M.Sc. Chemistry Programme (CBCS) Curriculum

Department of Chemistry
(DST-FIST Sponsored)
School of Basic and Applied Sciences
Central University of Tamil Nadu
Thiruvarur- 610 005
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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 PG programme in Science at CUTN. Besides the state-of-the-art PG and research laboratories, 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 is presently offering 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 provide hands-on experience to the students at all levels.

The focus of the department 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. As a part of the curriculum the students have to undergo Internships at industry, institutes, and Universities. The department aim is to produce highly sought after and knowledgeable graduates for pursuing careers with academia, industry and government.

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 24 courses in total with an overall credit of 92.

2. COURSE FEATURES

The 24 courses embrace core, department specific elective, skill enhancement, value added courses apart from research methodology course. In addition, 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 for theory courses (maximum marks 60%) will be conducted by the University at the end of each semester (odd and even). The student must register for the semester examination in order to be eligible for registration in the following semester examinations. To attend the examination 7 % attendance is mandatory.

4.3. QUESTION PAPER PATTERN

The end semester examination question paper comprises 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 ALL 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 based on 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) during second year for a period of 1-2 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 synchronized 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 integrated M.Sc. programme, the student will be able to

PO1: Think critically and analyze problems.

PO2: Prepare and present scientific and technical information resulting from laboratory outputs.

PO3: Design methodologies, analyze, 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 M.Sc. 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 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 position in Industry & Academics.

PSO5: Enhance employability through laboratory activities, solving problems and cocurricular activities

COURSE STRUCTURE

CC: Core Course; CCP: Core Course Practical; DSE: Department Specific Elective; OE: Open Elective; SEC: Skill Enhancement Course; VAC: Value Added Course; INT: Internship; Research Project/Dissertation

FIRST YEAR

No	Course Code	Course Title	Type	Credit	Hours / Week	Marks	
						Int	Ext
SEMESTER – I							
1	CHE2011	Inorganic Chemistry I	CC	4	4	40	60
2	CHE2012	Organic Chemistry I	CC	4	4	40	60
3	CHE2013	Physical Chemistry I	CC	4	4	40	60
4	CHE2014	Physical Methods in Chemistry I	CC	4	4	40	60
5	CHE2015	Organic Chemistry Laboratory	CCP	4	8	100	
6	CHEEXX	Elective	DSE	4	4	40	60
7	CHEVAXX	VAC-1	VAC	2	2	40	60
			Total	**26**	**30**		

No	Course Code	Course Title	Type	Credit	Hours / Week	Marks	
						Int	Ext
SEMESTER – II							
1	CHE2021	Inorganic Chemistry II	CC	4	4	40	60
2	CHE2022	Organic Chemistry II	CC	4	4	40	60
3	CHE2023	Physical Chemistry II	CC	4	4	40	60
4	CHE2024	Physical Methods in Chemistry II	CC	4	4	40	60
5	CHE2025	Physical Chemistry Laboratory	CCP	4	8	100	
6	CHEEXX	Elective	DSE	2	2	40	60
7	CHEVAXX	VAC-2	VAC	2 (not included)	--	40	60
			Total	**22**	**26**		
			Cumulative Total	**48**	**56**		

SECOND YEAR

No	Course Code	Course Title	Type	Credit	Hours / Week	Marks	
						Int	Ext
SEMESTER – III							
1	CHE2031	Inorganic Chemistry III	CC	4	4	40	60
2	CHE2032	Organic Chemistry III	CC	4	4	40	60
3	CHE2033	Physical Chemistry III	CC	4	4	40	60
4	CHE2034	Inorganic Chemistry Laboratory	CCP	4	8	100	
5	CHEEXX	Project Elective	DSE	4	4	40	60
6	CHESEXX	SEC-1	SEC	3	3	40	60
7		Open Elective	OE	3	3	40	60
			Total	**26**	**30**		
			Cumulative Total	**74**	**86**		

No	Course Code	Course Title	Type	Credit	Hours / Week	Marks	
						Int	Ext
SEMESTER – IV							
1	CHE2101	Research Project	CC	12	24	40	60
2	CHE2102	Internship-01	INT	2	--	100	
3	CHEEXX	Self-Study Course	DSE	4	4	40	60
			Total	**18**	**28**		
			OVERALL TOTAL	**92**	**114**		

CREDIT FRAMEWORK

Two years M.Sc. Degree

S. No.	Course Components / Name of the Course	Nos	Credits	Percentage
1	Core Courses (CC)	11	44	48
2	Core Courses Practical (CCP)	3	12	13
5	Department Specific Elective (DSE)	4	14	17
6	Open Elective (OE)	1	3	3
8	Skill Enhancement Course (SEC)	1	3	3
9	Value Added Course (VAC)	2	2	2
10	Internship	1	2	2
11	Research Project	1	12	13
	Total	**24**	92	100

Semester: I **Course Type: Theory** **Course Code: CHE2011**
Credit: 4 **Course Title: Inorganic Chemistry-II**

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**
CO4	Analyze the stability of complexes in solution	**Analyze**
CO-5	Understand reaction mechanisms in inorganic complexes	**Understand**

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 (S_N1-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.

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. G. L. Miessler and D. A. Tarr, Inorganic Chemistry, 3rd edition, Pearson, 2004.
14. C. E. Housecraft and A.G. Sharpe, Inorganic Chemistry, 4th edition, Pearson, 2012.
15. K. F. Purcell and, J. C. Kotz, Inorganic Chemistry, Cengage Learning, 2012.
16. M. C. Day Jr., J. Selbin, Theoretical Inorganic Chemistry, Literary Licensing, LC, 2012.
17. G. Wilkinson, R. D. Gillars and J. A. McCleverty, Comprehensive Co-ordination Chemistry, Pergamon Press, 1987.
18. G. Wulfberg, Inorganic Chemistry, University Science Books, 2000.
19. D.M. Adam, Inorganic Solids: An introduction to concepts in solid-state structural chemistry, John Wiley & Sons, 1974.
20. G.E. Rodger, Inorganic and Solid State Chemistry, Cengage Learning India, Edition, 2002.

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

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: 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-II

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, 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

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

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 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(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

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

Semester: I **Course Type: Theory** **Course Code: CHE2014**
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 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 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 IR 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 –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 INADEQUATE.

Unit-V Mass spectrometry

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

Reference Books:

1. J. R. Kalman, L. D. Field, S. Sternhell, Organic Structure from Spectra, Wiley, 6th Ed 2020
2. Pavia, Lampman and Kriz, Introduction to Spectroscopy, Brooks/Cole Pubs Co, 5th edition, 2015.
3. R. M. Silverstein and F. X. Webster, Spectrometric identification of organic compounds, John Wiley and Sons. Inc., 6th edition, 1997.
4. W. Kemp, Organic Spectroscopy, 3rd edition, MacMillan, 1994.
5. Jag Mohan, Organic Spectroscopy: Principles & Applications, Narosa Publishers, 2012.
6. Atta-ur-Rahman, Nuclear Magnetic Resonance-Basic Principles, Springer-Verlag, 1986
7. Atta-ur-Rahman, One- and Two- Dimensional NMR Spectroscopy, Elsevier, 1989
8. Paul S. Pregosin, NMR in Organometallic Chemistry, Wiley, 2013.
9. R. S. Drago, Physical Methods for Chemistry, 2nd Edition, Saunders College Publishing, 1992.
10. D. H. Williams and Ian Fleming, Spectroscopic methods in organic chemistry, Tata McGraw Hill, 1998.
11. William Kemp, NMR in chemistry: A multinuclear introduction, MacMillan, 1988.
12. L. D. S. Yadav, Organic Spectroscopy, Kulwer academic publishers, 2004.
13. A Carrington and A. D. Mclachlan, Introduction to Magnetic Resonance, Harper & Row, New York, 1979.
14. A. Carrington and Machlachlon, Magnetic Resonance, Harper & Row, 1967
15. A Derome, Modern NMR Technique, Pergamon, 1983.
16. Farrar and E. D. Becker, Pulsed FT NMR Spectroscopy.
17. A. E. Derome, Modern NMR Techniques for Chemistry Research, Pregamon, 1987.
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.

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

Semester: I **Course Type: Practical** **Course Code: CHE2015**
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**

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.
5. V. K. Ahluwalia, R. Aggarwal, Comprehensive Practical Organic Chemistry, Universities Press, 2004.

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

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 mechanistic aspects of organometallic chemistry and bio-inorganic chemistry	**Understand**

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, cyclo-oligomerisation, 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.

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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5. R. H. Crabtree, Organometallic Chemistry of the Transition Metals, 5thEd.Wiley, New York, 2009.
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.
7. S. J. Lippard and J. M. Berg, Principles of Bioinorganic Chemistry, Panima Publishing Company, New Delhi, 1997.
8. W. Kaim and, B. Schewederski, Bioinorganic Chemistry: Inorganic Elements in the Chemistry of Life, John Wiley & Sons, New York, USA, 2013.
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11. C. E. Housecraft and A.G. Sharpe, Inorganic Chemistry, 4thedition, Pearson, 2012.
12. C. Elschenbroich and A. Salzer, Organometallics: A Concise Introduction, 3rdedition, 1999.
13. N. N. Greenwood and A. Earnshaw, Chemistry of the Elements, 2nd edition, Elsevier, 2005.
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16. B. Douglas, D. H. McDaniel and J. J. Alexander, Concepts and Models of Inorganic Chemistry, 2nd edition, John Wiley & sons, New York, 2006.
17. M. Bochmann, Organometallics 1: Complexes with transition metal-carbon s-bonds; Oxford Chemistry Primers Series, No. 13,1994.

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.
20. Haiduc and J. J. Zuckerman, Basic Organometallic Chemistry, De Gruyter, 1st Ed., 1985.
21. R. Hoffmann, Angew. Chem. Int. Ed., Engl. 21, 711-800 1982.
22. F. A. Cotton, G. Wilkinson, C. A. Murillo and M. Bochmann, Advanced Inorganic Chemistry, 6th ed., A Wiley - Interscience Publication, John –Wiley & Sons, USA, 2007. Chem. Education, 62, No. 11, Bioinorganic Chemistry, State of the Art. 1985.
23. P. Atkins, T. Overton, J. Rourke, M. Weller and F. Armstrong, Inorganic Chemistry, 5thedition, Oxford University Press, 2010.
24. G. L. Miessler, and D. A. Tarr, Inorganic Chemistry, 3rd edition, Pearson, 2004.
25. Dong Soo Lee, Venugopal Rajendiran, Sanjana Ghosh and Jonathan F. Lovell, A book chapter on titled " Porphyrin and Phthalocyanine Radiolabeling", from Radio-nanomedicine - Combined Nuclear and Nanomedicine, Springer International Publishing AG, part of Springer Nature 2018. Pages 49-78
26. Shuai Shao, Venugopal Rajendiran and Jonathan F. Lovell, Metalloporphyrin nanoparticles: Coordinating diverse theranostic functions, *Coordination Chemistry Reviews* 2019, 379, 99–120.

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

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	Demonstrate the use of reducing reagents in the synthetic organic chemistry	**Understand**

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, $Al(iPrO)_3$. 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, NaBH4, Sodium cyanoborohydride, metal trialkylborohydrides. Electrophilic metal hydrides: BH_3 and AlH_3. Electron transfer reducing reagents: Li/Na in liquid NH3 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 - Wilinsons hydrogenation, 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.
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13. Daniel E. Levy, Arrow Pushing in Organic Chemistry-An easy approach to understanding reaction mechanisms, Wiley Publications, 2008
14. L. G. Wade, Organic Chemistry, 6th Ed. Pearson, 2006
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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

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 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**

Unit-I Quantum Chemistry-II

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-III

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-IV

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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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

Semester: II **Course Type: Theory** **Course Code: CHE2024**
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 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**

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 N_2O, ClF_3, NO^{3-}, ClO_4, 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 tensor 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 Spectroscopies

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.

Reference Books

1. R. S. Drago, Physical Methods for Chemistry, 2nd Ed, Saunders College Publishing, 1992.
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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.

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

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 QM methods for modeling simple organic/inorganic compounds for structural optimization and reaction modeling	**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.
3. B. Viswanathan, Practical Physical chemistry, Viva Pub., 2005.
4. S. Kumar and N. Kumar, Physical Chemistry Practical, New Central Book Agency,2012.
5. A.M. James, F.E. Prichard, Practical Physical Chemistry Paperback, 1974.
6. J. Foresman & A. Frisch, Exploring Chemistry with Electronic Structure Methods, Gaussian Inc., 2000.
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.
10. J. M. Haile, Molecular Dynamics Simulation: Elementary Methods, 2001.

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
4	3	3	3	3	3

Semester: III **Course Type: Theory** **Course Code: CHE2031**
Credit: 4 **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 medicine	**Remember**
CO-5	Gain knowledge on frontier areas of inorganic chemistry	**Knowledge**

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 Inorganic 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 medicine- 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 medicine: 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.

Reference Books

1. A. Earnshaw, Introduction to Magnetochemistry, Academic Press, 1968.
2. R. Dutta, Syama, 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.Medhi, Inorganic Chemistry - Principles of Structure and Reactivity, 4th edition, Pearson Education, 2006.
5. K. F. Purcelland, J. C. Kotz, Inorganic Chemistry, Cengage Learning, 2012.
6. A. W. Adamson, P. D. Fleischauer, Concepts of Inorganic Photochemistry, Wiley, 1975.
7. D. Bahnemann, A. O. T. Patrocinio, Springer Handbook of Inorganic Photochemistry, Springer Cham, 2022.
8. V. Ramamurthy, S. S. Kirk, Organic and Inorganic Photochemistry, Vol, 2, Marcel Dekkar Inc., New York, 1998.
9. H. J. Arnikar, Essentials of Nuclear Chemistry, 4th edition, New Age International Publishers Ltd., New Delhi, 1995.
10. W. D. Loveland, D. J. Morrissey and G. T. Seaborg, Modern Nuclear Chemistry, Wiley VCH Verlag GmbH Co. KGaA, 2006.
11. Glasstone, Source Book on Atomic Energy, 3rd edition, Affiliated East West Press, 1979.
12. G. R. Choppin, J-O Liljenzin, J. Rydberg, C. Ekberg, Radio Chemistry and Nuclear Chemistry 2016. (Unit II).
13. A. K. Das, Bioinorganic Chemistry, Books and Allied Ltd. Kolkatta, 2016. (Units I-III).
14. Nicholas P. F. Uses of Inorganic Chemistry in Medicine, The Royal Society of Chemistry 1999.
15. J. C. Dabrowiak, Metals in Medicine, 2nd Edition., John Wiley & Sons Ltd., 2017.
16. C. E. Housecraft and A.G. Sharpe, Inorganic Chemistry, 4th edition, Pearson, 2012.

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

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 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 E_2, prostacyclin (PGI_2). Structural features 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

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: 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, 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-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 and 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, 3rd Edn., 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. A.J. Bard, L.R Faulkner, Electrochemical Methods-Fundamentals and applications, 2nd Edn., 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: Practical** **Course Code: CHE2034**
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 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. 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 $[Co(NH_3)_5Cl]Cl_2$.
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. 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 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**

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.

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 Elective 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 & Catalysis	4
CHEE12	Chemistry of C-H Activation	4
CHEE13	Advanced Bioinorganic Chemistry	4
CHEE14	Principles of Biochemistry	4
CHEE15	Mathematics for Chemists and Biologists	4
CHEE16	Electrochemical Energy System	4
CHEE17	Fundamentals of Analytical Chemistry	4
CHEE18	Computational Chemistry	4
CHEE19	Supramolecular Chemistry	4
CHEE20	Computational Materials Modelling	4
CHEE21	Organometallics, Catalysis and Inorganic Spectroscopy	4
CHEE22	Physical Methods in Chemistry	4
CHEE23	Applications of Computational methods in Chemistry	4
CHEE24	Chemical Lab Safety and Management	4
CHEE25	Advances in Organic Chemistry	4
CHEE26	Green Chemistry	4
CHEE27	Selected Topics in Synthetic Organic Methods	4
CHEE28	Advanced Topics in Organometallic Chemistry	4
CHEE29	Industrial Chemistry	4
CHEE30	Advanced Organic Nanomaterials	4
CHEE31	Computer Software for Chemists	4
CHEE32	Selected Experiments in Applied Chemistry	4
CHEE33	Luminescence Spectroscopy for Advanced Research	4
CHEE34	Research Methodology	4
CHEE35	Chemistry in Nanoscience and Technology	4
CHEE36	Advanced NMR Techniques	4
CHEE37	Advanced Organic Synthesis	4
CHEE38	Nanoscience and Nanotechnology	4
CHEE39	Medicinal Chemistry	4
CHEE40	Introduction to Biochemistry	3
CHEE41	2D NMR Spectroscopy	2
CHEE42	Separation Techniques	2
CHEE43	Separation Techniques & 2D NMR Spectroscopy	4

*New electives will be appended based on the availability of course instructor.

Electives will be offered based on the individual faculty's availability

List of Skill Enhancement Courses

Course Code	Title of the Course	Credits
CHESE01	Computer software for Chemists	3
CHESE02	Selected Experiments in Applied Chemistry	3
CHESE03	Instrumentation Methods in Chemistry	3
CHESE04	Water & Waste Water Treatment	3
CHESE05	Pharmaceutical Chemistry	3

List of Value-Added Courses

Course Code	Title of the Course	Credits
CHEVA01	Instrumental Techniques for Chemical Analysis -01	2
CHEVA02	Instrumental Techniques for Chemical Analysis -02	2
CHEVA03	Basic Analytical Experiments	2
CHEVA04	Research Methodology and Publication Ethics	2
CHEVA05	Climate Change & Atmospheric Chemistry	2