nicolaou, E. J. Sorensen, Classics in Total Synthesis, Wiley-ECH, 1996
13. I. L. Finar, Organic Chemistry, Vol II, 6th Ed, Pearson Education, 2002.
14. R. T. Morrison, R. N. Boyd, Organic Chemistry, 7th Ed, Pearson Education, 2010.
15. J. Clayden, N. Greeves, S. Warren, Organic Chemistry, 2nd Ed, Oxford University Press, 2014.
16. Michael B. Smith, March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure, 8nd Ed., Wiley Publications, 2019
17. Graham Solomons, T. W. Fryhle, C. B. Snyder, S. A., Organic Chemistry, 12th Ed, Wiley, 2016.
18. J. E. McMurry, Fundamentals of Organic Chemistry, 7th Ed, Cengage Learning India Edition, 2013.
19. I. L. Finar, Organic Chemistry, Vol I, 6th Ed, Pearson Education, 2002.
20. P. Sykes, A Guidebook to Mechanism in Organic Chemistry, 6th Ed., Orient Longman, New Delhi, 1988.
21. Francis A. Carey and Richard J. Sundberg, Advanced Organic Chemistry, Part A: Structure and Mechanisms, Springer, 5th Ed. 2007
22. Daniel E. Levy, Arrow Pushing in Organic Chemistry-An easy approach to understanding reaction mechanisms, Wiley Publications, 2008
23. Robert B. Grossman, The Art of Writing Reasonable Organic Reaction Mechanisms, 2nd Ed, Springer, 2003

24. L. G. Wade, Organic Chemistry, 6th Ed. Pearson, 2006
25. Francis A. Carey, Robert M. Giuliano, Organic Chemistry, 8th Ed. 2008
26. Peter Vollhardt, Neil Schore, Organic Chemistry-Structure and Function, 6th Ed. W. H. Freeman and Company, 2011
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

C.O.	**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

Semester: III **Course Type: Theory** **Course Code: CHE2033**
Credit: 4 **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**

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-II

Activity and Activity coefficient of electrolytes, ionic strength, Debye Huckel theory of strong electrolytes, Mean ionic activity coefficient. 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-III

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 & Electroanalytical Techniques

Storage cells: Lead acid battery, lithium battery, nickel cadmium cell. Fuel Cell. Theory and working of fuel cell. H_2- O_2 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.

Reference Books:

1. R.P. Rastogi, R.R. Mishra, An introduction to Chemical Thermodynamics, Vikas Publishing house, 2009.
2. J. Rajaram, J.C. Kuriakose, Chemical Thermodynamics: Classical, Statistical and Irreversible, 1stEdn, S Chand and Co., 1999.
3. M.C. Gupta, Statistical Thermodynamics, New age international, 2007.
4. L.K. Nash, Elements of Classical & Statistical Mechanics, 2ndEd. Addison Wesley, 1972.
5. F.W. Sears, G.L. Salinger, Thermodynamics, Kinetic Theory and Statistical Thermodynamics, Addison Wesley, 1975.
6. J. Kestin, J.R. Dorfman, A Course in Statistical Thermodynamics, Academic Press, 1971.
7. John E. Freund. Modern elementary statistics, 2003, ISBN-13: 978-0131874398 20.
8. S. P. Gupta, Statistical Methods: S. Chand, 2014.
9. J. Bockris and A.K.N. Reddy, Modern Electrochemistry, 2ndEd, Wiley, New York, 1998.
10. D.R. Crow, Principles and Applications of Electrochemistry, Chapman & Hall, 3rdEdn., New York, 1994.
11. S. Glasstone, Introduction to Electrochemistry, Biblio Bazar, 2011.
12. B.K. Sharma, Electrochemistry, Krishna Prakashan, 1985.
13. A.I. Vogel, A Textbook of Quantitative Analysis including Instrumental Analysis, John Wiley & Sons, 1961.
14. H.H. Willard, J.A. Dean, L.L. Merritt, Instrumental Methods of Analysis, 7th Ed., Van Nostrand, 1965.
15. D.A. Skoog, D.M. West, F.J. Holler, S.R. Crouch, Fundamentals of Analytical Chemistry, 8thEdn. Saunders College Pub., 2007.
16. A.J. Bard, L.R Faulkner, Electrochemical Methods-Fundamentals and applications, 2ndEdn., Wiley India Ed.2004

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

Semester: III **Course Type: Theory** **Course Code: CHE2034**
Credit: 4 **Course Title: Research Methodology**

Course Outcomes		Level
CO-1	Understand the principles of research, literature survey and writing a research paper and thesis writing	**Understand**
CO-2	Gain knowledge of 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 of writing research papers and report	**Apply**

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 Analysis

Aim, objectives, expected outcome, and methodology to be adopted. Importance of reproducibility of results. Objectives and basic principles of designs of experiments. Data analysis: Accuracy, precision, significant figures, use of calculation in the estimation of errors. 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 scientific 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 Books:

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.

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

Semester: III **Course Type: Practical** **Course Code: CHE2035**
Credit: 4 **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 the working principle of cyclic voltammetry and differential pulse voltammetry techniques and determine the electrochemical properties of complexes	**Knowledge**

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

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

1. Tetramminecopper (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 $[Co(NH_3)_5Cl]Cl_2$.
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 Books:

1. J. Elias, A Collection of Interesting General Chemistry Experiments, Universities Press, Sangam Books Ltd, 2002.
2. J. D. Woollins, , Inorganic experiments, 3rd edition, Wiley-VCH Verlag GmbH @ Co. KGaA, 2012.
3. M. Hein, J. N. Peisen and R. L. Miner, Foundations of College Chemistry in the Laboratory, John Wiley and Sons, 2011.

4. G. S. Girolami, T. B. Rauchfuss and R. J. Angelici, Synthesis and Technique in Inorganic Chemistry: A Laboratory Manual, 3rd edition, University Science Books, 1999.
5. W. L. Jolly, The Synthesis and Characterization of Inorganic Compounds, Prentice-Hall, Inc.1970.
6. In-house Laboratory Manual, Department of Chemistry, CUTN.
7. Ghoshal, Mahapatra and Nad, An Advanced Course in Practical Chemistry, New Central Book Agency, 2011.
8. G. Svehla, Vogel's Qualitative Inorganic Analysis, Pearson Education, 2012.
9. J. Mendham, Vogel's Quantitative Chemical Analysis, Pearson, 2009.
10. Ghoshal, Mahapatra and Nad, An Advanced Course in Practical Chemistry, New Central Book Agency, 2011.
11. V. Venkateswaran, R.Veerasamy A. R Kulandaivelu, Basic principles of Practical Chemistry, 2nd edition, New Delhi, Sultan Chand & sons, 2016.

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

Semester: IV **Course Type: Practical** **Course Code: CHE2101**
Credit: 4 **Course Title: Research Project**

Course Outcomes		Level
CO-1	Understanding the nature of research problems and identifying the related area of knowledge	**Understand**
CO-2	Analyze literature reports 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**

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

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	3

List of Electives Courses

Course Code	Title of the Course	Credits
CHEE01	Principles of Polymer Science	4
CHEE02	Principles of Fluorescence Spectroscopy	4
CHEE03	Asymmetric Catalysis	4
CHEE04	Essentials of Carbohydrate Chemistry	4
CHEE05	Organic Electronics	4
CHEE06	Photochemistry in Molecules and Materials	4
CHEE07	Medicinal Inorganic Chemistry	4
CHEE08	Organic Semiconductors	4
CHEE09	Advances in Polymer Science	4
CHEE10	Advances in Carbohydrate Research	4
CHEE11	Advanced Organic Materials and Catalysis	4
CHEE12	Chemistry of CH Activation	4
CHEE13	Advanced Bio-inorganic Chemistry	4
CHEE14	Principles of Biochemistry	4
CHEE15	Mathematics for Chemists and Biologists	4
CHEE16	Electrochemical Energy Systems	4
CHEE17	Fundamentals of Analytical Chemistry	4
CHEE18	Computational Chemistry	4
CHEE19	Advanced NMR Techniques	4
CHEE20	Organometallics, Catalysis and Inorganic Spectroscopy	4
CHEE21	Applications of Computational Methods in Chemistry	4
CHEE22	Chemical Lab Safety and Management	4
CHEE23	Advanced Organic Synthesis	4
CHEE24	Green Chemistry	4
CHEE25	Advanced Topics in Organometallic Chemistry	4
CHEE26	Industrial Chemistry	4
CHEE27	Advanced Organic Nanomaterials	4
CHEE28	Computer software for Chemists	4
CHEE29	Selected Experiments in Applied Chemistry	4
CHEE30	Luminescence Spectroscopy for Advanced Research	4
CHEE31	Nanoscience and Technology	4

*New electives will be appended based on the availability of course instructor.
Electives will be offered based on the individual faculty's availability